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Dispersion, solvent and metal effects in the binding of gold cations to alkynyl ligands:implications for Au(I) catalysis

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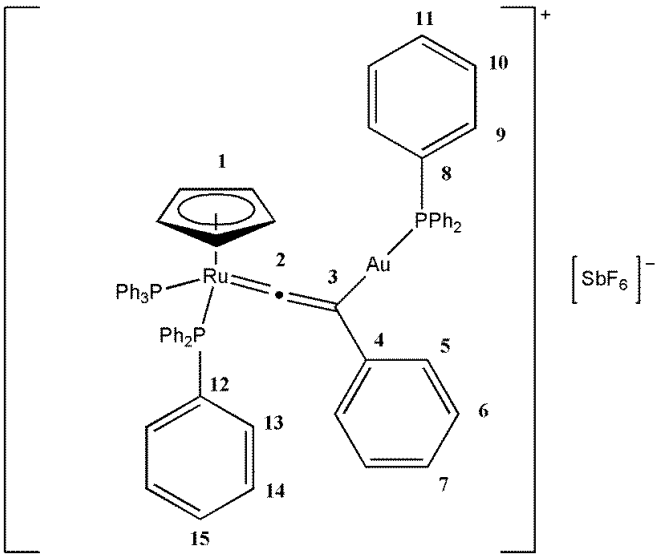
S1 Experimental Details

S1.1. General Considerations

All experiments were carried out under an atmosphere of dinitrogen using standard Schlenk line and glove box techniques. CH_2Cl_2 and pentane were purified with the aid of an Innovative Technologies anhydrous solvent engineering system. The CD_2Cl_2 and C_6D_6 used for NMR were dried over CaH_2 or Na, respectively, and degassed with three freeze-pump-thaw cycles. The solvent was vacuum transferred into NMR tubes fitted with PTFE Young's taps. NMR spectra were acquired on either a JEOL 400 (^{1}H 399.78 MHz, ^{13}C 100.52 MHz, ^{19}F 376.17 MHz and ^{31}P 161.83 MHz) or Bruker AVANCE 500 (^{1}H 500.23 MHz, ^{31}P 202.50 MHz, ^{13}C 125.77 MHz) spectrometer. Mass spectrometry measurements were performed on a Bruker micrOTOF (ESI) instrument. IR spectra were acquired on a Bruker Platinum ATR FT-IR instrument. All chemicals used were obtained from Sigma Aldrich Chemicals and used as supplied except for HC≡CPh which was obtained from Acros Organics and used without any further purification.

Complexes **1**,[1] **4**[2], [AuCl(PPh_3)][3] and [Au(C≡CPh)(PPh_3)][4] were prepared by literature methods.

S1.2. Synthesis of $[CpRu(PPh_3)_2(=C=CPh\{Au(PPh_3)\})]SbF_6$, [3]$SbF_6$.



[$AuCl(PPh_3)$] (125 mg, 0.25 mmol) was added to a backfilled Schlenk tube and dissolved in about 3 mL of CH_2Cl_2. $AgSbF_6$ (86 mg, 0.25 mmol) was added to the tube in a glove-box and the mixture was stirred for 10 min, during which time a precipitate formed, white in colour at the beginning and progressively turning to lilac and then dark purple. The supernatant solution was cannula filtered into a Schlenk tube containing a yellow solution of [Ru(η^5-C_5H_5)(-C≡CPh)$(PPh_3)_2$] (200 mg, 0.25 mmol) in 15 mL of CH_2Cl_2. The yellow solution turned into a dark yellow/orange colour and a precipitate was formed. The mixture was stirred at room temperature for 1 h, cannula filtered and solvent evaporated, leaving a bronze/orange coloured solid, which was washed with dry Et_2O and dried under vacuum.

Yield: 61 mg (0.04 mmol, 16%)

^{1}H NMR: (500 MHz, CD_2Cl_2) δ 7.60 (4H, m, **7** + **11**), 7.48 (6H, td, $^3J_{HH}$ = 7.6, $^4J_{PH}$ = 2.6, **10**) 7.42 (6H, m, **9**), 7.31 (6H, t, ^3J = 7.10, **15**), 7.14 (14H, m, **6** + **13** / **14**), 7.06 (12H, m, **13** / **14**), 6.90 (2H, m, **5**), 4.57 (5H, s, **1**).

^{13}C{^{1}H} NMR: (126 MHz, CD_2Cl_2) δ 354.1 (t, $^2J_{PC}$ = 15.7, **2**), 136.8 (vt, $^1J_{PC}$ + $^3J_{PC}$ = 44.4, **12**), 133.9 (d, $^2J_{PC}$ = 13.2, **9**), 133.7 (vt, $^nJ_{PC}$ + $^{n+2}J_{PC}$ = 10.3, **13** / **14**), 132.9 (s, **7**), 132.5 (d, $^4J_{PC}$ = 2.6, **11**), 130.6 (bs, **5**), 129.8 (s, **15**), 129.7 (d, $^3J_{PC}$ = 11.3, **10**), 128.3 (s, **6**), 128.1 (d, $^1J_{PC}$ = 59.9, **8**), 128.0 (vt, $^nJ_{PC}$ + $^{n+2}J_{PC}$ = 9.6, **13** / **14**), 126.7 (d, $^3J_{PC}$ = 2.4, **4**), 118.7 (d, $^2J_{PC}$ = 15.4, **3**), 85.9 (s, **1**).

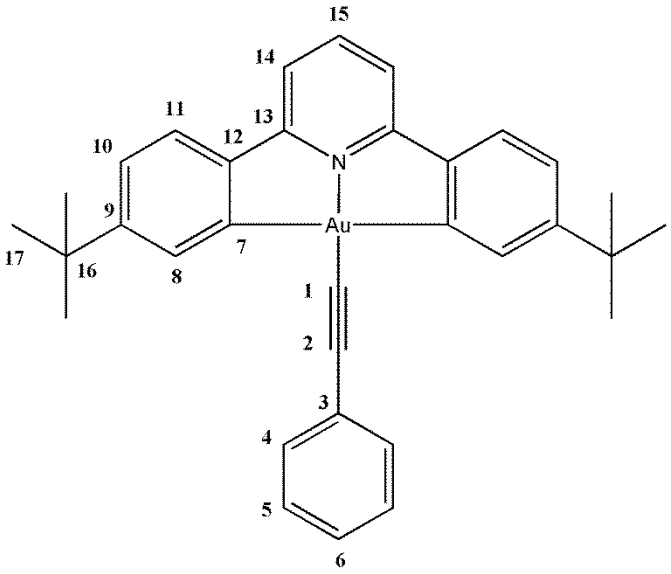
^{31}P{^{1}H} NMR: (162 MHz, CD_2Cl_2) δ 46.12 (Ru*P*Ph_3), 37.31 (Au*P*Ph_3).

ESI-MS: positive ion *m/z* 1251.2225 ($[M]^+$, calc. for $C_{67}H_{55}AuP_3Ru^+$: 1251.2238, error -0.5 mDa).

Elemental Analysis: for $C_{63}H_{55}AuF_6P_3RuSb$: Calc. C 52.59; H 3.85 %. Found C 52.33; H 3.76 %.

IR: 3502, 2970, 2156, 2070, 1914, 1590, 1571, 1479, 1433, 1309, 1184, 1158, 1087, 1071, 1026, 998, 833, 804, 743, 691, 654, 634, 497, 460, 421 cm^{-1}.

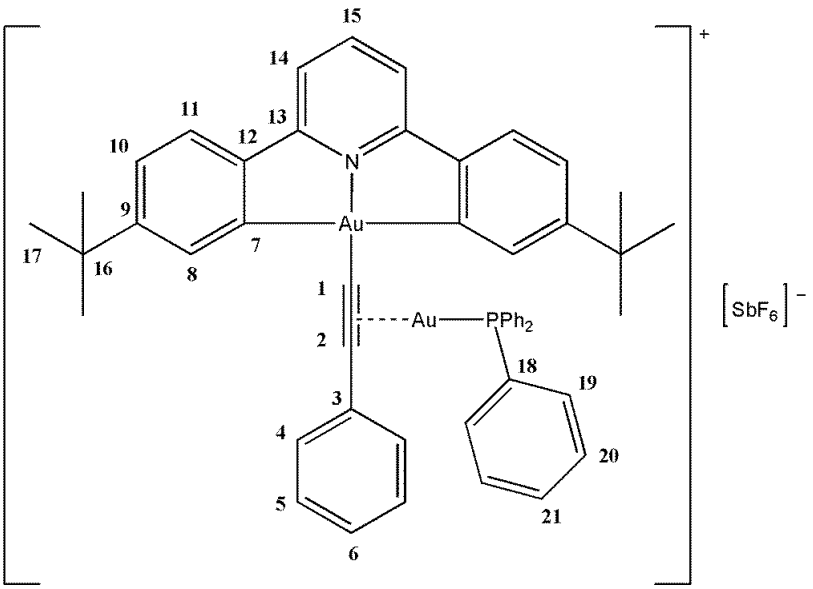
S1.3. Synthesis of [Au(^{t}Bu^C^N^C^{t}Bu)(-^{13}C≡CPh)], [4]-^{13}C.



To a Schlenk tube charged with [Au(^{t}BuC^N^C^{t}BuH)Cl][2] (100 mg, 0.174 mmol) and CuI (9 mg) was added anhydrous degassed CH_2Cl_2 followed by H^{13}C≡CPh (384 µL, 3.5 mmol) and triethylamine (1 mL). The yellow suspension was stirred under Ar for 17 hours. The solvents were removed *in vacuo* and the resulting solid was purified by flash column chromatography using EtOAc followed by CH_2Cl_2 to yield a yellow solid (90 mg, 81%).

^{1}H NMR: (400 MHz, C_6D_6) δ 8.74 (2H, dd, $^4J_{HH}$ = 2.0, $^4J_{HC}$ = 0.8, **8**), 7.97 (2H, m, **4**) 7.21 (2H, dd, $^3J_{HH}$ = 8.0, $^4J_{HH}$ = 2.0, **10**), 7.16 (partially overlapping with residual benzene signal, **5**), 7.12 (2H, d, $^3J_{HH}$ = 8.0, **11**), 7.06 (1H, tt, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.1, **6**), 6.74 (1H, t, $^3J_{HH}$ = 8.0, **15**), 6.48 (2H, d, $^3J_{HH}$ = 8.0, **14**), 1.35 (18H, s, **17**).
^{13}C{^{1}H} NMR: (400 MHz, C_6D_6) δ 168.3 (d, $^2J_{CC}$ = 3.0, **7**), 164.9 (**13**), 155.2 (**9**), 146.9 (**12**), 141.4 (**15**), 134.4 (d, $^3J_{CC}$ = 2.0, **8**), 132.3 (d, $^3J_{CC}$ = 3.0, **4**), 128.6 (**5**), 128 (**3**, under benzene signal, located by cross peaks in HMBC), 127.0 (**6**), 125.1 (**11**), 123.7 (**10**), 115.6 (d, $^4J_{CC}$ = 1.5, **14**), 101.7 (d, $^1J_{CC}$ = 145.9, **2**), 94.1 (**1**), 35.5 (**16**), 31.4 (**17**).

S1.4. Synthesis of [Au(^{t}BuC^N^C^{t}Bu)(-C≡CPh{η^2-AuPPh$_3$})]SbF$_6$, [5]SbF$_6$.



[AuCl(PPh$_3$)] (39 mg, 0.08 mmol) was added to a nitrogen filled Schlenk tube and dissolved in 2 mL of CH_2Cl_2. AgSbF$_6$ (27 mg, 0.08 mmol) was added to the reaction mixture in the glove-box and the mixture was stirred for 10 min, during which time a colourless precipitate formed, which progressively turned to lilac and then dark purple. The supernatant solution was cannula filtered into a Schlenk tube containing a yellow solution of [**4**] (50 mg, 0.08 mmol) in 10 mL of toluene. The yellow solution turned slowly into a lime yellow suspension. The mixture was stirred at room temperature for 16 h, toluene was concentrated down to about 3 mL and Et_2O added to the mixture to promote precipitation of the complex. The solid was isolated by cannula filtration and washed with Et_2O, then it was dried under vacuum and stored in the glove box.

Crystals suitable for X-ray diffraction were obtained from hot benzene (or toluene) in a Young's tap NMR tube, leaving the solution to cool down slowly to room temperature and stand for 16 h.

Yield: 76 mg (0.05 mmol, 71%).

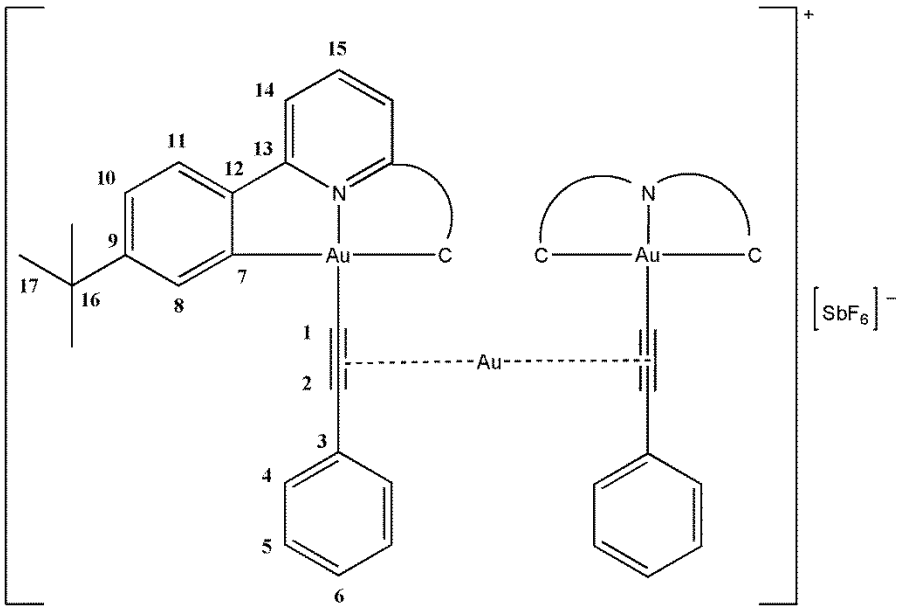
Due to the very low solubility in C_6D_6, it was impossible to obtain solution NMR spectra, even with ***C1*** ^{13}C enriched sample.

ESI-MS: positive ion *m/z* 1098.2790 ([M]$^+$, calc. for $C_{51}H_{47}Au_2NP^+$: 1098.2772, error -1.8 mDa).

Elemental Analysis: for $C_{51}H_{47}Au_2F_6NPSb$: Calc. C 45.90; H 3.55; N 1.05 %. Found C 45.88; H 3.40; N 1.07 %.

IR: 3056, 2961, 2904, 2865, 2053, 1585, 1561, 1483, 1435, 1259, 1100, 800, 746, 690, 653, 539, 502 cm^{-1}.

S1.5. Synthesis of [{Au(^{t}BuC^N^C^{t}Bu)(-C≡CPh)}$_2$(μ-Au)]$^+$, [6]SbF$_6$.

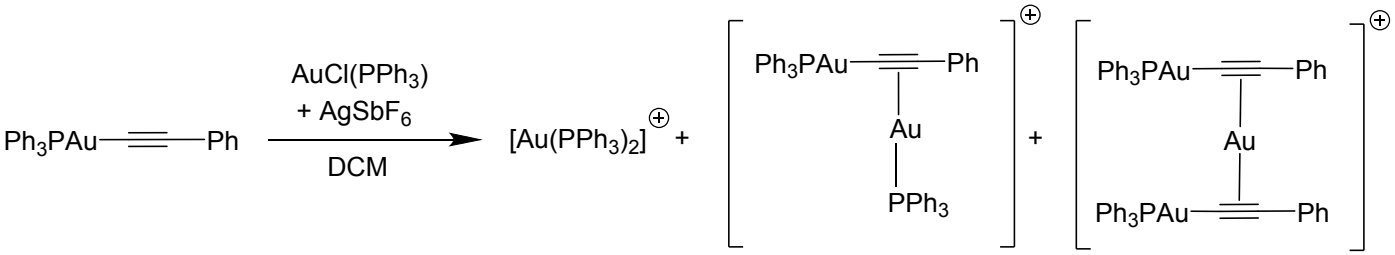


[AuCl(PPh$_3$)] (31 mg, 0.06 mmol) was added to a backfilled Schlenk tube and dissolved in about 2 mL of CH_2Cl_2. $AgSbF_6$ (22 mg, 0.06 mmol) was added to the tube in the glove-box and the mixture was stirred for 10 min, during which time a precipitate formed, white in colour at the beginning and progressively turning to lilac and then dark purple. The supernatant solution was cannula filtered into a Schlenk tube containing a yellow solution of [**4**] (40 mg, 0.06 mmol) in 10 mL of toluene. The yellow solution turned slowly into a lime yellow suspension. The mixture was stirred at room temperature for 5 h, toluene was concentrated down to about 3 mL and Et_2O added to the mixture to promote precipitation of the complex. The solid was isolated by cannula filtration, washed with Et_2O and re-dissolved in dichloromethane. The initially yellow solution turned green within a few minutes and the mixture was stirred under N_2 atmosphere for 16 h. The solution was cannula filtered, the CH_2Cl_2 concentrated to ~1 mL under vacuum and Et_2O added to help precipitation of the complex. The solid was isolated by cannula filtration, washed with Et_2O, dried and stored under nitrogen.
Crystals suitable for X-ray diffraction were obtained from slow diffusion of Et_2O layer into a DCM solution of the complex.
Yield: 18 mg (0.01 mmol, 35%)

Alternatively, [**6**]SbF_6 could be prepared by dissolving a sample of isolated [**5**]SbF_6 in CH_2Cl_2.

^{1}H NMR: (400 MHz, CD_2Cl_2) δ 7.97 (4H, d, $^4J_{HH}$ = 2.0, **8**), 7.93 (2H, t, $^3J_{HH}$ = 8.0, **15**) 7.83 (4H, m, **4**), 7.61 (4H, m (partially overlapped with **11**), **5**), 7.58 (4H, d, $^3J_{HH}$ = 8.0, **11**), 7.48 (4H, d, $^3J_{HH}$ = 8.0, **14**), 7.38-7.26 (6H, m, **10**+**6**), 1.23 (36H, s, **17**).
^{13}C{^{1}H} NMR: (400 MHz, CD_2Cl_2) δ 167.1 (**7**), 165.3 (**13**), 156.4 (**9**), 146.7 (**12**), 144.2 (**15**), 133.2 (**8**), 133.1 (**4**), 129.8 (**5**), 126.4 (**11**), 125.5 (**10**), 120.9 (**3**), 117.6 (**14**), 114.8 (**2**), 92.8 (**1**), 35.6 (**16**), 31.2 (**17**). **6** could not be identified.
ESI-MS: positive ion *m/z* 1475.4042 ([M]$^+$, calc. for $C_{66}H_{64}Au_3N_2^+$: 1475.4061, error -1.9 mDa).
Elemental Analysis: for $C_{66}H_{64}Au_3F_6N_2Sb$: Calc. C 46.31; H 3.77; N 1.64 %. Found C 45.92; H 3.49; N 1.04 %.
IR: 3057, 2950, 2903, 2859, 2034, 1992, 1980, 1584, 1561, 1544, 1486, 1434, 1360, 1258, 1182, 1102, 1024, 798, 753, 690, 654, 536, 522 cm^{-1}.

S1.6. Reaction of [Au(-C≡CPh)(PPh_3)], [7], with [Au(PPh_3)]SbF_6

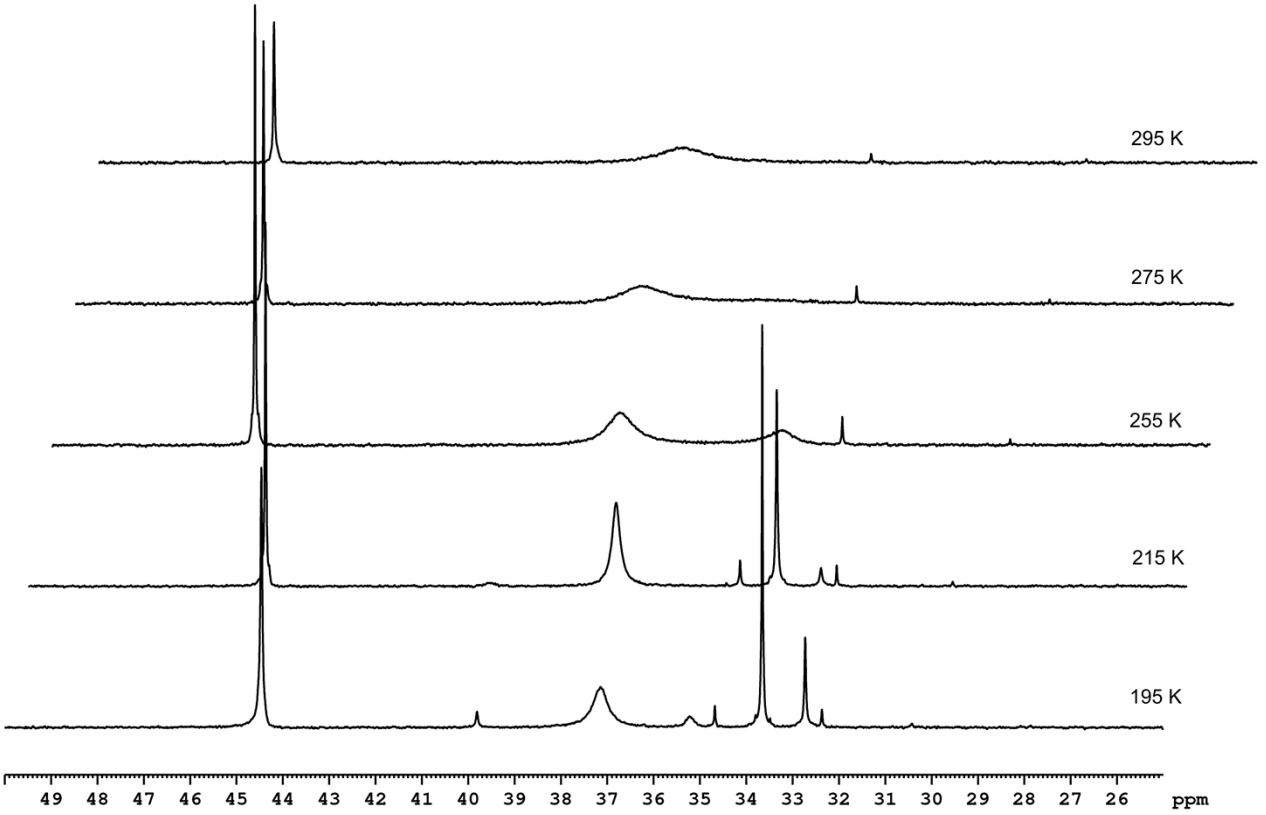


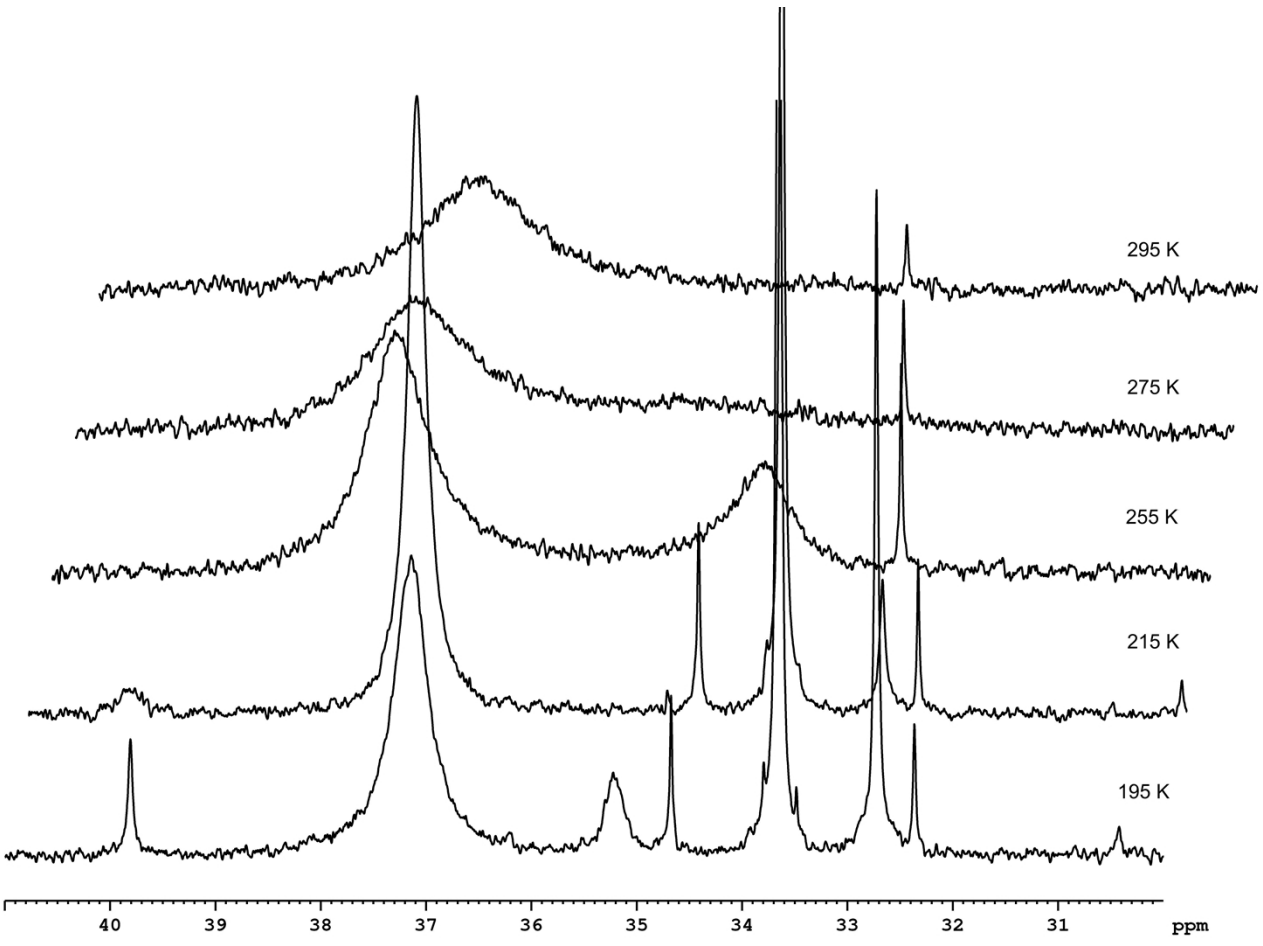
In a glove box, a solution of $AgSbF_6$ (10 mg, 0.029 mmol) in CH_2Cl_2 was added to a sample vial containing AuCl(PPh_3) (14 mg, 0.029 mmol), resulting in a lilac suspension of AgCl upon stirring. The suspension was filtered through a Pasteur pipette loaded with cotton wool to remove the precipitate and the remaining solution was added to a sample vial containing (PPh_3)Au(C_2Ph) (16 mg, 0.029 mmol). Over a period of 5 minutes, the initially colourless solution turned first to yellow with the formation of a yellow precipitate.

^{1}H NMR (400 MHz, CD_2Cl_2) Displays a multiplet in the aromatic region 7.71 - 7.39 ppm
^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2) δ 45.5 (sharp), 35.6 (broad);

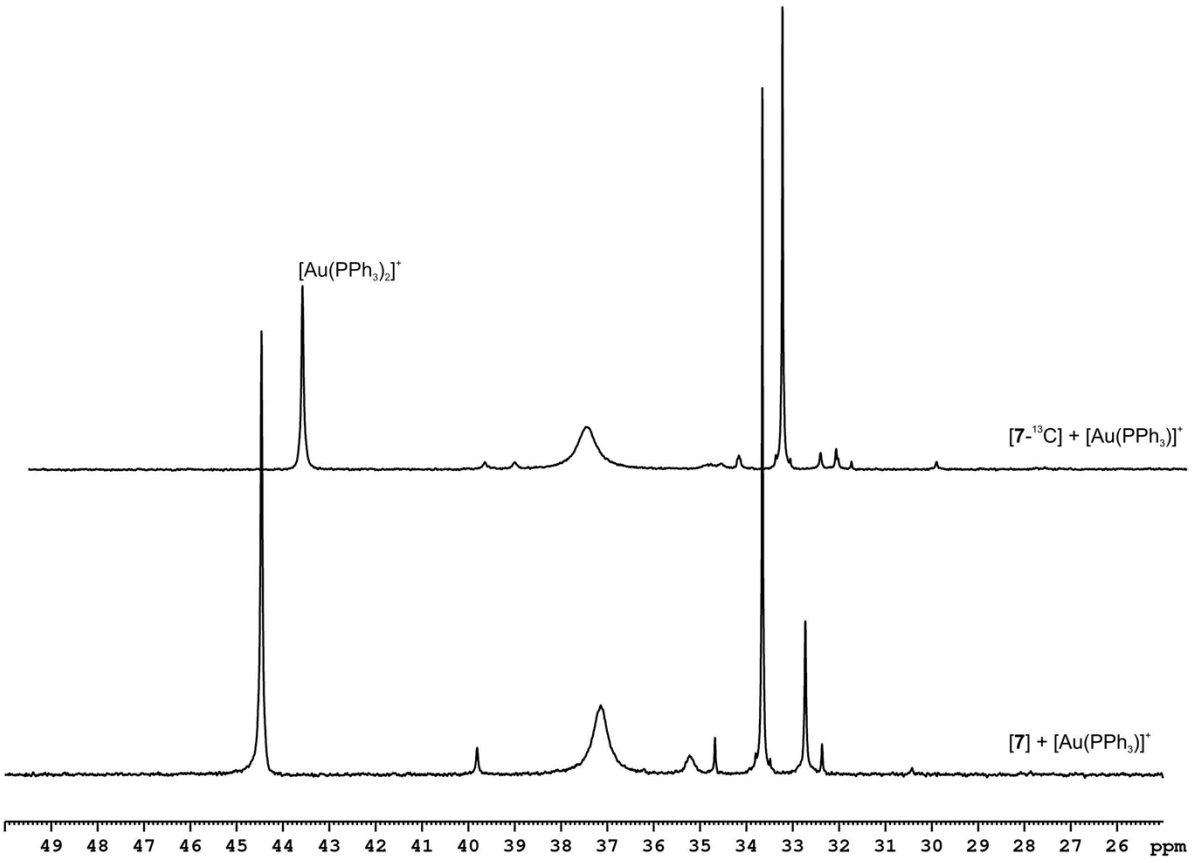
ESI-MS: positive ion *m/z* 721.1498 ($[M]^+$, calc. for $C_{36}H_{30}AuP_2^+$: 721.1483, error -1.6 mDa), *m/z* 1019.1556 ($[M]^+$, calc. for $C_{44}H_{35}Au_2P_2^+$: 1019.1540, error -1.6 mDa), *m/z* 1317.1643 ($[M]^+$, calc. for $C_{52}H_{40}Au_3P_2^+$: 1317.1596, error -4.6 mDa).

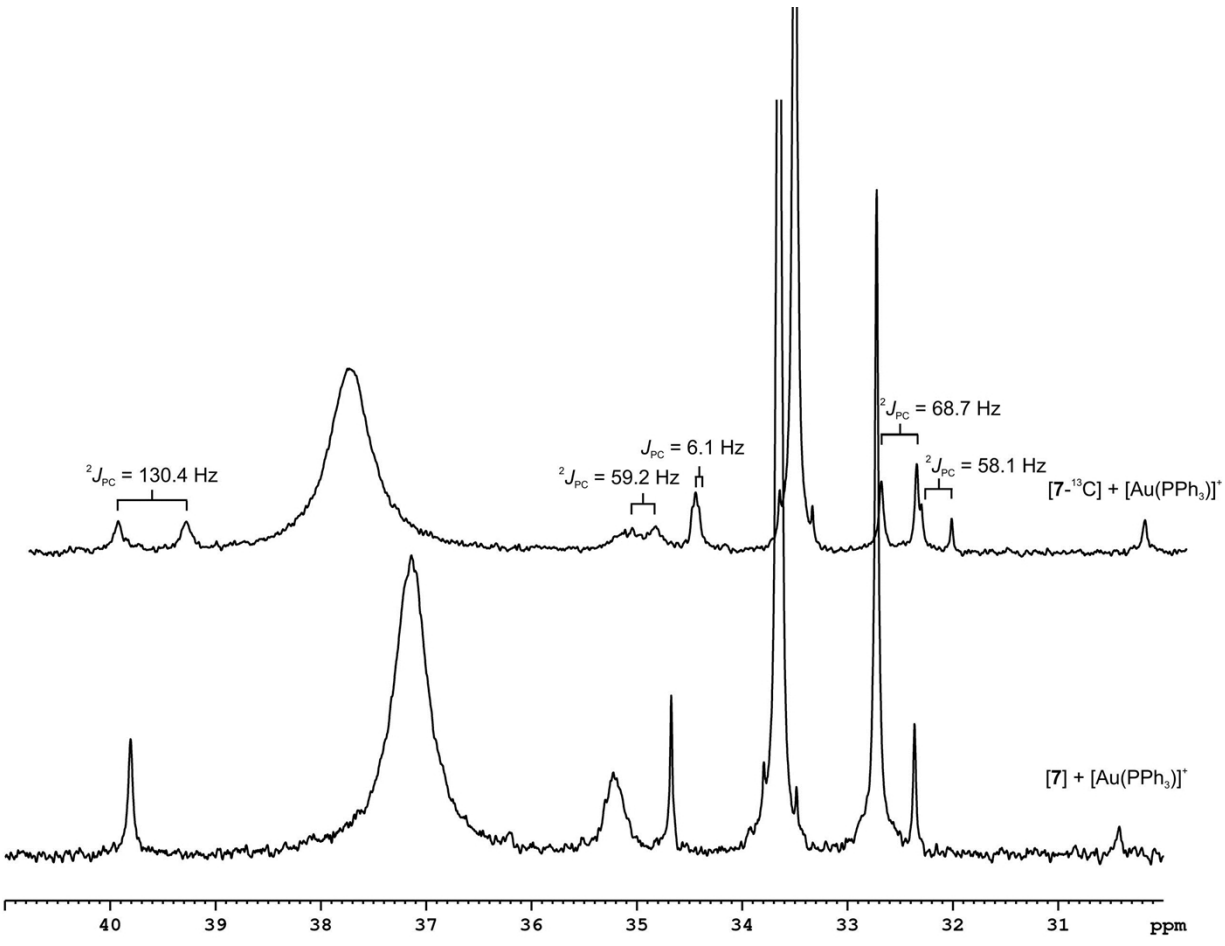
S1.7. Variable temperature $^{31}P\{^{1}H\}$ NMR spectra from the reaction of [7] with $[Au(PPh_3)]SbF_6$.
Spectra recorded in CD_2Cl_2 soution





S1.8. Comparision of $^{31}P\{^{1}H\}$ NMR spectra from the reaction of [7] and [7-^{13}C] with $[Au(PPh_3)]SbF_6$.
Spectra recorded at 195 K in CD_2Cl_2 soution



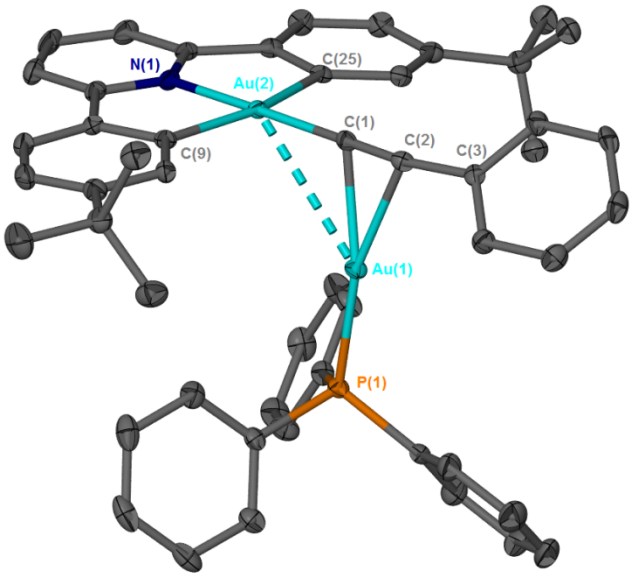


S2 X-ray Structure Determinations

Diffraction data for [**5**]$SbF_6.C_6D_6$ and **[6]**SbF_6 were collected at 110 K on an Oxford Diffraction SuperNova diffractometer with Mo-K_α radiation (λ = 0.71073 Å) using a EOS CCD camera. The crystal was cooled with an Oxford Instruments Cryojet. Diffractometer control, data collection, initial unit cell determination, frame integration and unit-cell refinement were carried out with "Crysalis".[5] Face-indexed absorption corrections were applied using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.[6] Data for **[5]**$SbF_6.C_6H_5CH_3$ were collected on a Bruker Microstar diffractometer using Cu-K_α radiation (λ = 1.54178 Å) using a Pt 135 CCD area detector. The crystal was cooled to 150 K during the data acquisition. The absorption correction was performed with SADABS.[7]

In all cases, OLEX2 was used for overall structure solution, refinement and publication data. Within OLEX2,[8] the algorithm used for structure solution was direct methods using the SHELXS-97,[9] refinement by full-matrix least-squares used the SHELXL-97. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using a "riding model" and included in the refinement at calculated positions.

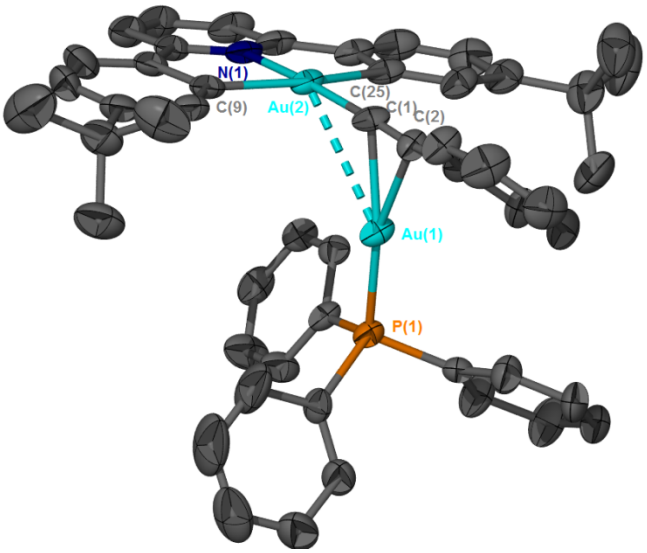
S2.1. Structure of [5]SbF_6.$(C_6D_6)_2$.



Solvent of crystallisation, anion and hydrogen atoms not shown.

CCDC code	1032551
Empirical formula	$C_{69}H_{65}Au_2F_6NPSb$
Formula weight	1568.87
Temperature/K	110.00(14)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.83401(14)
b/Å	18.45150(17)
c/Å	19.63900(17)
α/°	90
β/°	100.0543(8)
γ/°	90
Volume/Å^3	6006.44(9)
Z	4
ρ_{calc}mg/mm^3	1.735
m/mm^{-1}	5.407
F(000)	3056.0
Crystal size/mm^3	0.283 × 0.2022 × 0.0381
Radiation / Å	Mo-K_α (λ = 0.71073)
2Θ range for data collection	5.884 to 64.298°
Index ranges	-25 ≤ h ≤ 23, -27 ≤ k ≤ 27, -29 ≤ l ≤ 27
Reflections collected	37745
Independent reflections	18968 [R_{int} = 0.0251, R_{sigma} = 0.0406]
Data/restraints/parameters	18968/0/710
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0269, wR_2 = 0.0487
Final R indexes [all data]	R_1 = 0.0421, wR_2 = 0.0535
Largest diff. peak/hole / e Å^{-3}	1.09/-0.89

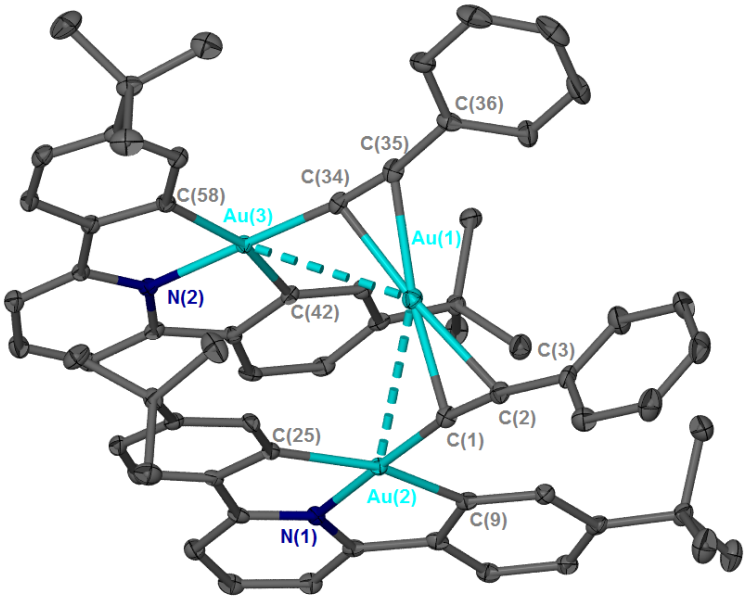
S2.2. Structure of [5]$SbF_6.C_6H_5CH_3$.



Solvent of crystallisation, anion and hydrogen atoms not shown.

CCDC code	1032552
Empirical formula	$C_{58}H_{55}Au_2F_6NPSb$
Formula weight	1426.78
Temperature/K	150
Crystal system	orthorhombic
Space group	Pbcn
a/Å	24.291(3)
b/Å	17.933(2)
c/Å	24.334(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	10600(2)
Z	8
ρ_{calc}mg/mm^3	1.788
m/mm^{-1}	14.988
F(000)	5504.8
Crystal size/mm^3	0.25 × 0.15 × 0.04
Radiation / Å	Cu-K_α (λ = 1.54178)
2Θ range for data collection	6.126 to 133.762°
Index ranges	-28 ≤ h ≤ 20, -21 ≤ k ≤ 21, -28 ≤ l ≤ 28
Reflections collected	167357
Independent reflections	9391 [R_{int} = 0.0635, R_{sigma} = 0.0211]
Data/restraints/parameters	9391/238/759
Goodness-of-fit on F^2	1.209
Final R indexes [I>=2σ (I)]	R_1 = 0.0437, wR_2 = 0.1033
Final R indexes [all data]	R_1 = 0.0446, wR_2 = 0.1038
Largest diff. peak/hole / e Å^{-3}	1.45/-1.36

S2.3. Structure of [6]SbF_6.

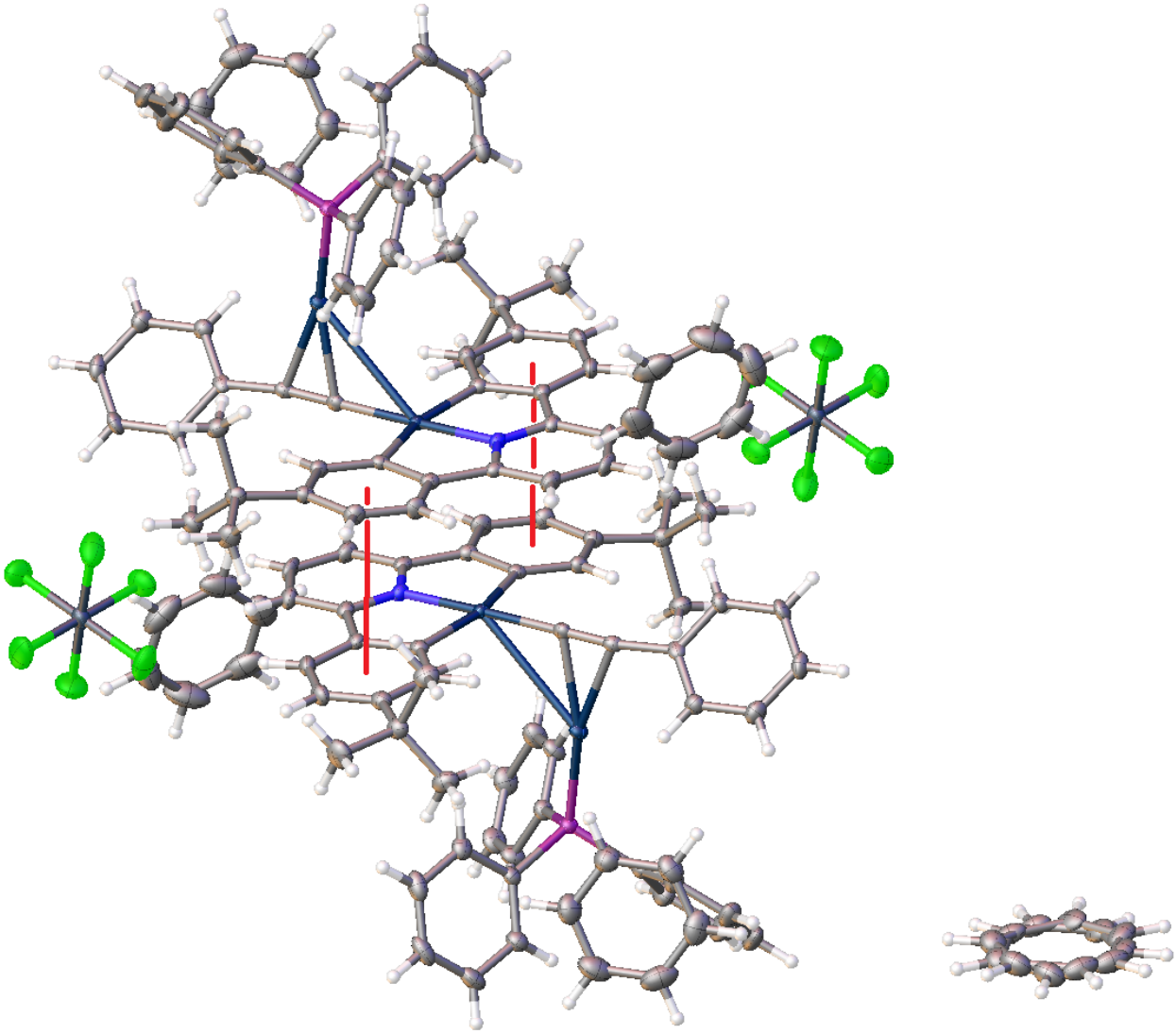


Anion and hydrogen atoms not shown.

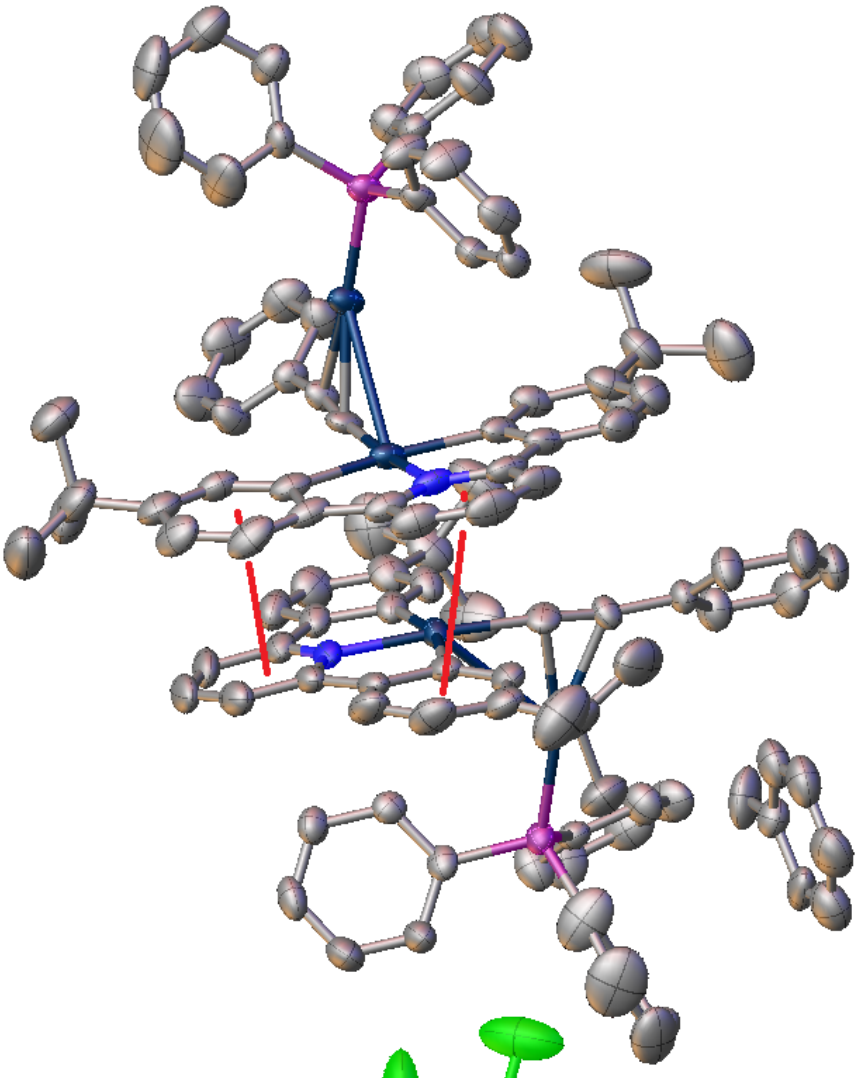
CCDC code	1032553
Empirical formula	$C_{66}H_{64}Au_3F_6N_2Sb$
Formula weight	1711.84
Temperature/K	110.05(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.33309(17)
b/Å	18.64797(16)
c/Å	18.79354(18)
α/°	90
β/°	91.0581(9)
γ/°	90
Volume/Å^3	5723.14(9)
Z	4
ρ_{calc}mg/mm^3	1.987
m/mm^{-1}	8.196
F(000)	3264.0
Crystal size/mm^3	0.145 × 0.0487 × 0.0483
Radiation	Mo-K_α (λ = 0.71073)
2Θ range for data collection	5.822 to 60.836°
Index ranges	-21 ≤ h ≤ 22, -24 ≤ k ≤ 25, -24 ≤ l ≤ 26
Reflections collected	33742
Independent reflections	15270 [R_{int} = 0.0255, R_{sigma} = 0.0372]
Data/restraints/parameters	15270/0/715
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0254, wR_2 = 0.0504
Final R indexes [all data]	R_1 = 0.0371, wR_2 = 0.0546
Largest diff. peak/hole / e Å^{-3}	1.22/-1.57

S2.4. Discussion of π-π interactions

Analysis of the interactions between neighbouring ligands was performed using Platon.[10] In the structure of [**5**]SbF_6 C_6D_6, interactions between the rings shown were found with a centroid-to-centroid distance of 3.9018(16) Å. Interactions between ligand and benzene atoms-of-crystallisations were also found 3.634(2) Å and 3.638(4) Å.



In the structure of [**5**]SbF_6 C_7H_8,the complexes are found in the crystal lattice almost at 90˚ to each other considering the N-Au-acetylide axes, with π-interactions between the ^{t}BuC^N^C^{t}Bu ligands.

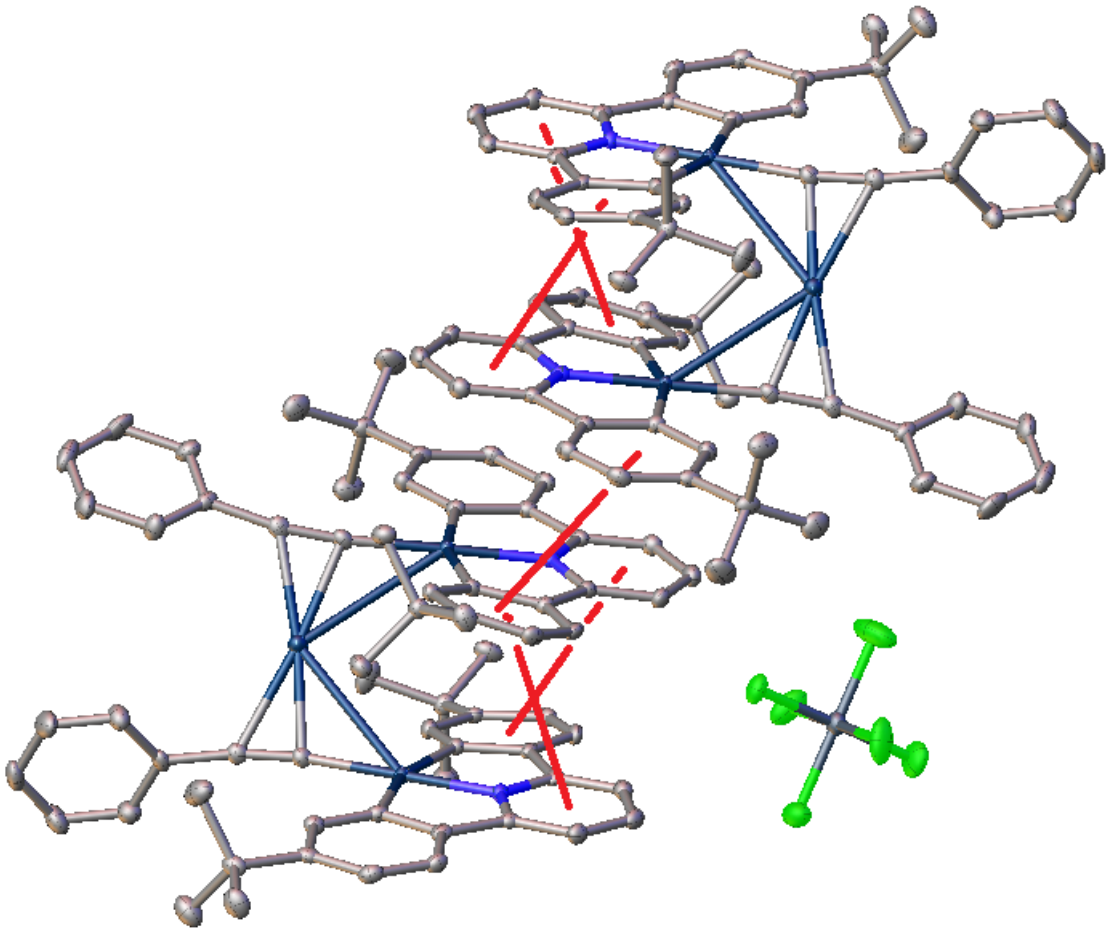


Ring designation used in PLATON:Ring(4) made by N(1) and C(15) to C(19) atoms
Ring(6) made by C(9) to C(14) atoms
Ring(8) made by C(34) to C(39) atoms
Ring(11) made by C(52) to C(57) atoms
Ring(13) made by C(52B) to C(57B) atoms

Distance between centroids (Cg)
Cg(6) – Cg(4) 3.6086 Å
A π-π interaction between ring(8) and the disordered toluene molecule was also present:
Cg(8) – Cg(11) 3.8642 Å
Cg(8) – Cg(13) 3.9430 Å

The torsion angle between N-Au-Au-N was found to be 100.23°.

In the structure of [**6**]PF_6 the packing is head-to-tail, considering two consecutive trigold complexes. The π-π interactions are both intra- and inter- molecular



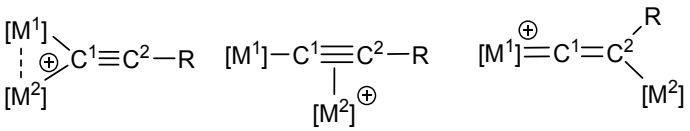
Ring designation used in PLATON:
Ring(7) made by N(1) and C(15) to C(19) atoms
Ring(8) made by N(2) and C(48) to C(52) atoms
Ring(11) made by C(20) to C(25) atoms
Ring(13) made by C(42) to C(47) atoms
Ring(14) made by C(53) to C(58) atoms

Distance between centroids (Cg)
Intramolecular
Cg(7) – Cg(13) 3.9320(19) Å
Cg(8) – Cg(11) 3.9745(19) Å
Intermolecular
Cg(13) – Cg(14) 3.945(2) Å

The torsion angle between Au-N-N-Au (intramolecular) was measured as -20.52°, while the Au-N-N-Au (intermolecular) was 180.00°.

S2.5. Comparison of Structural Metrics

$\delta_1 = l_{[M1]-C1} - l_{[M1]-C2}$
$\delta_2 = l_{[M2]-C1} - l_{[M2]-C2}$
$\Delta\delta = |\delta_1| - |\delta_2|$

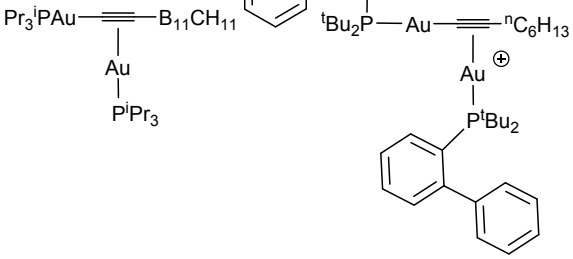


D	E	F
δ_1 = < 0	δ_1 < 0	δ_1 < 0
δ_2 = < 0	$\delta_2 \approx 0$	δ_2 > 0
$\Delta\delta \approx 0$	$\Delta\delta \neq 0$	$\Delta\delta$ varied

In order to evaluate the position of a given complex on the **D**, **E**, **F** continuum, three structural metrics, δ_1, δ_2 and $\Delta\delta$ are proposed (Figure 3). In the case of [**3**]$^+$, the DFT-calculated structure gives δ_1 =1.283 Å, δ_2 = 0.734 Å and $\Delta\delta$ = 0.549 Å, reinforcing the notation that the organic ligand in this case is best considered as a vinylidene. In contrast, for the majority of case in which [M_1] = [M_2] = Au(I), δ_1 is typically -1.2 Å, $\delta_2 \approx$ -0.1 and $\Delta\delta \approx$ 1.1 Å. This is also the case for the [**5**]$^+$ (δ_1 =1.218(4) Å, δ_2 = -0.034(4) Å and $\Delta\delta$ = 1.184 Å), although for [**6**]$^+$, the interaction between Au(2) and Au(I) shows the greatest tendency towards the **D**-bonding extreme (δ_1 =1.216(6) Å, δ_2 = -0.213(4) Å and $\Delta\delta$ = 1.003 Å) in any type of this complex studied to date. The trigold complex the Au(I) is not bound identically to both alkynyl ligands (for Au(1)-Au(3) δ_1 =1.218(6) Å, δ_2 = -0.080(4) Å and $\Delta\delta$ = 1.136 Å), however, this must be tensioned against a comparison with the germinal σ-alkenyl complex prepared by Fürstner[11] (WAGGAO) in which δ_1 = -0.79(1) Å, δ_2 = -0.63(4) Å and $\Delta\delta$ = 0.16 Å) illustrating that the distortion in [**6**]$^+$ is small at best.[12]

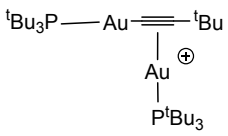
Complex	Ref.	[M1]-[M2]	[M1]-C1	[M1]-C2	δ1	[M2]-C1	[M2]-C1	δ2	Δδ
[**3**]$^+$ 1a	a	4.553	1.905	3.188	-1.283	2.837	2.103	0.734	0.549
[**3**]$^+$ 1b	a	4.118	1.915	3.213	-1.298	2.744	2.114	0.630	0.668
[**5**]SbF_6	a	3.2937(5)	1.984(3)	3.202(3)	-1.218(4)	2.221(3)	2.255(3)	-0.034(4)	1.184
[**6**]SbF_6	a	3.2477(5)	1.974(4)	3.190(4)	-1.216(6)	2.145(3)	2.358(3)	-0.213(4)	1.003
[**6**]SbF_6	a	3.3687(5)	1.976(4)	3.192(4)	-1.216(6)	2.174(3)	2.254(3)	-0.080(4)	1.136
AMOYAD	13	3.288(5)	2.043(8)	3.245(8)	-1.202(11)	2.222(8)	2.308(7)	-0.086(11)	1.116
FIJKUG	14	3.3989(6)	2.050(1)	3.220(1)	-1.170(1)	2.250(1)	2.310(1)	-0.060(1)	1.110
KUVSAW	5	3.4311(3)	2.021(5)	3.234(6)	-1.213(8)	2.209(5)	2.307(6)	-0.098(8)	1.115
NIZMAM00	15	3.5845(3)	2.021(3)	3.216(3)	-1.195(4)	2.213(4)	2.265(4)	-0.052(6)	1.143
PEXTUJ	16	3.6381(9)	1.980(1)	3.210(1)	-1.230(1)	2.210(1)	2.220(1)	-0.010(1)	1.220
QAVNAE	17	3.373(4)	2.025(8)	3.229(7)	-1.204(11)	2.198(8)	2.336(8)	-0.138(11)	1.066
QAVNEI	17	3.5327(3)	2.022(5)	3.224(5)	-1.202(7)	2.199(4)	2.309(4)	-0.110(6)	1.092
RERKIK	18	3.6486(5)	2.050(1)	3.210(1)	-1.160(1)	2.228(9)	2.274(9)	-0.046(13)	1.114
VIKMIN		3.4507(6)	2.000(1)	3.200(1)	-1.200(1)	2.230(1)	2.200(1)	0.030(1)	1.170
YEDQEF	7	3.6235(9)	1.997(7)	3.183(7)	-1.186(10)	2.193(8)	2.234(9)	-0.041(12)	1.145
ZEXMUM(1)	19	3.62(1)	2.000(1)	3.200(1)	-1.200(1)	2.194(7)	2.217(8)	-0.023(11)	1.177
ZEXMUM(2)	19	3.745(1)	2.001(7)	3.208(7)	-1.207(10	2.221(7)	2.194(8)	0.027(11)	1.180
WAGGAO	11	2.7591(9)	2.130(1)	2.920(1)	-0.790(1)	2.180(2)	2.810(2)	-0.630(3)	0.160
VAKVOS	20	2.759(1)	2.162(8)	4.600(1)	-2.438(8)	2.160(1)	4.660(1)	-2.500(1)	-0.062
LAXJOL	21	2.696(7)	2.180(1)	4.650(1)	-2.470(1)	2.170(2)	4.680(1)	-2.510(2)	-0.040
BEFKAA	22	2.7906(5)	2.125(9)	4.510(1)	-2.385(9)	2.122(9)	4.680(1)	-2.558(9)	-0.173

TableS3. 1: comparision of selected σ-π complexes and gem-diaurates. a this work. Complexes are listed by CCDC reference code. See page S18 for key to the gold componets involved.

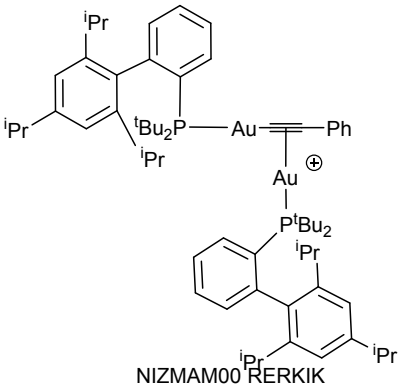


AMOYAD

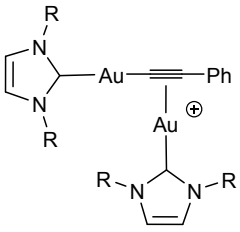
FIJKUG



KUVSAW

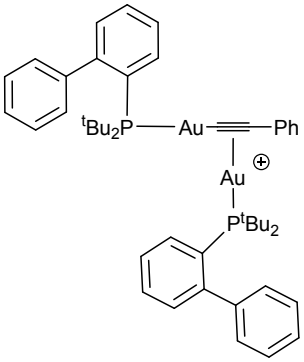


NIZMAM00 RERKIK

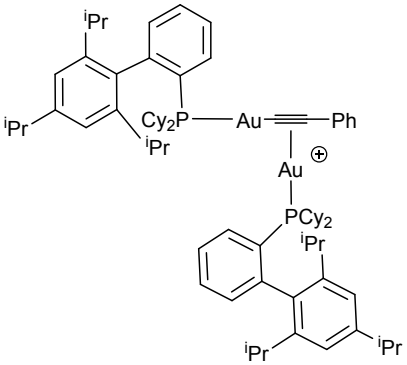


R = C_6H_3-2,6-^{i}Pr

PEXTUJ VIKMIN



QAVNAE



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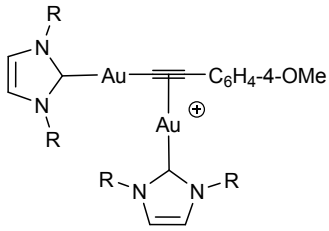
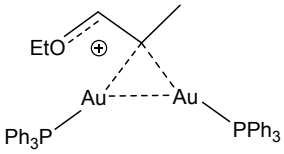
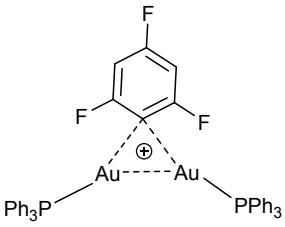


R = C_6H_3-2,6-^{i}Pr

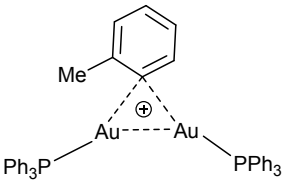
ZEXMUM



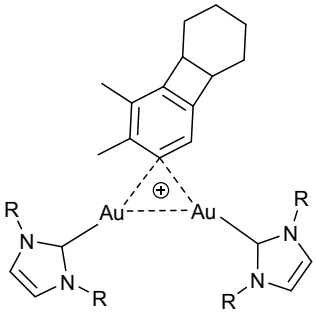
WAGGAO



VAKVOS



LAXJOL



R = C_6H_3-2,6-^{i}Pr

BEFKAA

S3 Computational Details

S3.1. Level of Theory

Unless stated otherwise, structures discussed here were optimised in Jaguar[23] with the standard BP86[24] density functional as implemented. The Jaguar triple-ζ form of the standard Los Alamos ECP basis set (LACV3P*) was used on the transition metal atoms, employing the 6-31G* basis for all other atoms with five spherical harmonic components of the polarization functions. "Loose" convergence (5 times larger than default criteria) was used for geometry optimizations and calculations were performed on isolated molecules. Vibrational frequencies were not routinely computed, and so, unless indicated, the energetic data do not include a correction for zero-point energy, although we would expect this to be quite small. In the absence of frequency calculations, stationary points have not been verified as minima; for most of these large complexes, optimisation to transition states is unlikely.

Angle restraints (C≡C-R = 120 °) were necessary to locate some of the conformers **D**-**F** when comparing the effect of different metal centres, as not all were stable local minima. These have been indicated in the data shown in section 3.2 below.

Optimisations with the standard B3LYP[24a, 25] density functional as implemented in Jaguar gave somewhat longer M-L distances in the complexes considered here (see section 3.2 for representative examples), and we were concerned that, in the absence of dispersion corrections, this functional might overestimate the relative stability of sterically crowded complexes, as well as underestimating some of the binding energies considered below. Where available, results are shown for comparison, but we have based our main discussion on the BP86 functional unless stated otherwise.

Trial optimisations with the dispersion-corrected version[26] of the functional used (BP86-D3), as well as the M06[27] density functional as implemented in Jaguar, on the other hand, resulted in significant flattening of complex [**6**]$^+$, with distances between the CNC units reduced by at least 0.3 Å. Presumably this geometry would maximise intramolecular attractive interactions in the gas phase, whereas the geometry observed in the single crystal represents a balance between intra- and intermolecular forces. Where shown in section 3.2 below, dispersion corrections were therefore calculated and added after geometry optimisation with the standard, non-dispersion corrected functional, *i.e.* these results have been derived from single point energy corrections.

For the discussion of complexes shown in Scheme 2 (**4**, [**5**]$^+$ and [**6**]$^+$) and the data in Table 4 of the main paper, a more extensive computational study was undertaken, including corrections for solvation, dispersion and Gibbs energies. In Jaguar, geometries were re-optimised with BP86 as above, standard convergence criteria, tight cutoffs (iacc=1) and fine grids (gdftfine/gdftgrad/gdftmed=13), and these calculations were followed by frequency calculations. Solvent effects were considered explicitly, by coordinating the solvent molecule shown into the vacant site of [Au(PPh_3)]$^+$. Unfortunately, small negative frequencies were found for several of the complexes considered, even with these tighter cutoffs, and not all optimisations converged fully with these settings. (Table S3.4)

The relevant structures were then re-optimised in Gaussian (the full citations are given at the end of this section), using the two standard density functionals BP86[24c, 24d, 25a] and B3LYP[24a, 25a-e] as implemented. Calculations used the standard 6-31G* basis set, but with only the five spherical harmonic components of the polarization functions, on all atoms apart from gold, where the corresponding Stuttgart relativistic ECP basis set [28a , 28b] was used to describe 60 core electrons (denoted as BS1). Vibrational frequencies were calculated at this level of theory, allowing the determination of zero-point energies and gas-phase thermodynamic corrections (298 K). Solvation effects were considered with explicit solvent coordination in the vacant site of [(PPh_3)Au]$^+$, for which structures were re-optimised, and followed by single point calculations on the gas-phase optimised geometries using a continuum dielectric field. For the latter, the Integral Equation Formalism Polarizable Continuum Model (IEF-PCM) continuum dielectric solvation model[29] was used with benzene and dichloromethane as the solvents. These were not corrected for solvation free energy effects. Basis set effects were also captured through single point calculations with the

larger 6-311+G* on all atoms apart from gold, where the aug-cc-pVTZ-PP small-core relativistic PP correlation consistent basis set[30] was used (60 core electrons, denoted as BS2). The BS2 single point calculations were generally run with tight SCF convergence, but in some cases neither this nor invoking the quadratically-convergent option would complete, so the SCF=sleazy option, applying looser SCF convergence criteria, had to be used. These data are indicated by footnotes in the tables below. Empirical dispersion corrections according to Grimme's scheme (D3[26c] and D3BJ[31]) were derived from single point calculations on the gas-phased optimised geometries. (Tables S3.5, S3.6)

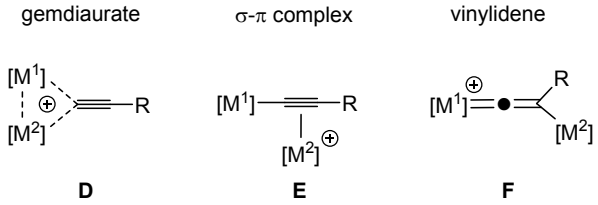
Full Gaussian citations:

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT **2010**.

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. , lmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.

S3.2. Results and Discussion

TableS3. 2: Relative potential energies of isomers for different metal complexes (BP86, kJ mol^{-1}).



a) Metal effect

Complex	M^1 = [CpRu(PPh$_3$)$_2$]$^+$, M^2 = [Au(PPh$_3$)]$^+$	M^1, M^2 = [Au(PPh$_3$)]$^+$	M^1 = [Au(^{t}BuC^N^C^{t}Bu)]$^+$, M^2 = [Au(PPh$_3$)]$^+$
D	(90)[a]	0.0	(10)[a]
E	19	10	0.0 **[5]**$^+$
F	0.0 **[3]**$^+$	(78)[a]	(59)[a]

[a] Angle restraints used.

These data show that the preferred conformation is determined by the identity of M^1, with **F** more accessible for the Au(III) complex than for Au(I), although **D** and **E** are still preferred. The data suggest that when [M^1] = Au, **D** and **E** are close in energy, agreeing with previous predictions about the exchange of Au atoms in σ–π complexes. [7]

b) Functional effect for M^1 = [CpRu(PPh$_3$)$_2$]$^+$, M^2 = [Au(PPh$_3$)]$^+$

Complex	BP86 opt	BP86-D3[a] @BP86	B3LYP opt	B3LYP-D3[a] @B3LYP
D	(90)[b]	(81)[b]	(61)[b]	(55)[b]
E	19	11	13	7
F	0.0	0.0	0.0	0.0

[a] Single Point energy; [b] Angle restraints used.

Key bond lengths (Å)

	BP86 opt	B3LYP opt
complex D		
Au-P	2.337	2.342
Au-C	2.054	2.076
Ru-P	2.381, 2.401	2.432, 2.413
Ru-C	2.229	2.273
C=C	1.266	1.250
complex E		
Au-P	2.316	2.334
Au-C(η^2-C=C)	2.195, 2.397	2.213, 2.449
Ru-P	2.368, 2.361	2.400, 2.387
Ru-C	1.978	1.995
C≡C	1.281	1.263
complex F		
Au-P	2.336	2.347
Au-C	2.114	2.135
Ru-P	2.361, 2.400	2.394, 2.428
Ru-C	1.915	1.941
C=C	1.307	1.285

c) Functional effect for M^1 = [Au(^{t}BuC^N^C^{t}Bu)]$^+$, M^2 = [Au(PPh_3)]$^+$

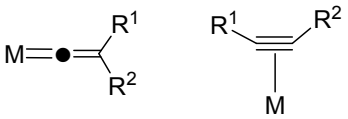
Complex	BP86 opt	BP86-D3[a] @BP86	B3LYP opt	B3LYP-D3[a] @B3LYP
D	(10.3)[b]	(23.6)[b]	(19.0)[b]	(24.5)[b]
E	0.0	0.0	0.0	0.0
F	(59.3)[b]	(62.7)[b]	(62.6)[b]	(59.7)[b]

[a] Single Point energy; [b] Angle restraints used.

Key bond lengths (Å)

	BP86 opt	B3LYP opt
complex D		
Au(I)-P	2.326	2.347
Au(I)-C	2.051	2.058
C=C	1.271	1.265
C-Au(III)	2.066	2.087
complex E		
Au(I)-P	2.314	2.326
Au(I)-C (η^2-C=C)	2.198, 2.366	2.227, 2.415
C≡C	1.261	1.244
Au(III)-C	1.987	1.996
complex F		
Au(I)-P	2.332	2.342
Au(I)-C	2.087	2.103
c=C	1.289	1.272
Au(III)-C	1.927	1.940

Structural analysis of the optimised geometries shows systematically longer M-L distances with the B3LYP functional. These geometries may be better able to accommodate the steric hindrance encountered in conformers **D**, and, to some extent, **E**, likely contributing to the lowering of energy differences observed. For the corresponding Au(III) complexes, functional effects on relative energies are smaller and less clear, suggesting perhaps that structural and steric effects are less important here.



v a

In our previous work, we explored the effect of different metal centres (changing metal identity, oxidation state and ligands) on the calculated energy differences between alkynes and vinylidenes.[32] For the exploration of metal effects, we focussed on six representative tautomer pairs, with the following substituents R^1/R^2: H/Me (A), H/Ph (B), Ph/Ph (C), F/F (D), Me/CO_2Me (E) and Ph/C(O)Ph (F). For the Au(III) complex with ^{t}BuC^N^C^{t}Bu pincer ligand used in the present work, some of the alkynyl complexes (C and F) showed pronounced metal-slippage such that only one of the C atoms in the triple bond could be considered bound to the metal atom; in addition, the substituent on this C would bend away from the Au(III)-C bond. This type of complex is perhaps better described by a carbocationic resonance structure and can be more favourable than a "classic" alkyne complex. For pairs A, B, D and E, standard alkyne and vinylidene complexes could be optimized and the energy difference determined. Throughout the study, the F/F substituted pair would always favour the vinylidene form, and this is the case with Au(III)-^{t}BuC^N^C^{t}Bu as well ($E_{v\text{-}a}$ = -80.6 kJ mol^{-1}). For A, B and E, the calculations predict that the alkyne tautomer remains most stable, but this preference is small (and smaller than that observed for Au(I) complexes) for A, B and E. Indeed, for A and E, an energy difference of <20 kJ mol^{-1} might lie within computational noise. Table S3.2 shows results for both the Au(III)/CNC system and representative Au(I) complexes.

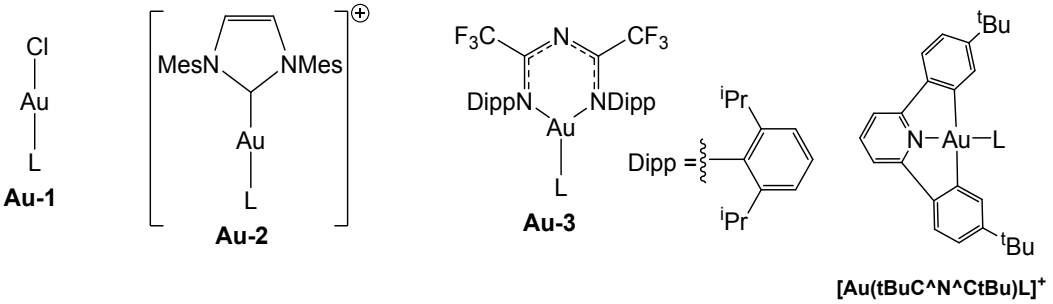


Table S3.3: Calculated tautomer energy differences, $\Delta E_{v\text{-}a}$ (kJ mol^{-1}) for different metal complexes.[32]

No.	Substituents R^1/R^2	Au-1[32]	Au-2[32]	Au-3[32]	[Au(III)(^{t}BuC^N^C^{t}Bu)L]$^+$
A	H/Me	39	61	36	13
B	H/Ph	41	77	37	(40)[a]
C	Ph/Ph	67	74	63	46
D	F/F	-33	-28	-22	-81
E	Me/CO_2Me	51	47	34	18
F	Ph/C(O)Ph	49	71	54	(40)[a]

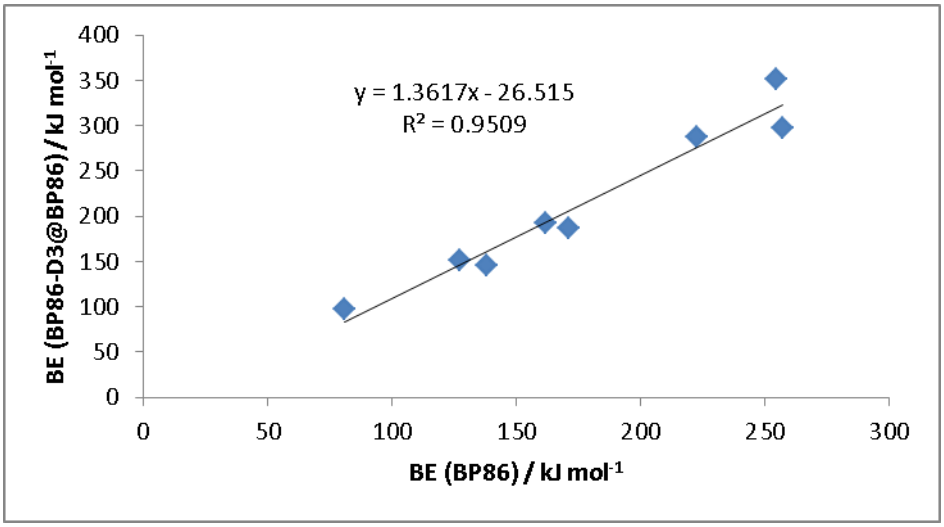
[a] Carbocation instead of alkyne.

Table S3.4: $(Au(PPh_3)]^+$ fragment binding energies, BE = E(sum of all fragments) – E(complex) (kJ mol^{-1})

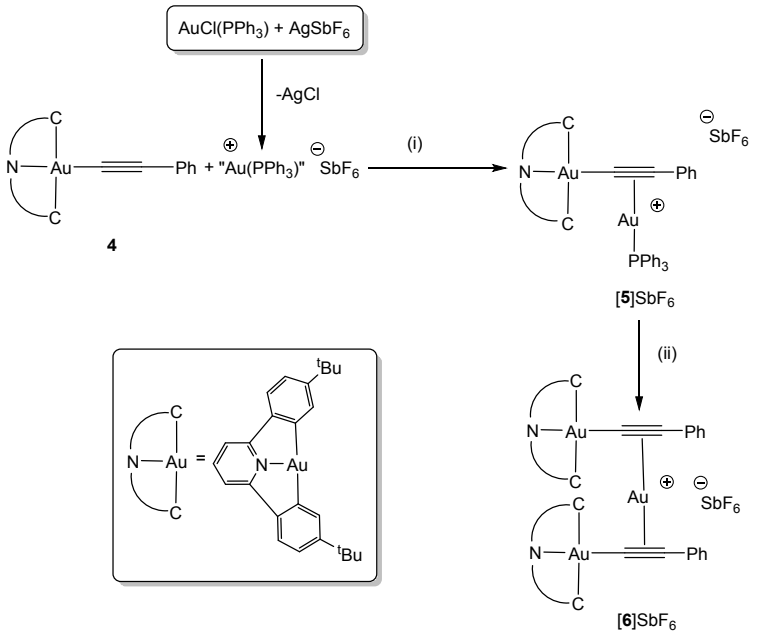
Complex	BP86 opt	BP86-D3 @BP86[a]
[**3**]$^+$ [(Ru(η^5-C_5H_5)(PPh_3)$_2$(=C=CPh{$AuPPh_3$})]	255	352
[**5**]$^+$ [Au(^{t}BuC^N^C^{t}Bu)(C≡CPh{$AuPPh_3$})]	222	288
[Au(PPh_3)(C_6H_6)]$^+$	127	152
[Au(PPh_3)(CH_2Cl_2)]$^+$	81	98
[Au(PPh_3)$_2$]$^+$	257	297
[Au(PPh_3)(η^2-HC≡CH)]$^+$	138	146
[Au(PPh_3)(η^2-HC≡CPh)]$^+$	171	186
[Au(PPh_3)((η^2-PhC≡CPh)]$^+$	162	192

[a] Single Point energy.

Figure S3.1: Comparison of binding energies calculated with BP86 and BP86-D@BP86 (data in Table S3.2, kJ mol^{-1})



The correlation between standard and dispersion-corrected BP86 binding energies is reasonably good, with bigger differences observed for the larger complexes ([**3**]$^+$ and [**5**]$^+$), as might be expected due to their increased steric hindrance.



Scheme 2. (i) Toluene 16 hrs, r.t., (ii) CH_2Cl_2, 16 hrs, r.t. - $[Au(PPh_3)_2]SbF_6$

Table S3.5: Relative energies (kJ mol^{-1}) calculated for gold complexes shown in Scheme 2 (main paper, reproduced above), Jaguar results:

a) free $[Au(PPh_3)]^+$

Complex	BP86 opt	BP86-D3 SP @ BP86
([**4**] + $[Au(PPh_3)]^+$) × 2	0.00	0.00
([**5**]$^+$) × 2	-445	-576
[**6**]$^+$ + $(Au(PPh_3)_2]^+$	-415/-438[a]	-621/-582[a]

[a] Two conformers were found for [**6**]$^+$ in Jaguar, one quite similar to the crystal structure geometry, where the two CNC ligands are stacked (Au(III)-C…C-Au(III) = -27.5 °, changing to -38.2 ° with tighter settings (data shown are for standard optimisations, as not all optimisations completed)) and a second one where the two ^{t}BuC^N^C^{t}Bu ligands are perpendicular to each other (Au(III)-C…C-Au(III) = -98.5 °), with the latter lower in energy by 23.05 kJ mol^{-1} with BP86, but 38.93 kJ mol^{-1} higher in energy with BP86-D3 at the same geometry. Both conformers could also be located with B3LYP, giving Au(III)-C…C-Au(III) = -31.3 and -92.0 °, with the latter 19.10 kJ mol^{-1} lower in energy at this level of theory.

b) Using $[Au(PPh_3)(C_6H_6)]^+$ (explicit benzene solvation)

Complex	BP86 opt	BP86-D3 SP@ BP86
([**4**] + $[Au(PPh_3)(C_6H_6)]^+$) × 2	0.00	0
([**5**]$^+$ + (C_6H_6)) × 2	-190	-272
[**6**]$^+$ + $(Au(PPh_3)_2]^+$ + 2 C_6H_6	-160/-183[a]	-318/-278[a]

[a] see Table S3.4a).

c) Using $[Au(PPh_3)(CH_2Cl_2)]^+$ (explicit dcm solvation)

Complex	BP86 opt	BP86-D3 SP@ BP86
([**4**] + $[Au(PPh_3)(CH_2Cl_2]^+$) × 2	0	0
([**5**]$^+$ + (CH_2Cl_2)) × 2	-283	-380
[**6**]$^+$ + $(Au(PPh_3)_2]^+$ + 2 CH_2Cl_2	-254/-277[a]	-426/-387[a]

([a] see Table S3.5a).

Table S3.6: Relative energies (kJ mol^{-1}) calculated for gold complexes shown in Scheme 2 (main paper, reproduced above), Gaussian results:

a) free [Au(PPh$_3$)]$^+$ (implicit solvation (continuum dielectric medium (CDM) only, vacant site in Au(PPh$_3$) complex)

Complex	**BP86 ΔE/BS1**	**B3LYP ΔE/BS1**	**B3LYP-D3 ΔE/BS1**	**B3LYP-D3BJ ΔE/BS1**	**B3LYP ΔG/BS1**	**B3LYP ΔE$_{sl}$/BS1 (benzene/CH$_2$Cl$_2$)[a]**	**B3LYP ΔE/BS2**	**B3LYP-D3BJ ΔG+ΔE$_{sl}$/BS2 (benzene/CH$_2$Cl$_2$)[a]**
([**4**] + [Au(PPh$_3$)]$^+$) × 2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
([**5**]$^+$) × 2	-445.6	-428.6	-540.0	-543.1	-324.4	-341.1/-271.8	-408.8	-331.5/-262.2
[**6**]$^{+b}$ + (Au(PPh$_3$)$_2$]$^+$	-442.3	-419.1	-546.1	-547.0	-310.0	-334.2/-267.1	-399.8[c]	-333.6/-266.6[c]

[a] CDM solvation only. [b] In G09, only a single conformer of complex [**6**]$^+$ could be located on optimization, even when starting from the crystal structure geometry. This conformer has the C^N^C groups almost perpendicular to each other, with Au(III)-C…C-Au(III) = -81.1 ° (BP86) and -84.9 ° (B3LYP). [c] Sleazy SCF convergence had to be used for [**6**]$^+$.

b) [(PPh$_3$)Au(benzene)]$^+$, benzene CDM

	B3LYP					**BP86**				
Complex	ΔE/BS2	ΔE$_{sl}$/BS2	ΔE - D3BJ/BS2	ΔG/BS2	ΔG-D3BJ+ΔE$_{sl}$/BS2	ΔE/BS2	ΔE$_{sl}$/BS2	ΔE - D3BJ/BS2	ΔG/BS2	ΔG-D3BJ+ΔE$_{sl}$/BS2
([**4**] + [Au(PPh$_3$)(C$_6$H$_6$)]$^+$) × 2	0	0	0	0	0	0	0	0	0	0
([**5**]$^+$ + (C$_6$H$_6$)) × 2	-190	-144	-245	-173	-182	-192	-147	-259	-184	-207
[**6**]$^+$ + (Au(PPh$_3$)$_2$]$^+$ + 2 C$_6$H$_6$	-181[a]	-138[a]	-249[a]	-159[a]	-185[a]	-188[a]	-146[a]	-272[a]	-170[a]	-211[a]

[a] Sleazy SCF convergence had to be used for [**6**]$^+$.

c) [(PPh$_3$)Au(CH$_2$Cl$_2$)]$^+$, CH$_2$Cl$_2$ CDM

	B3LYP					**BP86**				
Complex	ΔE/BS2	ΔE$_{sl}$/BS2	ΔE - D3BJ/BS2	ΔG/BS2	ΔG-D3BJ+ΔE$_{sl}$/BS2	ΔE/BS2	ΔE$_{sl}$/BS2	ΔE - D3BJ/BS2	ΔG/BS2	ΔG-D3BJ+ΔE$_{sl}$/BS2
([**4**] + [Au(PPh$_3$)(C$_6$H$_6$)]$^+$) × 2	0	0	0	0	0	0	0	0	0	0
([**5**]$^+$ + (C$_6$H$_6$)) × 2	-241	-144	-317	-225	-203	-256	-161	-343	-241	-234
[**6**]$^+$ + (Au(PPh$_3$)$_2$]$^+$ + 2 C$_6$H$_6$	-232[a]	-139[a]	-321[a]	-211[a]	-208[a]	-253[a]	-162[a]	-357[a]	-226[a]	-240[a]

[a] Sleazy SCF convergence had to be used for [**6**]$^+$.

While two conformers could be found when optimizing in Jaguar, the one more closely resembling the geometry observed crystallographically did not appear to be a stable minimum in Gaussian with standard DFT approaches, suggesting perhaps that it is at best a very shallow local minimum (a small imaginary frequency was found for this conformer in Jaguar, although this happened for a number of the complexes needed and may just be an artefact of the way frequencies are calculated).

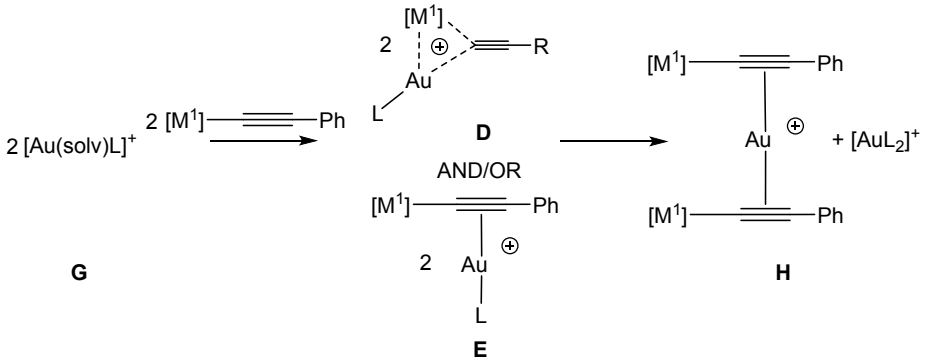
As indicated above, optimization with dispersion-corrected functionals gave rise to what might best be described as a "flattening" of the trigold complex, shortening contacts between the two C^N^C ligands by around 0.3 Å, and retaining the stacking of these ligands observed crystallographically (Au(III)-C…C-Au(III) = -18.9 with BP86-D3 in

Jaguar). This suggests that the geometry observed in the crystal structure is a compromise between intra- and intermolecular dispersion effects, and that, if these are not present, as is the case for the standard density functionals used, it becomes more favourable to twist the two units away from each other. The BP86-D3 single point energies for the two Jaguar BP86 conformers further support this: while the perpendicular conformer is 23.0 kJ mol^{-1} more favourable with BP86, it is 38.9 kJ mol^{-1} less favourable with BP86-D3.

This method sensitivity strongly suggests that the balance between [**5**]$^+$ and [**6**]$^+$ should be considered with caution. The Gaussian results above show that it is also affected by the other corrections applied, as well as the choice of solvent (note also the stronger basis set effect for explicit CH_2Cl_2). With all computational approaches showing (familiar) flaws, perhaps the strongest conclusion we can draw from the computational data is that these two complexes are likely to be close in energy.

Table S3.7: Key structural parameters for [**6**]$^+$

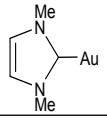
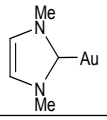
	BP86 (Jag)	**BP86 (Jag)**	**BP86-D3 (Jag)**	**B3LYP (Jag)**	**B3LYP (Jag)**	**BP86 (G09)**	**B3LYP(G09)**
Au(III)-C…C-Au(III)	-27.5	-98.5	-18.9	-31.3	-92.0	-81.1	-84.9
rel. E (kJ mol^{-1})	23.0	0.0	N/A	19.1	0.0	N/A	N/A
C≡C	1.271, 1.272	1.269, 1.270	1.269, 1.269	1.249, 1.250	1.250, 1.249	1.275, 1.275	1.252, 1.252
Au(III)-C	1.989, 1.993	1.985, 1.988	1.999, 1.996	1.999, 2.001	1.994, 1.995	1.983, 1.983	1.994, 1.994
Au(I)-C	2.188, 2.250; 2.196, 2.237	2.158, 2.244; 2.169, 2.255	2.222, 2.254; 2.214, 2.271	2.224, 2.317; 2.232, 2.295	2.186, 2.296; 2.190, 2.302	2.178, 2.191; 2.178, 2.191	2.202, 2.275; 2.202, 2.275



Scheme S3. Model reaction used to explore preference for gold(I) sandwich complex **H**

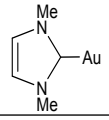
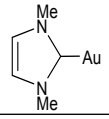
Table S3.8: Calculated energy balance between complexes **D**/**E** and **H** (Scheme 3, reproduced from main paper) with different alkyne substituents [M¹]. ΔG-D3BJ + ΔE_{solv}, kJ mol^{-1}, using both explicit solvent on $[Au(PPh_3)]^+$ and CDM solvent model.

a) BP86 Data

Solvent	L	[M¹]	G	D/E[a]	H	D/E-H
C_6H_6	PPh_3	Au(^{t}BuC^N^C^{t}Bu)	0.0	-207	-211	+4
CH_2Cl_2	PPh_3	Au(^{t}BuC^N^C^{t}Bu)	0.0	-234	-240	+6
C_6H_6	PPh_3	H	0.0	-47	-43	-4
CH_2Cl_2	PPh_3	H	0.0	-100	-99	-1
C_6H_6	PPh_3	Au(PPh_3)	0.0	-200	-192	-8
CH_2Cl_2	PPh_3	Au(PPh_3)	0.0	-219	-213	-6
C_6H_6	PPh_3		0.0	-184	-196	+12
CH_2Cl_2	PPh_3		0.0	-202	-216	+14
C_6H_6	PPh_3	Au(IPr)	0.0	-225	-211	-14
CH_2Cl_2	PPh_3	Au(IPr)	0.0	-233	-223	-10

[a]Starting from geometry **E** (σ-π), these complexes optimised to geometries better described by **D** (gem). [b] Sleazy SCF convergence used for **H**.

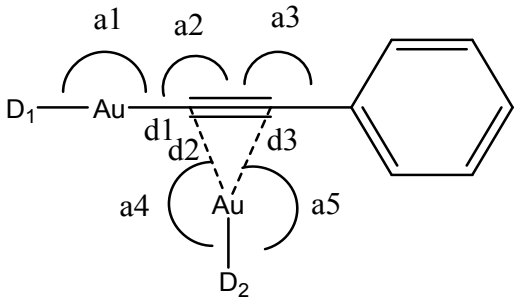
b) B3LYP Data

Solvent	L	[M¹]	G	D/E[a]	H	D/E-H
C_6H_6	PPh_3	Au(^{t}BuC^N^C^{t}Bu)	0.0	-182	-184[b]	3
CH_2Cl_2	PPh_3	Au(^{t}BuC^N^C^{t}Bu)	0.0	-203	-207[b]	4
C_6H_6	PPh_3	H	0.0	-33	-26	-7
CH_2Cl_2	PPh_3	H	0.0	-82	-75	-7
C_6H_6	PPh_3	Au(PPh_3)	0.0	-188[a]	-179	-9
CH_2Cl_2	PPh_3	Au(PPh_3)	0.0	-198[a]	-193	-5
C_6H_6	PPh_3		0.0	-181[a]	-182	1
CH_2Cl_2	PPh_3		0.0	-190[a]	-193	3
C_6H_6	PPh_3	Au(IPr)	0.0	-219[a]	-206[b]	-13
CH_2Cl_2	PPh_3	Au(IPr)	0.0	-220[a]	-212[b]	-8.0

[a]Starting from geometry **E** (σ-π), these complexes optimised to geometries better described by **D** (gem). [b] Sleazy SCF convergence used for **H**.

While both density functionals give the same trends in preferences, BP86 gives more negative relative energies for **D**/**E** and **H**, possibly because bonds are shorter (Tables S3.6 and S3.8) and so the dispersion effect is larger, and shows a more pronounced preference for **H** when M¹ corresponds to the smaller carbene, while this becomes smaller when M¹ = H. Functional choices also affect the balance between **D** and **E** when M¹ = Au(IPr), with BP86 favouring the σ-π form, while B3LYP optimises to give the gem form. As indicated previously, this method sensitivity suggests that these results should be considered with some caution, but that these complexes are similar in energy.

Table S3.9: Key structural parameters for **D**/**E** (optimisations started from the σ-π complex **E** in all cases), highlights correspond to gem **D**.



	D_1Au = H, D_2 = PPh_3		**D_1 = ^{t}BuC^N^C^{t}Bu, D_2 = PPh_3**		**D_1 = D_2 = PPh_3**		**D_1 = NHC-Me, D_2 = PPh_3**		**D_1 = IPr, D_2 = PPh_3**	
DFT	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
a1			179.6	179.3	176.9	174.7	176.3	174.8	174.2	174.4
a2	142.2	139.5	161.6	164.4	132.0	132.4	141.0	140.1	138.5	161.1
a3	177.6	177.3	176.3	172.9	179.9	180.0	179.8	179.8	179.7	173.6
a4	172.2	170.9	169.9	168.6	177.0	174.7	178.2	176.1	175.2	173.6
a5	160.9	162.2	160.1	159.7	159.3	157.1	157.2	156.3	154.2	155.0
d1			2.000	1.987	2.089	2.072	2.062	2.053	2.064	2.007
d2	2.159	2.123	2.212	2.200	2.089	2.072	2.114	2.092	2.107	2.189
d3	2.704	2.716	2.492	2.383	3.059	3.066	2.961	3.007	2.956	2.415
H-C...Au	116.1	116.8	110.9	113.3	96.5	95.1	97.5	94.0	99.9	114.8
(Ph)C-C...Au	126.2	127.9	121.2	120.6	149.1	150.1	142.7	145.8	142.9	122.0

S4 References

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S5 Coordinates of Optimized Geometries

S5.1. BP86 (Jaguar)

$M^1 = [CpRu(PPh_3)_2]^+$, $M^2 = [Au(PPh_3)]^+$

Ru Isomer D, E = -3839.648535 Hartree

Ru1	1.4500347436	2.7565024216	-1.9218350667
Au2	1.5070718249	1.6734420818	1.6258424909
C2	3.2734520278	3.3290597783	-0.6965573420
C3	2.2570600784	4.3350482775	-0.4876191814
C4	1.9834760502	4.9624623236	-1.7412599537
C5	2.8279494874	4.3507569990	-2.7472078755
C6	3.6198680682	3.3497499715	-2.0897343396
H7	1.7863290877	4.5701939363	0.4707500803
H8	1.2765813288	5.7742888621	-1.9175828912
H9	2.8832832232	4.6524543141	-3.7942441888
H10	4.3777338742	2.7185832445	-2.5570415365
H11	3.7170353322	2.6954739479	0.0710988677
P40	-0.4948540234	3.4237938186	-3.1609458403
P41	1.9741843796	0.6219439284	-2.8370015650
C36	0.6975103089	6.4791110170	-6.5432333762
C37	-0.1808751007	6.8883211100	-5.5221378254
C38	-0.5604298773	5.9969429238	-4.4970038197
C39	-0.0442281729	4.6740720554	-4.4729149986
C40	0.8550910992	4.2893732924	-5.4890850051
C41	1.2043235413	5.1770659219	-6.5175292607
H42	0.9864128033	7.1708082353	-7.3503818304
H43	-0.5821289358	7.9003185774	-5.5225594965
H44	-1.2644053100	6.3389812268	-3.7289992331
H45	1.2874901636	3.2900031250	-5.4732586700
H46	1.8802715630	4.8515263252	-7.3028084213
C43	3.2004845726	0.4894187357	-7.3577151351
C44	2.5268953314	-0.5939052928	-6.7836617917
C45	2.1308433703	-0.5795331443	-5.4400143805
C46	2.3916212810	0.5488216044	-4.6495397316
C47	3.0656449634	1.6428401443	-5.2370093352
C48	3.4772393305	1.6120257452	-6.5739793979
H49	3.5125260896	0.4674637455	-8.4070187170
H50	2.3152929870	-1.4647294785	-7.3826697586
H51	1.6209138667	-1.4434472530	-5.0093054795
H52	3.2685641548	2.5362595214	-4.6378286686
H53	4.0119478011	2.4658544918	-6.9970609739
C50	5.9168829692	-0.9890565301	-0.8550470627
C51	5.8395445636	-0.8500090471	-2.2455849560
C52	4.6660881612	-0.3866906205	-2.8557211213
C53	3.5543851847	-0.0316894564	-2.0815905156
C54	3.6463758139	-0.1719923930	-0.6760099275
C55	4.8091694456	-0.6580058479	-0.0664576041
H56	6.8306170566	-1.3636662900	-0.3863341525
H57	6.6950236920	-1.1104229023	-2.8599569574
H58	4.6120277674	-0.3014950221	-3.9263745069
H59	2.8016773717	0.0834792172	-0.0599271696
H60	4.8384926851	-0.7810872590	1.0170526872
C57	-0.7591379990	-3.1801975236	-2.7041199560
C58	0.4175950167	-3.1450535037	-1.9468207994
C59	1.2267936575	-2.0007866152	-1.9423196360
C60	0.8698064035	-0.8691121952	-2.6908658327
C61	-0.3262948567	-0.9054399164	-3.4426428768
C62	-1.1295494949	-2.0519599639	-3.4544598029
H63	-1.3821719546	-4.0776996638	-2.7146060541
H64	0.7214929724	-4.0213819848	-1.3638471255
H65	2.1586036931	-2.0016980708	-1.3694132395
H66	-0.6296677127	-0.0364331433	-4.0579867568
H67	-2.0536683123	-2.0502514617	-4.0656612470
C64	-3.4455811212	0.5991896282	-5.5150134015
C65	-3.6330402537	0.8625257503	-4.1449713670
C66	-2.7551827355	1.7257982754	-3.4692119653
C67	-1.6733574811	2.3379286697	-4.1322697880
C68	-1.5000535023	2.0780990226	-5.5147312939
C69	-2.3808856363	1.2156189925	-6.1986685946
H70	-4.1339600450	-0.0673612247	-6.0511560579
H71	-4.4698548635	0.3915553117	-3.5858497118
H72	-2.9340271477	1.9283717017	-2.4115958509
H73	-0.6849732851	2.5590546847	-6.0791213906
H74	-2.2307757439	1.0309531073	-7.2738780314
C71	-3.6000940723	5.9619451665	-0.7024170710
C72	-3.8947222541	5.5551449856	-2.0151286076
C73	-2.9792389509	4.7759391664	-2.7405918096
C74	-1.7516918376	4.3843530015	-2.1679000348
C75	-1.4689731040	4.7924390026	-0.8482671031
C76	-2.3865186734	5.5784871535	-0.1233537310
H77	-4.3157325727	6.5726360762	-0.1386083946
H78	-4.8416019917	5.8491539192	-2.4803433421
H79	-3.2136065121	4.4758015391	-3.7651338261
H80	-0.5377747924	4.4635296203	-0.3838377764
H81	-2.1486416528	5.8822258629	0.9015896150
C82	-0.6984514908	1.3679732707	-0.2347657774
P86	2.5118894816	1.3913793004	3.7165784514
C89	6.1979805875	4.1477752681	4.2150887158
C90	5.1766176954	4.2049483099	5.1571288382
C91	4.0624806656	3.3688285584	5.0344592319
C92	3.9728376845	2.4681874434	3.9537834034
C93	5.0087911939	2.4095315908	2.9916622430
C94	6.1177354275	3.2486443074	3.1344117657
H95	7.0612134680	4.8007533534	4.3152299803
H96	5.2371547676	4.9001878221	5.9934596934
H97	3.2607385985	3.4184646934	5.7801034556
H98	4.9554886272	1.7004502371	2.1453709143
H99	6.9126276173	3.2026526982	2.3964956548
C99	-0.3217029203	2.4549429583	7.2086244490
C100	-0.4729911551	3.0812278238	5.9568762191
C101	0.3610356445	2.7445069559	4.8990113185
C102	1.3779477204	1.7802347433	5.1022955809
C103	1.5321975596	1.1463420723	6.3719188736
C104	0.6779565871	1.4852741138	7.4157009850
H105	-0.9823098802	2.7122369921	8.0290125731
H106	-1.2415136983	3.8285594591	5.7971282920
H107	0.2262722214	3.2219530217	3.9163242474
H108	2.3208945433	0.3856277453	6.5430131031
H109	0.7893571682	0.9906776844	8.3913631277
C109	3.7561073495	-3.0205974978	4.4563500957
C110	4.5963481503	-1.9890779467	4.8927780900
C111	4.2439606863	-0.6472115510	4.6720467264
C112	3.0497851394	-0.3371081643	3.9969223141
C113	2.2213917791	-1.3856874911	3.5494952432
C114	2.5707920493	-2.7154412481	3.7859567474
H115	4.0248826054	-4.0616744261	4.6308841603
H116	5.5373435979	-2.2283632622	5.4090208250
H117	4.9055868288	0.1480735602	5.0179172986
H118	1.3045903239	-1.1553965083	3.0105586159
H119	1.9201750009	-3.5217153280	3.4409243692
C119	-4.5586774639	-0.3077097361	0.1700207609
C120	-3.4813130562	-1.1194346530	-0.2307215529
C121	-2.2115636489	-0.5659217389	-0.3977988031
C122	-2.0009070889	0.8198812765	-0.1652168810
C123	-3.0992756338	1.6306116464	0.2373027788
C124	-4.3638406780	1.0656380602	0.4055940558
H125	-5.5516901648	-0.7477323468	0.3013885949
H126	-3.6321281705	-2.1853285440	-0.4136589231
H127	-1.3602544764	-1.1842427805	-0.7005779317
H128	-2.9408574747	2.6913003434	0.4203981910
H129	-5.2021587166	1.6969754878	0.7212563436

Ru Isomer E

E = -3839.675524 Hartree

Ru1	1.4879898125	2.7435479168	-1.8741800262
Au2	1.0243713582	1.3807279058	1.5289382955
C2	3.2950879236	3.1172478553	-0.5268627484
C3	2.2738316119	4.0715140066	-0.1811114577
C4	2.0315115770	4.9024677781	-1.3160340331
C5	2.9233047483	4.4895985666	-2.3781086952
C6	3.6912410547	3.3893605089	-1.8852067870
H7	1.7683681417	4.1394624648	0.7834934436
H8	1.3250580699	5.7305300352	-1.3632960122
H9	3.0006838179	4.9589887763	-3.3590879821

H10	4.4608756906	2.8459062753	-2.4357513141
H11	3.7196339512	2.3587888440	0.1290969542
P40	-0.3622613500	3.5533819370	-3.1111557949
P41	2.0440812041	0.7243367986	-2.9634042442
C36	0.8750706667	7.2021148523	-5.8424340788
C37	0.3994075170	7.4043727665	-4.5381669167
C38	0.0131382703	6.3125018304	-3.7448605933
C39	0.0959130140	4.9881824972	-4.2342054507
C40	0.5795577181	4.7989367971	-5.5471579554
C41	0.9591889670	5.8928271590	-6.3413005090
H42	1.1674037543	8.0542994849	-6.4654594438
H43	0.3148510518	8.4191752899	-4.1326506171
H44	-0.3858787848	6.5035075163	-2.7429785108
H45	0.6467686888	3.7966064697	-5.9763909797
H46	1.3140656345	5.7141498218	-7.3629609389
C43	3.5322813293	1.0801860080	-7.3974077211
C44	3.0432740050	-0.1497375509	-6.9284936584
C45	2.5771107357	-0.2730191858	-5.6105374166
C46	2.5879187880	0.8403057684	-4.7417871986
C47	3.0690659333	2.0753013601	-5.2270025397
C48	3.5449902892	2.1930856097	-6.5427334363
H49	3.8969421688	1.1711449724	-8.4268049735
H50	3.0233184417	-1.0222842933	-7.5915928820
H51	2.1976445910	-1.2386834364	-5.2615269420
H52	3.0474064538	2.9519470916	-4.5714903427
H53	3.9179317852	3.1594749951	-6.9011430768
C50	5.7861611971	-1.0737569889	-0.7659161447
C51	5.9309129202	-0.5615824549	-2.0649633711
C52	4.8229858543	-0.0261693083	-2.7482949761
C53	3.5568715660	0.0186353442	-2.1310658088
C54	3.4200019997	-0.4921062640	-0.8182010630
C55	4.5221518125	-1.0413575458	-0.1472953088
H56	6.6470260238	-1.5050801740	-0.2426248969
H57	6.9074883876	-0.5881299276	-2.5620113588
H58	4.9487073284	0.3452828576	-3.7720370627
H59	2.4400060055	-0.4730090888	-0.3256780279
H60	4.3900774413	-1.4593333913	0.8587792280
C57	-0.7157312033	-3.0732157114	-3.1290188328
C58	0.6796549832	-3.2148829633	-3.0546312768
C59	1.5030943451	-2.0801327309	-2.9695127826
C60	0.9434502059	-0.7785470439	-2.9586533650
C61	-0.4591740151	-0.6503674042	-3.0142232881
C62	-1.2795179466	-1.7875143407	-3.1033091720
H63	-1.3570735516	-3.9593750813	-3.1976815610
H64	1.1357497555	-4.2121564910	-3.0631529681
H65	2.5884663304	-2.2125992596	-2.9070169319
H66	-0.9203995964	0.3395489766	-2.9838047241
H67	-2.3665610184	-1.6595358921	-3.1431241900
C64	-2.8629167891	0.8113991699	-5.9917298419
C65	-3.4871651362	1.4159546248	-4.8911715033
C66	-2.7528232347	2.2341648144	-4.0170468478
C67	-1.3751836678	2.4617219513	-4.2300402694
C68	-0.7492317722	1.8065570416	-5.3153218497
C69	-1.4874541079	1.0032579755	-6.1949782390
H70	-3.4407227588	0.1805899192	-6.6767441066
H71	-4.5555564683	1.2548188429	-4.7057958143
H72	-3.2625374016	2.6915990673	-3.1645832918
H73	0.3321029178	1.8871544313	-5.4601289945
H74	-0.9776775223	0.5128893012	-7.0316352290
C71	-3.6182067720	5.6997455060	-0.5069237401
C72	-3.6985265148	5.7359041495	-1.9102461821
C73	-2.7274666337	5.0883907006	-2.6876087408
C74	-1.6645389065	4.3815672321	-2.0732929553
C75	-1.5906962332	4.3580404957	-0.6670014136
C76	-2.5613604374	5.0146727961	0.1109832390
H77	-4.3756399001	6.2097885930	0.0999541340
H78	-4.5162409823	6.2756947547	-2.4020778673
H79	-2.7914916227	5.1379336284	-3.7810371279
H80	-0.7745110852	3.8101374468	-0.1860630653
H81	-2.4891461181	4.9882829892	1.2051417748
C82	-0.4576277559	0.9033461882	-0.0178473451
P86	2.2264797636	1.4522953502	3.5070340811
C89	6.3242959932	3.6011977952	3.0211117821
C90	5.3383131219	4.1702997704	3.8432957280
C91	4.1037188997	3.5246626533	4.0203434883
C92	3.8509654804	2.3004496774	3.3683492763
C93	4.8424354122	1.7348506534	2.5316411554
C94	6.0753106656	2.3814352838	2.3677071680
H95	7.2873168524	4.1072644806	2.8878374183
H96	5.5293973123	5.1195769400	4.3569464893
H97	3.3428478545	3.9684886881	4.6730485921
H98	4.6553670384	0.7850592101	2.0146637486
H99	6.8419182807	1.9329045739	1.7241066524
C99	-0.0854134660	3.7537719881	6.8191831882
C100	-0.2842832902	4.0664244631	5.4642057855
C101	0.4005920605	3.3500113061	4.4714314087
C102	1.3002287944	2.3228870935	4.8312081754
C103	1.4936228919	2.0094984878	6.1937601006
C104	0.7998048754	2.7245463937	7.1812979767
H105	-0.6265854919	4.3080815742	7.5944738623
H106	-0.9808945449	4.8632099612	5.1795994083
H107	0.2342534253	3.5774088262	3.4110103376
H108	2.1763846326	1.2025282442	6.4824990059
H109	0.9491525930	2.4734725681	8.2372240615
C109	3.1150527391	-2.7879019153	5.1843822117
C110	3.9933751113	-1.7311658178	5.4727078368
C111	3.7447903332	-0.4495353429	4.9587010679
C112	2.6082525217	-0.2214296110	4.1507552042
C113	1.7302016389	-1.2870880134	3.8596087499
C114	1.9850824812	-2.5649400612	4.3793691144
H115	3.3151229581	-3.7887041870	5.5838442317
H116	4.8785534870	-1.9043961660	6.0959156522
H117	4.4415020389	0.3685364202	5.1722043500
H118	0.8515376498	-1.1126633616	3.2247885274
H119	1.3026091270	-3.3901797466	4.1493327887
C119	-3.7703175214	-1.4121171166	1.3818838608
C120	-2.6250140421	-2.0501801814	0.8779740755
C121	-1.5402371010	-1.2936374696	0.4164073567
C122	-1.5890267103	0.1217100015	0.4495805854
C123	-2.7496767030	0.7564153270	0.9554559109
C124	-3.8292778372	-0.0085643805	1.4152768241
H125	-4.6150697677	-2.0068258382	1.7477547267
H126	-2.5751392237	-3.1449384176	0.8452307024
H127	-0.6470273725	-1.7857207538	0.0169328303
H128	-2.7935822881	1.8511240655	0.9754478532
H129	-4.7224435278	0.4940411508	1.8043296893

Ru Isomer F

E = -3839.68264 Hartrees

Ru1	1.2120132538	2.4360397879	-1.6149410758
Au2	-0.3750720080	0.5419291669	1.6786419669
C2	2.7172729490	2.3408430033	0.0987631100
C3	1.7710487928	3.3859003968	0.3881477319
C4	1.8967908588	4.3943593789	-0.6131173291
C5	2.9589565503	3.9942861477	-1.5168422357
C6	3.4600534218	2.7405767846	-1.0732446909
H7	1.0549176976	3.3792332180	1.2111981668
H8	1.3210771080	5.3189664388	-0.6577397933
H9	3.3056323622	4.5627463224	-2.3801221396
H10	4.2626266695	2.1650577847	-1.5368453185
H11	2.8791511310	1.4356833341	0.6831530535
P40	-0.0539033712	3.6374640222	-3.2619705257
P41	1.6656902476	0.3907375937	-2.7042791392
C36	2.6073870303	6.4972091935	-5.8956045403
C37	2.3008252796	6.8135221434	-4.5613046250
C38	1.4955395654	5.9557347497	-3.7977637807
C39	0.9766367175	4.7597504779	-4.3488199049
C40	1.2789953793	4.4613122552	-5.6937829936
C41	2.0869378058	5.3220932683	-6.4566439994
H42	3.2324062536	7.1686733143	-6.4942107903
H43	2.6803151603	7.7386798491	-4.1125487256
H44	1.2443554106	6.2395928373	-2.7702168154
H45	0.8671286580	3.5663620197	-6.1678224675
H46	2.2974155849	5.0703211163	-7.5024306165
C43	3.9148965982	0.6393743384	-6.8122881740
C44	3.1515003403	-0.5002624319	-6.5072690085
C45	2.4482301897	-0.5819485171	-5.2949281894
C46	2.4936711414	0.4841976376	-4.3689843254
C47	3.2488360815	1.6325813199	-4.6912933978
C48	3.9598249310	1.7063653154	-5.9006425988
H49	4.4660621607	0.6967436330	-7.7574025974
H50	3.1034123734	-1.3354947670	-7.2154644141

H51	1.8592169104	-1.4777852767	-5.0706832186
H52	3.2654319343	2.4779622438	-3.9939654035
H53	4.5421182181	2.6055830600	-6.1314961326
C50	4.7926612504	-1.9865155318	-0.1286891319
C51	5.1653826017	-1.4986306597	-1.3892563019
C52	4.2413027185	-0.7955272837	-2.1836400309
C53	2.9289426746	-0.5675755243	-1.7215074452
C54	2.5613203876	-1.0601837154	-0.4481795207
C55	3.4842747775	-1.7663137882	0.3371589860
H56	5.5132526481	-2.5374289098	0.4859686427
H57	6.1803746206	-1.6679662677	-1.7670687319
H58	4.5471344447	-0.4345008511	-3.1715358594
H59	1.5437613921	-0.8884318887	-0.0720200617
H60	3.1789057422	-2.1465338869	1.3192811071
C57	-1.6835643436	-2.8388163843	-3.2421071387
C58	-0.3421336248	-3.2296058938	-3.0973503201
C59	0.6609496696	-2.2629308856	-2.9274435411
C60	0.3372281118	-0.8854414822	-2.9105909687
C61	-1.0124857887	-0.5037389267	-3.0556568621
C62	-2.0135374732	-1.4748609190	-3.2178667549
H63	-2.4675196181	-3.5947207672	-3.3634856291
H64	-0.0713888127	-4.2918614189	-3.1084444193
H65	1.6991987885	-2.5852359962	-2.7907208853
H66	-1.2902610955	0.5519055172	-3.0335252044
H67	-3.0570589317	-1.1554911803	-3.3104580951
C64	-2.7844596612	1.4933556018	-6.4252146438
C65	-3.3380068028	2.4430112915	-5.5535693671
C66	-2.5359879652	3.0882202862	-4.5973028356
C67	-1.1612745920	2.7846447302	-4.4904165203
C68	-0.6189754163	1.8087418749	-5.3573897257
C69	-1.4201949597	1.1797122040	-6.3216448156
H70	-3.4113888719	0.9966437681	-7.1738261146
H71	-4.4033613700	2.6927005648	-5.6164156628
H72	-2.9878578447	3.8371622560	-3.9398176105
H73	0.4349134975	1.5237793018	-5.2760990868
H74	-0.9731285220	0.4311703452	-6.9844862909
C71	-2.9382179027	6.7730826063	-1.2946159836
C72	-2.5475932260	6.9126283307	-2.6379015357
C73	-1.6819228227	5.9777931228	-3.2244586423
C74	-1.1911239850	4.8827905467	-2.4738960798
C75	-1.5907251250	4.7495898868	-1.1280842782
C76	-2.4590706169	5.6885998562	-0.5445444375
H77	-3.6124287418	7.5061116514	-0.8381215777
H78	-2.9164577310	7.7550673609	-3.2339730040
H79	-1.3829242300	6.1021869150	-4.2711313312
H80	-1.2268380543	3.9002894450	-0.5391364676
H81	-2.7618722225	5.5653114255	0.5016232269
C81	-1.2993187105	1.0701807645	-0.1482351956
C82	-0.3436778311	1.6322706900	-0.8394802904
C84	-5.5378017630	0.3616859984	-0.4978863193
C85	-4.9200648069	1.3659661851	-1.2610090431
C86	-3.5431778531	1.5995067780	-1.1522304757
C87	-2.7426091155	0.8270106794	-0.2742823703
C88	-3.3801797944	-0.1882812871	0.4816927415
C89	-4.7578013534	-0.4159063447	0.3725097556
H90	-6.6160613632	0.1855613159	-0.5825171690
H91	-5.5177060866	1.9803443362	-1.9448083436
H92	-3.0785303640	2.3975060181	-1.7395363444
H93	-2.7728522913	-0.8175410057	1.1446648594
H94	-5.2230767927	-1.2111823579	0.9669735515
P95	0.2686652575	-0.0404564819	3.8470446064
C98	-2.9396699879	1.2016065682	6.9871450767
C99	-1.5795554795	1.2297237771	7.3359431624
C100	-0.5996696692	0.8781410991	6.3940778959
C101	-0.9785257583	0.4910820328	5.0899735530
C102	-2.3463181985	0.4749599239	4.7402276994
C103	-3.3197066959	0.8256552126	5.6877240618
H104	-3.7011290396	1.4795029439	7.7239789419
H105	-1.2757447891	1.5307842223	8.3448514789
H106	0.4598282539	0.9168162522	6.6711889526
H107	-2.6483534204	0.1955198582	3.7233583478
H108	-4.3783218029	0.8124710102	5.4058009400
C108	4.1818622455	2.1241769605	5.1370409243
C109	3.0571226749	2.8535876652	4.7135579482
C110	1.8893042754	2.1819124805	4.3289434412
C111	1.8321042884	0.7700814383	4.3768204278
C112	2.9620289586	0.0431378021	4.8011433539
C113	4.1321312709	0.7230212623	5.1785539975
H114	5.0958267986	2.6500921122	5.4347283678
H115	3.0906095948	3.9484112250	4.6816960202
H116	1.0118568385	2.7543964401	4.0034484068
H117	2.9289170304	-1.0506934510	4.8443009112
H118	5.0062272819	0.1514012190	5.5102054957
C118	0.9415015175	-4.6089767113	4.4649240001
C119	0.7446029425	-3.7739311245	5.5782562301
C120	0.5224238383	-2.4002308147	5.4014972412
C121	0.5026058915	-1.8461000909	4.1022246548
C122	0.6849968518	-2.6913796413	2.9868308349
C123	0.9062504510	-4.0661051793	3.1701967399
H124	1.1118996250	-5.6816927532	4.6073516364
H125	0.7584784965	-4.1935579982	6.5903805031
H126	0.3561035661	-1.7597211191	6.2750623302
H127	0.6370260831	-2.2711062013	1.9747922350
H127	0.6370260831	-2.2711062013	1.9747922350
H128	1.0429668356	-4.7139895931	2.2972835726

M^1, M^2 = $[Au(PPh_3)]^+$

Au(I) Isomer D

E = -2651.418617

Au1	1.9070051589	-1.2298795831	1.2527753550
Au2	1.1186930581	-1.6438324256	-1.7067784678
C3	2.4324212520	-2.4557425843	-0.3290874614
C4	3.2472141309	-3.4110528930	-0.4122346096
C6	5.9702540185	-6.6361111133	-0.6819837571
C7	4.6281132868	-6.8808837318	-0.3391270602
C8	3.7240766079	-5.8195214186	-0.2474804548
C9	4.1592081984	-4.4897414089	-0.5032467806
C10	5.5180640726	-4.2549342437	-0.8504073714
C11	6.4124769942	-5.3250197703	-0.9359674997
H12	6.6754917345	-7.4715718421	-0.7514043085
H13	4.2890478394	-7.9035216849	-0.1426559190
H14	2.6770256336	-5.9944037587	0.0186381264
H15	5.8476083281	-3.2297601113	-1.0456605559
H16	7.4586857769	-5.1403164218	-1.2016676633
P17	-0.3358476133	-0.8373976295	-3.3325055999
C18	-3.7132146377	-3.8733734006	-4.3098120828
C19	-3.2214339741	-3.7522114056	-2.9993959989
C20	-2.1884490797	-2.8477391030	-2.7181187431
C21	-1.6476218944	-2.0492538967	-3.7494441397
C22	-2.1410658982	-2.1758935248	-5.0652171699
C23	-3.1716311344	-3.0881138202	-5.3398537668
H24	-4.5154347844	-4.5864216971	-4.5295384105
H25	-3.6373589106	-4.3700108758	-2.1959562028
H26	-1.7938470633	-2.7624852296	-1.6978400293
H27	-1.7160659461	-1.5706608037	-5.8733334027
H28	-3.5483954547	-3.1871985204	-6.3637877887
C29	1.8492686610	0.0783261135	-7.3278510874
C30	2.2271475476	-1.0252066268	-6.5446213058
C31	1.5726133775	-1.2832276550	-5.3325100643
C32	0.5254869956	-0.4392166082	-4.9022011415
C33	0.1496621275	0.6692206037	-5.6897154929
C34	0.8137575842	0.9235723527	-6.8995403257
H35	2.3675147797	0.2828237214	-8.2710814746
H36	3.0393920038	-1.6821177434	-6.8742181691
H37	1.8745445315	-2.1383898429	-4.7150205962
H38	-0.6533704768	1.3350778205	-5.3559268484
H39	0.5217971040	1.7878483343	-7.5061833270
C40	-2.4207682088	3.1559137157	-2.1921281313
C41	-3.1724350690	2.1338435012	-2.7924247333
C42	-2.5660625055	0.9101375994	-3.1181493484
C43	-1.1986091397	0.7069014815	-2.8386813387
C44	-0.4494457544	1.7318525470	-2.2206841092
C45	-1.0599632764	2.9533909674	-1.9054007652
H46	-2.8963120620	4.1115892155	-1.9447540586
H47	-4.2346050221	2.2877268898	-3.0132051558
H48	-3.1539030204	0.1176522989	-3.5936323836
H49	0.6116058887	1.5724857290	-1.9929062178
H50	-0.4737120822	3.7468266920	-1.4295333478
P51	1.3348959840	0.0669899205	3.0960371125
C52	-0.1812351348	-2.5831666696	6.6004590580
C53	-0.8204216913	-1.3622860052	6.3342235932
C54	-0.3813387958	-0.5507599859	5.2764690835

C55	0.7051896846	-0.9646721864	4.4779812096
C56	1.3413986582	-2.1969730664	4.7446473138
C57	0.9005114163	-2.9989295780	5.8059768439
H58	-0.5305514811	-3.2155496472	7.4241064627
H59	-1.6683543852	-1.0395502548	6.9483836737
H60	-0.8885094414	0.3974131876	5.0683888752
H61	2.1783961383	-2.5275591759	4.1170884691
H62	1.3964680962	-3.9546551356	6.0076583459
C63	-2.1670586897	2.9920170639	2.2216309413
C64	-2.1424008001	1.7130568797	1.6403837930
C65	-1.0626758921	0.8528680565	1.8815754534
C66	-0.0045881878	1.2656303235	2.7207413660
C67	-0.0271726872	2.5537793126	3.2943434956
C68	-1.1087353022	3.4125234288	3.0422320973
H69	-3.0116152837	3.6636575324	2.0312155248
H70	-2.9614487360	1.3883150352	0.9898149731
H71	-1.0382591158	-0.1427648948	1.4226872122
H72	0.7952174386	2.8836699350	3.9385958869
H73	-1.1233765803	4.4118140339	3.4913088032
C74	4.8564645563	2.6297870950	4.7217587971
C75	3.9317794074	2.0744760851	5.6210587393
C76	2.8725488908	1.2833181697	5.1484969241
C77	2.7355559035	1.0455432231	3.7641356996
C78	3.6740825508	1.5955246118	2.8639655846
C79	4.7260592839	2.3886909880	3.3433963893
H80	5.6825546955	3.2444949319	5.0952959382
H81	4.0345156696	2.2534469052	6.6969722994
H82	2.1577797563	0.8474868415	5.8551706925
H83	3.5799582442	1.3969291431	1.7889750279
H84	5.4504724950	2.8125856450	2.6394754613

Au(I) Isomer E

E = -2651.414992 Hartree

Au1	1.3822923032	-1.0776944403	-0.0608585719
Au2	2.5223105042	-2.8937881274	-2.4953207562
C3	2.8126770869	-2.4623329880	-0.3889740106
C4	3.7194122427	-3.3347673486	-0.3192498595
C6	6.7429549582	-6.2623204323	0.1927259117
C7	5.3886142929	-6.6286101974	0.2853823151
C8	4.3884583196	-5.6661455153	0.1157805445
C9	4.7414193599	-4.3178011933	-0.1519549993
C10	6.1100263380	-3.9560086557	-0.2434468728
C11	7.1005922291	-4.9280784085	-0.0700171299
H12	7.5230131426	-7.0197765621	0.3269831710
H13	5.1131092872	-7.6681908556	0.4926965945
H14	3.3299125896	-5.9360676755	0.1893240489
H15	6.3755132780	-2.9142914983	-0.4470419370
H16	8.1564753844	-4.6453939262	-0.1384843244
P17	1.9498854357	-3.2421239614	-4.7121364193
C18	-1.2842503836	-6.5594900643	-5.0937057498
C19	-1.2840273712	-5.6874945065	-3.9921167130
C20	-0.2905652176	-4.7059761228	-3.8746066552
C21	0.7066380904	-4.5844278180	-4.8671056123
C22	0.7070876547	-5.4661826860	-5.9684402667
C23	-0.2886141544	-6.4496097792	-6.0771034433
H24	-2.0573028331	-7.3308169357	-5.1811610325
H25	-2.0534881206	-5.7783078880	-3.2175107629
H26	-0.2811814988	-4.0358128788	-3.0057281326
H27	1.4853615855	-5.3890476732	-6.7354166806
H28	-0.2824526838	-7.1342781597	-6.9322727391
C29	5.5094341595	-4.6124663985	-7.3690459091
C30	5.4015124058	-5.0499337752	-6.0378527219
C31	4.3397070250	-4.6101226562	-5.2353567488
C32	3.3688079124	-3.7331541427	-5.7667984816
C33	3.4824179011	-3.2904733389	-7.1016282043
C34	4.5518035395	-3.7319138009	-7.8963242319
H35	6.3425643265	-4.9536221705	-7.9926831303
H36	6.1498951514	-5.7318179282	-5.6196962057
H37	4.2615880433	-4.9484020171	-4.1946402137
H38	2.7404419682	-2.6019503145	-7.5200633110
H39	4.6345929735	-3.3828965660	-8.9314869898
C40	0.2070067338	0.5171857080	-6.8290920354
C41	-0.3092202695	-0.7528690998	-7.1344005677
C42	0.1868202378	-1.8938781754	-6.4834978621
C43	1.2097466864	-1.7664094242	-5.5187050482
C44	1.7194592457	-0.4869863453	-5.2076099053
C45	1.2202885237	0.6473978778	-5.8642751645
H46	-0.1813988166	1.4046375298	-7.3403704000
H47	-1.1014507277	-0.8602227440	-7.8838889205
H48	-0.2214738652	-2.8811265274	-6.7263319513
H49	2.5071779934	-0.3820027922	-4.4513834733
H50	1.6206438292	1.6365563566	-5.6171384492
P51	-0.3189448858	0.4802366500	0.2562500249
C52	-3.5388737215	-1.0348855825	3.2452511796
C53	-3.9403424072	-0.3148141837	2.1088336307
C54	-2.9845955392	0.1418050521	1.1875602479
C55	-1.6162620027	-0.1242172810	1.4048037856
C56	-1.2177463681	-0.8566989733	2.5445043512
C57	-2.1774413639	-1.3048471747	3.4622529495
H58	-4.2883128610	-1.3914208978	3.9605311777
H59	-5.0021661251	-0.1083142117	1.9345723158
H60	-3.3041328761	0.6978411268	0.2995846785
H61	-0.1557705056	-1.0765327809	2.7102281571
H62	-1.8617887600	-1.8720136035	4.3447098622
C63	-2.5951093308	1.3845426182	-3.6948226041
C64	-2.0535852693	0.1101478027	-3.4595924425
C65	-1.3426153871	-0.1443055318	-2.2788900084
C66	-1.1803431201	0.8764031867	-1.3173657799
C67	-1.7141793620	2.1586601196	-1.5629576022
C68	-2.4210389632	2.4077086295	-2.7498010594
H69	-3.1491080391	1.5818115250	-4.6192954996
H70	-2.1747570521	-0.6840587120	-4.2039525770
H71	-0.9115449130	-1.1356857218	-2.0980375830
H72	-1.5778539938	2.9610693442	-0.8295602309
H73	-2.8360727273	3.4048493227	-2.9341323820
C74	1.2040902967	4.5705499073	1.8429271952
C75	-0.0174424467	4.0623223486	2.3121641284
C76	-0.4860690340	2.8194151614	1.8583335563
C77	0.2738586941	2.0800253181	0.9283193462
C78	1.5071308331	2.5894416708	0.4670810805
C79	1.9657031275	3.8334315487	0.9207512056
H80	1.5672486665	5.5399505565	2.2014199929
H81	-0.6087892673	4.6323403636	3.0371704675
H82	-1.4371566090	2.4232857581	2.2310454885
H83	2.1067001803	2.0083964007	-0.2446426065
H84	2.9235392800	4.2243477826	0.5604331787

Au(I) Isomer F

E = -2651.389094, Hartree

Au1	2.5561246227	-1.0191458011	-0.8629645766
Au2	4.5809030446	-3.5229448932	-1.2524757768
C3	4.4598154524	-1.3855214211	-1.4393317538
C4	5.6290931046	-1.2224997168	-1.8825786014
C6	9.5276944307	-0.5801036145	-3.4258687195
C7	9.2923310033	-0.4552246068	-2.0447130482
C8	8.0096573493	-0.6657071684	-1.5271097630
C9	6.9404907046	-1.0018866253	-2.3985090774
C10	7.1851432659	-1.1224012026	-3.7927309662
C11	8.4732303933	-0.9130850822	-4.2958607509
H12	10.5347676194	-0.4179984807	-3.8251512570
H13	10.1142822717	-0.1951515567	-1.3691339865
H14	7.8153218986	-0.5737550382	-0.4536338098
H15	6.3567668288	-1.3791179836	-4.4601512157
H16	8.6587141740	-1.0082482293	-5.3711424022
P17	4.5245013136	-5.8241114478	-0.9988414831
C18	2.8563690706	-7.9788950938	-4.7714998605
C19	3.6871629768	-6.8523634653	-4.8984817922
C20	4.1667265499	-6.1981773536	-3.7546904393
C21	3.8252701579	-6.6749726363	-2.4697889671
C22	2.9850581645	-7.8017438436	-2.3451993247
C23	2.5051150284	-8.4485267835	-3.4955812732
H24	2.4787349056	-8.4860228039	-5.6659887604
H25	3.9599539408	-6.4784900594	-5.8914850217
H26	4.8091759428	-5.3147330764	-3.8561720213
H27	2.7041140058	-8.1726375028	-1.3534378676
H28	1.8527177524	-9.3226310038	-3.3914492421
C29	1.8801680042	-7.1455145507	2.5922875339
C30	1.5661903361	-5.9838321353	1.8667405158
C31	2.3790990843	-5.5816094926	0.7973291000
C32	3.5122956679	-6.3444026735	0.4416584790
C33	3.8307581647	-7.5052024726	1.1789531282
C34	3.0130482456	-7.9014954469	2.2489379603

H35	1.2481292246	-7.4570023500	3.4310796000
H36	0.6933014918	-5.3808812973	2.1396366930
H37	2.1412732751	-4.6664767628	0.2411233274
H38	4.7188641966	-8.0935872259	0.9227320073
H39	3.2668752298	-8.8025150886	2.8182460607
C40	8.7418562678	-7.6345087043	-0.2278425324
C41	7.8501690526	-8.2979613129	-1.0853077552
C42	6.5786947586	-7.7584712663	-1.3405394449
C43	6.1951600047	-6.5435147894	-0.7346464566
C44	7.0982388137	-5.8736730722	0.1198939459
C45	8.3631190906	-6.4218144635	0.3735886634
H46	9.7331706811	-8.0576126424	-0.0326868819
H47	8.1427325949	-9.2400860744	-1.5619682679
H48	5.8905561502	-8.2802283110	-2.0140211486
H49	6.8096899276	-4.9226478631	0.5842439850
H50	9.0582071012	-5.8967626959	1.0378950126
P51	0.3476245284	-0.5432557860	-0.3102501517
C52	-2.5082430162	-1.8327216898	-3.7472358028
C53	-2.7354459846	-0.6185707167	-3.0811598605
C54	-1.8844097546	-0.2125361328	-2.0409038959
C55	-0.7965632690	-1.0270537128	-1.6640850297
C56	-0.5678957354	-2.2453272048	-2.3419107391
C57	-1.4245384068	-2.6462515392	-3.3759040631
H58	-3.1706661418	-2.1422326647	-4.5631620971
H59	-3.5746067544	0.0213267258	-3.3749519864
H60	-2.0594227240	0.7411385249	-1.5315136595
H61	0.2877877184	-2.8736950842	-2.0656325042
H62	-1.2403438461	-3.5908705307	-3.8996402106
C63	-0.2997472494	4.0085707123	0.3384441954
C64	0.6166109209	3.5462941857	-0.6204261158
C65	0.8140924193	2.1696816154	-0.7956654651
C66	0.0830647574	1.2463095489	-0.0159632266
C67	-0.8335493724	1.7136285666	0.9487128248
C68	-1.0207135571	3.0937710916	1.1221330848
H69	-0.4460894100	5.0849123993	0.4802955644
H70	1.1868473411	4.2584662985	-1.2266476331
H71	1.5377935508	1.8081474055	-1.5369835851
H72	-1.3903990859	1.0027285120	1.5689547307
H73	-1.7307017740	3.4537649046	1.8746595145
C74	-1.0724332070	-2.6747534196	3.5747437789
C75	-1.9462906942	-2.5839536636	2.4788331371
C76	-1.5322259655	-1.9552009770	1.2932008671
C77	-0.2335730279	-1.4133765806	1.2008324286
C78	0.6472675702	-1.5158661217	2.3004396946
C79	0.2244719876	-2.1391011237	3.4834455701
H80	-1.4008179897	-3.1622984108	4.4991965717
H81	-2.9570063722	-3.0020494713	2.5443280959
H82	-2.2166321296	-1.8901380082	0.4401708434
H83	1.6628219555	-1.1072516163	2.2278491554
H84	0.9112170046	-2.2105514977	4.3340909551

M^1 = [Au(^{t}Bu^C^N^C^{t}Bu)]$^+$, M^2 = [Au(PPh_3)]$^+$

Au(III) Isomer D

E = -2638.723371 Hartree

Au1	1.0045994324	-2.2052662149	1.3886573959
Au2	1.2001675820	-1.6940841521	-2.1332552274
C3	0.9044354341	-0.6345441239	3.8600284480
C4	0.4375473700	-0.2865577814	5.1417314532
C5	-0.6076826776	-1.0254779212	5.7147154289
C6	-1.1932379098	-2.1015230985	5.0327693787
C7	-0.7160397556	-2.4379542400	3.7513154621
N8	0.3026322104	-1.6892263508	3.2343195784
H9	0.8892482201	0.5494167218	5.6811082902
H10	-0.9713278702	-0.7575716244	6.7127183341
H11	-2.0064629231	-2.6750551513	5.4841916515
C12	4.0264407245	1.1528479251	1.4704370288
C13	3.2853024519	0.0250133707	1.0227220492
C14	2.2754448027	-0.5606647110	1.7908388179
C15	1.9783686653	-0.0026161620	3.0776076113
C16	2.7090804236	1.1105568788	3.5356445441
C17	3.7156848305	1.6772223744	2.7422111492
H18	3.5119075442	-0.4019889496	0.0378505714
H19	2.4986053477	1.5495600237	4.5186222008
H20	4.2612254075	2.5423353974	3.1295444472
C21	-2.0302947399	-5.5377279595	1.0567619223
C22	-0.9582998718	-4.6631209199	0.7318781477
C23	-0.5206703495	-3.6612666051	1.6003099037
C24	-1.1794328603	-3.5142409980	2.8652996963
C25	-2.2348742685	-4.3814169294	3.2058359416
C26	-2.6505482337	-5.3761298220	2.3119211459
H27	-0.4575267093	-4.7715277413	-0.2376143942
H28	-2.7476031203	-4.2871260870	4.1702900091
H29	-3.4764223151	-6.0299575578	2.6059381726
C30	-2.4828569094	-6.6124912797	0.0473267663
C31	-3.6349442804	-7.4863881717	0.5927051411
H32	-3.3427760465	-8.0322879670	1.5080264317
H33	-4.5361337674	-6.8876152129	0.8174498453
H34	-3.9185404125	-8.2389468043	-0.1644951803
C35	-1.2827149461	-7.5397519056	-0.2845195266
H36	-0.9112940064	-8.0496159365	0.6225052425
H37	-1.5867002629	-8.3139898125	-1.0130359647
H38	-0.4408843324	-6.9758115487	-0.7256950623
C39	-2.9742904824	-5.9165975628	-1.2511625786
H40	-3.2935571031	-6.6733389171	-1.9916151551
H41	-3.8353696276	-5.2556042970	-1.0448179851
H42	-2.1807535588	-5.3040830690	-1.7153957291
C43	5.1226678084	1.7579908522	0.5683550230
C44	5.8039641899	2.9865833745	1.2117111538
H45	5.0855232199	3.8042402266	1.4033876969
H46	6.3018955709	2.7315128122	2.1647543500
H47	6.5783732487	3.3807987201	0.5294596066
C48	4.4883386501	2.2021590696	-0.7777235983
H49	3.7162028429	2.9758765638	-0.6155666549
H50	5.2631537395	2.6278777095	-1.4416125641
H51	4.0168495113	1.3573577505	-1.3107791105
C52	6.2116566867	0.6845131006	0.2961623042
H53	7.0046622530	1.1015271847	-0.3519293245
H54	6.6817600480	0.3479965089	1.2379147735
H55	5.7952464803	-0.2035220853	-0.2122323388
C56	1.7513669548	-2.7460699312	-0.4432498662
C57	2.5869788767	-3.6992034223	-0.5325242739
C58	5.4041637901	-6.8156836408	-0.9247697213
C60	4.0316450615	-7.0985987040	-1.0543179508
C61	3.0943608372	-6.0723131255	-0.9263329251
C62	3.5276029531	-4.7405917416	-0.6669881173
C63	4.9203221603	-4.4693571787	-0.5357011674
C64	5.8469536041	-5.5049591438	-0.6646054074
H65	6.1358205407	-7.6251262341	-1.0256242954
H66	3.6989137214	-8.1225311690	-1.2538184452
H67	2.0221632441	-6.2727599792	-1.0175892493
H68	5.2440149846	-3.4437751700	-0.3315056429
H70	6.9172487785	-5.2978169526	-0.5618939706
P71	0.5614676316	-0.4576089320	-3.9965308608
C72	-1.5298102415	-3.0335300949	-7.2466462486
C73	-1.7475824181	-3.2929679144	-5.8830988283
C74	-1.0983897681	-2.5222305595	-4.9089972565
C75	-0.2328506727	-1.4762609540	-5.2975730290
C76	-0.0131053998	-1.2206168673	-6.6674836022
C77	-0.6630753197	-2.0005955493	-7.6364114138
H78	-2.0329127622	-3.6414329386	-8.0066647991
H79	-2.4193356555	-4.1024407035	-5.5770321717
H80	-1.2615502655	-2.7292291684	-3.8440723183
H81	0.6658869272	-0.4185503068	-6.9761756142
H82	-0.4879132725	-1.8003672405	-8.6991917335
C83	4.1636403198	1.5984533683	-6.0885423635
C84	4.2780356770	0.2864426408	-5.5983978706
C85	3.1933165030	-0.3178471065	-4.9483211848
C86	1.9794701287	0.3877046758	-4.7962074165
C87	1.8687643767	1.7057208942	-5.2854615311
C88	2.9620508893	2.3060976532	-5.9294124850
H89	5.0146448563	2.0712908955	-6.5911328149
H90	5.2171756931	-0.2651873279	-5.7170406474
H91	3.2853356365	-1.3390386483	-4.5580265902
H92	0.9336304473	2.2624876935	-5.1601039240
H93	2.8723744948	3.3311173392	-6.3058554332
C94	-2.4043101342	2.9120314918	-2.8109898145
C95	-2.6111123245	2.2021006488	-4.0037682555
C96	-1.7316701308	1.1728959449	-4.3747892344
C97	-0.6374044732	0.8532484055	-3.5451887922
C98	-0.4379303933	1.5617482175	-2.3398186506
C99	-1.3170288494	2.5918860894	-1.9801791339

H100	-3.0948105528	3.7129426630	-2.5243780303
H101	-3.4614338121	2.4468162275	-4.6497494664
H102	-1.8972227630	0.6199629338	-5.3058768590
H103	0.4038110436	1.3038897624	-1.6849331525
H104	-1.1577418411	3.1402050643	-1.0452418466

Au(III) Isomer E
E = -2638.727311 Hartree

Au1	0.8569553667	-1.3848915659	-0.1065329827
Au2	2.4423818910	-3.2088885317	-2.5629467313
C2	0.2803364980	1.4753322136	0.1669576294
C3	-0.5175157384	2.6032484544	0.4320087387
C4	-1.8686411908	2.4222491578	0.7611850410
C5	-2.4317425072	1.1401827406	0.8232756894
C6	-1.6210948990	0.0213265265	0.5556439103
N7	-0.3078180353	0.2444944505	0.2479905202
H8	-0.0846304254	3.6056212229	0.3821163183
H9	-2.4941626644	3.2966232933	0.9712779861
H10	-3.4865775855	1.0048108647	1.0753679779
C11	4.4310228029	1.2507988208	-0.9997632091
C12	3.6401176359	0.0857513311	-0.7954178306
C13	2.2968832785	0.1486801761	-0.4125286492
C14	1.7005544048	1.4363501321	-0.2109716843
C15	2.4763384694	2.5965041014	-0.3949547409
C16	3.8182332471	2.5022760033	-0.7861088765
H17	4.1005021315	-0.8986962277	-0.9425204955
H18	2.0393264186	3.5901127976	-0.2391369425
H19	4.3878053846	3.4253703041	-0.9252183789
C20	-2.6491421840	-4.1680725715	0.4156765467
C21	-1.3229995332	-3.7092256255	0.1880731669
C22	-0.9845384634	-2.3562518872	0.2471357960
C23	-2.0053185922	-1.3962048081	0.5451901358
C24	-3.3190406088	-1.8397265172	0.7854752313
C25	-3.6309508872	-3.2034765384	0.7203371021
H26	-0.5384322723	-4.4384083380	-0.0445440628
H27	-4.1165234635	-1.1243436545	1.0187241752
H28	-4.6638673440	-3.5105211149	0.9074398156
C29	-2.9706351939	-5.6719861851	0.3126805769
C30	-4.4528212236	-5.9778287863	0.6236584968
H31	-4.7297848585	-5.6782796283	1.6506197814
H32	-5.1357584007	-5.4709925218	-0.0823566732
H33	-4.6338218850	-7.0639772546	0.5360173060
C34	-2.0860463498	-6.4574888226	1.3191381846
H35	-2.2881694089	-6.1378911879	2.3571506136
H36	-2.2973703741	-7.5403098249	1.2478846600
H37	-1.0083130598	-6.3107992618	1.1267624060
C38	-2.6702132583	-6.1534773267	-1.1334607144
H39	-2.8826022431	-7.2345847113	-1.2278754617
H40	-3.2987548543	-5.6167282329	-1.8671932949
H41	-1.6127962993	-5.9913063066	-1.4101510427
C42	5.9006822571	1.1150614228	-1.4441255419
C43	6.5838139138	2.4869700102	-1.6395610875
H44	6.0789871655	3.0934316223	-2.4137586557
H45	6.6117096431	3.0722313201	-0.7026985787
H46	7.6284234768	2.3376003328	-1.9661117279
C47	5.9553514774	0.3482735629	-2.7930424960
H48	5.4093714437	0.8957291158	-3.5826681074
H49	7.0039840277	0.2325247014	-3.1233498705
H50	5.5157002858	-0.6621361000	-2.7148288691
C51	6.6895589608	0.3256892924	-0.3656198056
H52	7.7439054001	0.2077247103	-0.6767088301
H53	6.6763336313	0.8567278714	0.6029126088
H54	6.2704449284	-0.6831207131	-0.2040959034
C55	1.9643490959	-3.0029985031	-0.4272317704
C56	2.6197503503	-4.0790762908	-0.3701182618
X57	2.4834136084#	-3.4494366013#	-0.4006262824#
C58	4.6083369241	-7.7686937507	0.3185062189
C59	3.2353162255	-7.7559719738	0.0180977102
C60	2.5796366834	-6.5433573340	-0.2173133558
C61	3.2992532914	-5.3234299284	-0.1500599988
C62	4.6843034419	-5.3447176164	0.1489727296
C63	5.3289545803	-6.5636774388	0.3844799154
H64	5.1177822194	-8.7206915107	0.5034007600
H65	2.6740921792	-8.6953076208	-0.0311420139
H66	1.5102163389	-6.5216398576	-0.4514761311
H67	5.2347780554	-4.4003866812	0.2038271646
H68	6.3978343869	-6.5750233585	0.6230777755
P70	2.5486513610	-2.9332330954	-4.8582660495
C71	0.4501200325	-6.4090852141	-7.1071882186
C72	-0.1116911138	-5.8744760560	-5.9350425799
C73	0.5414685171	-4.8400711176	-5.2517398481
C74	1.7596282668	-4.3258378445	-5.7488759199
C75	2.3221523371	-4.8640987903	-6.9240551706
C76	1.6644020523	-5.9054203894	-7.5982646456
H77	-0.0591995384	-7.2220930865	-7.6362377637
H78	-1.0582419582	-6.2682821780	-5.5488560027
H79	0.1061350735	-4.4266443894	-4.3333322198
H80	3.2692251801	-4.4733144794	-7.3113440693
H81	2.1050780804	-6.3228623947	-8.5102218110
C82	6.8505245417	-2.6386090191	-6.5933129085
C83	6.5732827867	-3.4874313909	-5.5083895842
C84	5.2776038850	-3.5512906557	-4.9755791672
C85	4.2435273896	-2.7693248724	-5.5341499536
C86	4.5258794950	-1.9138097783	-6.6208881253
C87	5.8266774635	-1.8527825813	-7.1457210659
H88	7.8644185888	-2.5874999044	-7.0046070194
H89	7.3700247924	-4.0987388355	-5.0707707185
H90	5.0649161041	-4.2105431004	-4.1247822493
H91	3.7334851998	-1.2937687951	-7.0542350788
H92	6.0384353995	-1.1858970231	-7.9888977422
C93	0.2893422055	0.9480116088	-6.0321460360
C94	0.1454206555	-0.2010375714	-6.8256902801
C95	0.8120416243	-1.3865608668	-6.4783964450
C96	1.6291665645	-1.4196672839	-5.3293415995
C97	1.7642337340	-0.2658047516	-4.5251675057
C98	1.0989896479	0.9146404501	-4.8841186826
H99	-0.2344053360	1.8705516579	-6.3063853133
H100	-0.4894476510	-0.1784377518	-7.7184023261
H101	0.6938464589	-2.2828352275	-7.0971848489
H102	2.3835183330	-0.2901633041	-3.6204507795
H103	1.2092713689	1.8083885671	-4.2604271645

Au(III) Isomer F
E = -2638.704744

Au1	1.0204863883	-1.3086040021	0.0741351708
Au2	2.4797572375	-4.7916145822	-2.5066226389
C2	0.4164701956	1.4327050535	0.9358434736
C3	-0.4081210733	2.5225869121	1.2689118232
C4	-1.8006842410	2.3764661338	1.1940656200
C5	-2.3803234279	1.1641951009	0.7922586753
C6	-1.5411376175	0.0833506341	0.4664399376
N7	-0.1892653580	0.2666531667	0.5556713682
H8	0.0364449470	3.4700820373	1.5821818051
H9	-2.4452472927	3.2232524056	1.4531313386
H10	-3.4658526697	1.0547121219	0.7334129973
C11	4.7239399028	1.1571820616	0.7837965776
C12	3.8870821816	0.0450082425	0.4945135963
C13	2.4954547310	0.1353288015	0.5580459311
C14	1.8834910979	1.3738515288	0.9285914303
C15	2.7063665172	2.4746429319	1.2334512815
C16	4.1008591372	2.3637002495	1.1602361485
H17	4.3504074449	-0.9048096505	0.2075514325
H18	2.2651984421	3.4362756972	1.5203447473
H19	4.7070428135	3.2426521547	1.3971854224
C20	-2.5632386047	-3.9511031567	-0.6645465716
C21	-1.2128941530	-3.5120392967	-0.5830339759
C22	-0.8827505524	-2.1998466319	-0.2391970092
C23	-1.9301162566	-1.2668677708	0.0424481980
C24	-3.2702922937	-1.6842991409	-0.0580771178
C25	-3.5763532241	-3.0054857536	-0.4077023101
H26	-0.4078387550	-4.2298961286	-0.7777941868
H27	-4.0887056943	-0.9855395856	0.1516104781
H28	-4.6283145054	-3.2981268020	-0.4659513803
C29	2.2047871570	-2.7573387685	-0.3865242044
C30	2.9913948623	-3.6862417179	-0.8119804714
C31	-2.8710712008	-5.4249074325	-0.9985270146
C32	-4.3888600126	-5.7131964432	-1.0538838141
H33	-4.8798358200	-5.5342980184	-0.0802788192
H34	-4.8988273966	-5.0993619567	-1.8185894601
H35	-4.5553729877	-6.7734829272	-1.3148597861
C36	-2.2390466540	-6.3292317408	0.0958346743
H37	-2.6628360371	-6.1038826297	1.0909786868

H38	-2.4396711149	-7.3931881184	-0.1282014287
H39	-1.1439985818	-6.1979748227	0.1566518038
C40	-2.2581004581	-5.7799023922	-2.3782875173
H41	-2.4702937216	-6.8350438330	-2.6298237474
H42	-2.6840446744	-5.1465306191	-3.1775480935
H43	-1.1604390147	-5.6531317270	-2.3869417474
C44	6.2547336450	1.0103073375	0.6742243900
C45	6.9901775226	2.3382691512	0.9581924388
H46	6.7203894759	3.1245536725	0.2300276047
H47	6.7805658107	2.7173985536	1.9750173096
H48	8.0807232106	2.1791530664	0.8843495777
C49	6.6219042594	0.5468812357	-0.7626670099
H50	6.2910478437	1.2844636032	-1.5159941167
H51	7.7178532203	0.4338706059	-0.8535387525
H52	6.1640058615	-0.4259027311	-1.0144503607
C53	6.7409465034	-0.0482895494	1.7013545374
H54	7.8373713413	-0.1702212079	1.6273940335
H55	6.5015718489	0.2625322346	2.7342641579
H56	6.2819670507	-1.0372272077	1.5276774655
C57	6.7515024217	-4.4341161045	1.2097804883
C58	5.6296561204	-3.9924871731	1.9318986776
C59	4.4135923047	-3.7452097101	1.2801664170
C60	4.3006126423	-3.9390786955	-0.1177555245
C61	5.4304511351	-4.3931281369	-0.8348223170
C62	6.6453355624	-4.6319760497	-0.1757288586
H63	7.6966092504	-4.6346362383	1.7258458575
H64	5.6962539208	-3.8468891136	3.0160502939
H65	3.5358241512	-3.4337687753	1.8562702877
H66	5.3535009234	-4.5570879666	-1.9162619972
H67	7.5095701833	-4.9860037791	-0.7493298295
P69	2.1563014569	-6.0947918527	-4.4128822356
C70	-0.3151563369	-3.8802263920	-7.6733243628
C71	0.7206027214	-4.7472720608	-8.0570141593
C72	1.4856756974	-5.4115833287	-7.0848963470
C73	1.2101075717	-5.2112965761	-5.7150848546
C74	0.1753562585	-4.3290844965	-5.3320372078
C75	-0.5860082075	-3.6727968434	-6.3100134626
H76	-0.9056082625	-3.3601168128	-8.4353286057
H77	0.9405449243	-4.9060123758	-9.1184489106
H78	2.2954794296	-6.0825604264	-7.3914092481
H79	-0.0326411876	-4.1562998483	-4.2692098871
H80	-1.3853049372	-2.9882883067	-6.0053183547
C81	6.1998338979	-7.2718004728	-6.3903246686
C82	5.9828463996	-5.9607070079	-5.9322002352
C83	4.7673078317	-5.6194032956	-5.3222951774
C84	3.7519253279	-6.5911549481	-5.1751004397
C85	3.9724334852	-7.9059781739	-5.6348994637
C86	5.1950425399	-8.2402961174	-6.2396189700
H87	7.1522868404	-7.5376187948	-6.8613311130
H88	6.7645946043	-5.2016399777	-6.0457119225
H89	4.6013689322	-4.5947612472	-4.9665807253
H90	3.1937114360	-8.6674332589	-5.5197287875
H91	5.3600718905	-9.2641465808	-6.5927277649
C92	-0.0112335362	-10.1057610976	-3.4929607746
C93	-0.3317185130	-9.3977713453	-4.6627603715
C94	0.2971305957	-8.1742375976	-4.9457826629
C95	1.2550386583	-7.6532087735	-4.0506006289
C96	1.5684348484	-8.3625026752	-2.8697206387
C97	0.9393941629	-9.5857070462	-2.5976734975
H98	-0.5039242095	-11.0598854694	-3.2766292108
H99	-1.0748613269	-9.7972212088	-5.3617831674
H100	0.0437054485	-7.6274383672	-5.8605118734
H101	2.3050008793	-7.9565733431	-2.1652004278
H102	1.1889773200	-10.1314797979	-1.6811571697

Fragments for Binding Energies

C_6H_6

E = -232.233419 Hartree

C1	-0.1716026521	2.5825812687	-0.0000017959
C2	-0.8738699335	3.7988806574	-0.0000007358
C3	-2.2782926388	3.7988746784	0.0000014285
C4	-2.9805416140	2.5825749230	0.0000001422
C5	-2.2783572084	1.3662519476	0.0000000242
C6	-0.8738177197	1.3662503332	0.0000011039
H7	0.9243839463	2.5825781884	-0.0000023814
H8	-0.3258423049	4.7480053130	-0.0000005972
H9	-2.8262979904	4.7480075345	0.0000019929
H10	-4.0765294974	2.5825465231	-0.0000021564
H11	-2.8263728810	0.4170983687	-0.0000023330
H12	-0.3258034935	0.4170996592	0.0000034845

CH_2Cl_2

E = -959.7459647 Hartree

Cl36	2.3357314419	-3.7689636505	-0.0907028511
H38	1.2892511492	-2.5533014748	1.6602182158
H40	0.2522844638	-2.6608388583	0.1749834765
C39	1.2635762775	-2.4897924316	0.5650400951
Cl40	1.7649183275	-0.8324563175	0.0948802617

$[Au(PPh_3)]^+$

E = -1171.642125 Hartree

Au1	2.2305024313	-3.4740732681	-2.5265492101
P70	2.1306236797	-3.2333560327	-4.7937765767
C71	1.7188103200	-7.3998207024	-6.7430272197
C72	0.8543960610	-7.0178696395	-5.7006086907
C73	0.9926765859	-5.7610402313	-5.1007528224
C74	2.0006560741	-4.8767061049	-5.5539230515
C75	2.8678562652	-5.2591146570	-6.6008644715
C76	2.7186722282	-6.5225646855	-7.1916823974
H77	1.6122974083	-8.3873206300	-7.2042791048
H78	0.0763142833	-7.7037938892	-5.3501721571
H79	0.3229996447	-5.4669453877	-4.2836683287
H80	3.6486023905	-4.5775762566	-6.9527783802
H81	3.3893684926	-6.8205627091	-8.0041927955
C82	5.9974618020	-1.1401945937	-6.2104025505
C83	6.0715546451	-2.3035929210	-5.4219652567
C84	4.8991257615	-2.9333155245	-4.9878979756
C85	3.6411584689	-2.4002865032	-5.3577767461
C86	3.5649855424	-1.2300053655	-6.1445210490
C87	4.7485561362	-0.6085681607	-6.5703112850
H88	6.9171570267	-0.6449901280	-6.5386473072
H89	7.0450355658	-2.7154017405	-5.1363952887
H90	4.9588503831	-3.8337870020	-4.3648377696
H91	2.5932908315	-0.8120769027	-6.4257359063
H92	4.6911188954	0.2972696679	-7.1826394513
C93	-1.5519616466	-0.6660566449	-5.8870020427
C94	-1.2837207468	-1.8409015270	-6.6070378333
C95	-0.1793983245	-2.6388065374	-6.2731685936
C96	0.6605203961	-2.2478506452	-5.2063742018
C97	0.3912200888	-1.0633006107	-4.4814209471
C98	-0.7127609636	-0.2751901009	-4.8280497928
H99	-2.4220241325	-0.0539211801	-6.1467736877
H100	-1.9397716859	-2.1451875296	-7.4291740711
H101	0.0229801835	-3.5574133210	-6.8326055310
H102	1.0406690353	-0.7627008634	-3.6503256760
H103	-0.9267834433	0.6374773834	-4.2625136387

HCCH

E = -77.317212 Hartree

C3	0.6080915147	-0.0000000167	-0.0000003125
C4	-0.6080915399	-0.0000000449	0.0000002477
H5	-1.6825820418	0.0000003722	0.0000002852
H6	1.6825823421	0.0000003621	0.0000004865

HCCPh

E = -308.37452 Hartree

C3	0.5737207280	-0.0000181311	0.0000171008
C4	-0.6487726849	-0.0001232811	0.0000579295
H5	-1.7224743713	-0.0002011658	0.0001010313
C6	4.8297703491	-0.0001038548	0.0000499519
C7	4.1251268903	-1.2156418021	-0.0000143063
C8	2.7251553826	-1.2206730059	-0.0000089764
C9	2.0054609387	0.0001079716	-0.0000340855
C10	2.7250558842	1.2209252814	-0.0000946129
C11	4.1251265737	1.2155462146	0.0000251246
H12	5.9254835126	-0.0002373164	0.0001097036
H13	4.6700915449	-2.1661020472	-0.0000729411
H14	2.1721703090	-2.1650607782	-0.0000344745
H15	2.1719247045	2.1654006542	-0.0001873841
H16	4.6702933208	2.1658697479	0.0001063811

PhCCPh

E = -539.4339535 Hartree

C3	0.6076545729	-0.0056758827	0.0048757648
C4	-0.6218819211	-0.0033562761	0.0069111534
C8	-4.8740122324	0.0026290473	-0.0056700317
C9	-4.1728591318	-0.7047305680	0.9861912278
C10	-2.7733966258	-0.7099388254	0.9967409688
C11	-2.0463008280	-0.0004124553	0.0051759824
C12	-2.7647795865	0.7096685844	-0.9921119425
C13	-4.1641172023	0.7082233232	-0.9923814849
H14	-5.9696834347	0.0038082981	-0.0098526359
H15	-4.7215111322	-1.2574287041	1.7572310039
H16	-2.2236939967	-1.2603905428	1.7665362739
H17	-2.2076931577	1.2584314466	-1.7583470202
H18	-4.7054402239	1.2618187739	-1.7679904196
C15	4.8601944576	0.0043640980	-0.0041827495
C16	4.1583934632	-0.5979617712	1.0541175918
C17	2.7590409666	-0.6052331370	1.0619362701
C18	2.0321090710	-0.0045248444	0.0012252558
C19	2.7513105483	0.6016412151	-1.0617424144
C20	4.1506331121	0.6026953284	-1.0596218569
H21	5.9558354778	0.0077852084	-0.0063038826
H22	4.7060942610	-1.0650881296	1.8804241986
H23	2.2087859083	-1.0721638256	1.8848730588
H24	2.1950664579	1.0659793463	-1.8821537574
H25	4.6921812516	1.0737639150	-1.8877772942

PPh_3

E = -1036.27999 Hartree

P70	2.5160143764	-2.8844387031	-4.9487311425
C71	2.6015203612	-6.8225027127	-7.4843830674
C72	1.7923139232	-6.7008333634	-6.3427064351
C73	1.7972117481	-5.5096907122	-5.6021532350
C74	2.5949682964	-4.4139014927	-6.0011984760
C75	3.4051385218	-4.5479345039	-7.1490781154
C76	3.4098863253	-5.7452467259	-7.8823180552
H77	2.6050620574	-7.7557313876	-8.0592719721
H78	1.1623635641	-7.5389369737	-6.0225713545
H79	1.1760203113	-5.4257052144	-4.7016549226
H80	4.0362779327	-3.7116095822	-7.4686685240
H81	4.0458107154	-5.8349474899	-8.7710548926
C82	6.3155793709	-0.5387553745	-6.3648403921
C83	6.3837562586	-1.5016442400	-5.3441416952
C84	5.2244715087	-2.1790066212	-4.9390460217
C85	3.9819534157	-1.9199753779	-5.5600810581
C86	3.9249274592	-0.9498312602	-6.5836425558
C87	5.0834997010	-0.2623476506	-6.9794327944
H88	7.2194230282	-0.0029120989	-6.6769192908
H89	7.3408787994	-1.7196948783	-4.8560987733
H90	5.2803035385	-2.9184087878	-4.1303143644
H91	2.9686747811	-0.7309236321	-7.0709910869
H92	5.0232973490	0.4893901893	-7.7753985280
C93	-1.0699338260	-0.4421266320	-6.7160307159
C94	-0.5796642833	-1.5406301840	-7.4401647883
C95	0.4991537643	-2.2911040320	-6.9453254780
C96	1.0987483529	-1.9566501239	-5.7126233278
C97	0.5869008757	-0.8581801322	-4.9855143306
C98	-0.4812448774	-0.1006308921	-5.4869460966
H99	-1.9104946166	0.1437618045	-7.1053290376
H100	-1.0358929780	-1.8139916089	-8.3990273682
H101	0.8778262957	-3.1432468975	-7.5199347225
H102	1.0312892836	-0.5972955188	-4.0168009977
H103	-0.8609882312	0.7525021910	-4.9127282688

[Au(^{t}Bu^C^N^C^{t}Bu)(C≡CPh})]

E = -1467.000509 Hartree

Au1	1.0676930098	-1.1614511936	-0.1587758256
C2	0.7500998258	1.7357911952	0.1690663712
C3	0.0489360739	2.9342521218	0.4035063926
C4	-1.3418769843	2.8856006077	0.5790732303
C5	-2.0385113318	1.6692280606	0.5260351345
C6	-1.3206504134	0.4808079278	0.2915544535
N7	0.0314095904	0.5755418110	0.1254755644
H8	0.5855888071	3.8856749086	0.4485497653
H9	-1.8938629173	3.8143236276	0.7622871623
H10	-3.1224377078	1.6387629673	0.6652926137
C11	4.9690999343	1.0607481659	-0.4617390696
C12	4.0336166939	-0.0066312858	-0.4263374227
C13	2.6674429944	0.2050042642	-0.2229489959
C14	2.1958545665	1.5474230179	-0.0386534615
C15	3.1144849695	2.6137128394	-0.0683916323
C16	4.4778910340	2.3699709287	-0.2775119045
H17	4.3798581085	-1.0375120224	-0.5647275270
H18	2.7753528514	3.6481994901	0.0683476180
H19	5.1626785694	3.2231320653	-0.2983193982
C20	-2.7059810853	-3.6023146915	0.0355494618
C21	-1.3331400881	-3.2640114743	-0.0906557250
C22	-0.8792503462	-1.9446952728	-0.0137262681
C23	-1.8344892613	-0.8967326095	0.2040872315
C24	-3.1988987439	-1.2195298659	0.3300563101
C25	-3.6235649070	-2.5517908841	0.2454992054
H26	-0.5918883356	-4.0553061336	-0.2523994184
H27	-3.9465160839	-0.4337948950	0.4959956398
H28	-4.6916741618	-2.7659674586	0.3479760885
C29	-3.1426640722	-5.0793965348	-0.0574602353
C30	-4.6716628627	-5.2535171815	0.0811313909
H31	-5.0421985630	-4.8854970218	1.0554955273
H32	-5.2209579429	-4.7256156898	-0.7198858011
H33	-4.9316377007	-6.3254149534	0.0107927689
C34	-2.4561292506	-5.8862512885	1.0774083343
H35	-2.7565662753	-5.5055949478	2.0704329345
H36	-2.7445789965	-6.9524707725	1.0165548404
H37	-1.3555211593	-5.8291639529	1.0147431075
C38	-2.7105371019	-5.6534842112	-1.4334172437
H39	-3.0007598823	-6.7180843111	-1.5117085958
H40	-3.1955273096	-5.1040152588	-2.2603756246
H41	-1.6186263345	-5.5885905965	-1.5812425020
C42	6.4645954947	0.7618608362	-0.6966776659
C43	7.3319542561	2.0405637582	-0.6906793452
H44	7.0313981513	2.7462467982	-1.4867782028
H45	7.2806810539	2.5694824831	0.2786118284
H46	8.3896398194	1.7726652271	-0.8666390973
C47	6.6363796394	0.0656076299	-2.0734542337
H48	6.2866672086	0.7192852855	-2.8928372837
H49	7.7024450690	-0.1689131062	-2.2529385509
H50	6.0681254176	-0.8787512661	-2.1308843334
C51	6.9774796305	-0.1794430981	0.4255733132
H52	8.0442950867	-0.4220921719	0.2625792912
H53	6.8819961053	0.2987994878	1.4172978878
H54	6.4142174848	-1.1283897585	0.4546931726
C55	2.0719544049	-2.8241261553	-0.4004596470
C56	2.7094640246	-3.8716841297	-0.5398132867
C58	4.9179122721	-7.4866409268	-0.9986004776
C59	3.5183359417	-7.5235233034	-0.8809735730
C60	2.7895687023	-6.3383124373	-0.7310605481
C61	3.4490009907	-5.0828758756	-0.6946224391
C62	4.8622206949	-5.0610842674	-0.8151206015
C63	5.5845730138	-6.2501679064	-0.9649097798
H64	5.4860591196	-8.4165016353	-1.1161317239
H65	2.9906002285	-8.4841634764	-0.9066378306
H66	1.6984116098	-6.3638474684	-0.6400575058
H67	5.3790193056	-4.0957690722	-0.7887507820
H68	6.6764791009	-6.2126749489	-1.0563579357

[($Ru(\eta^5$-$C_5H_5)(PPh_3)_2$(=C=CPh)]

E = -2667.936473 Hartree

Ru1	1.4852593635	2.5721423237	-1.8895114072
C2	3.2522826151	2.6414024535	-0.4544676886
C3	2.1795187781	3.4174626462	0.1054013884
C4	1.9180064905	4.5162387135	-0.7696248044
C5	2.8454500127	4.4445994348	-1.8811505677
C6	3.6552418897	3.2852409058	-1.6829541050
H7	1.6362983196	3.1839860494	1.0216516891
H8	1.1717278051	5.2928669030	-0.6037905655
H9	2.9107837697	5.1583773161	-2.7028473291
H10	4.4564378259	2.9401214451	-2.3387353981
H11	3.6862187229	1.7369639818	-0.0293055847
P40	-0.3750260535	3.4844015978	-2.9762422909
P41	2.0750915180	0.7961341872	-3.2806247887
C36	0.8492977113	7.4654002053	-5.1909855548
C37	0.5324950022	7.4692552748	-3.8235139656
C38	0.1368763606	6.2840954876	-3.1855515758
C39	0.0509717247	5.0646575140	-3.8966900773

C40	0.3635551439	5.0795384881	-5.2727997127
C41	0.7582946139	6.2655613013	-5.9117239502
H42	1.1543815927	8.3914489637	-5.6917890179
H43	0.5832766834	8.4011134841	-3.2478606860
H44	-0.1364308913	6.3173641492	-2.1258552232
H45	0.2808239187	4.1663225378	-5.8670888320
H46	0.9853187021	6.2475349331	-6.9843503224
C43	3.7267826396	1.9576481355	-7.5342304605
C44	3.2523380537	0.6534862416	-7.3165069035
C45	2.7391476470	0.2828645467	-6.0631064173
C46	2.6872586695	1.2143812678	-5.0021940649
C47	3.1471671539	2.5275848967	-5.2393388512
C48	3.6700414215	2.8947140958	-6.4903262748
H49	4.1285473600	2.2428417144	-8.5133202764
H50	3.2792594159	-0.0841985047	-8.1274576865
H51	2.3668552167	-0.7359115696	-5.9159672659
H52	3.0676826282	3.2665115681	-4.4332746056
H53	4.0235833677	3.9201947884	-6.6493596031
C50	5.7188032818	-1.3850215340	-1.3012328477
C51	5.9120197240	-0.7128663700	-2.5161763850
C52	4.8371055469	-0.0546576279	-3.1418280521
C53	3.5601802734	-0.0574931091	-2.5480945602
C54	3.3733142775	-0.7305426852	-1.3179633247
C55	4.4448900763	-1.3933284514	-0.7048650366
H56	6.5561534001	-1.9023916117	-0.8184117710
H57	6.9017810033	-0.7017955840	-2.9880943407
H58	4.9967108122	0.4532387941	-4.0992919327
H59	2.3834231420	-0.7207241023	-0.8443654802
H60	4.2845800375	-1.9171435658	0.2449730193
C57	-0.6027625064	-2.9736331025	-4.0843757090
C58	0.7951809987	-3.0687749875	-4.1699045530
C59	1.5931062929	-1.9448776687	-3.9071886548
C60	1.0059871993	-0.7034729502	-3.5677327430
C61	-0.3954304738	-0.6293266431	-3.4538554461
C62	-1.1932129299	-1.7546219573	-3.7184227336
H63	-1.2278021564	-3.8521523364	-4.2843647790
H64	1.2700742432	-4.0222382485	-4.4301229857
H65	2.6839031577	-2.0420820703	-3.9445049381
H66	-0.8637500730	0.3005976376	-3.1301013082
H67	-2.2818114911	-1.6745232390	-3.6225751514
C64	-2.8082638950	1.1506307484	-6.2545335999
C65	-3.4719122681	1.6610519716	-5.1295563718
C66	-2.7622195458	2.3639374773	-4.1413805692
C67	-1.3701377702	2.5627739509	-4.2594444043
C68	-0.7082934479	2.0082291324	-5.3792332108
C69	-1.4205651255	1.3245591059	-6.3741073416
H70	-3.3657410830	0.6060413082	-7.0255258004
H71	-4.5523781754	1.5144272081	-5.0137445569
H72	-3.3003504904	2.7538549526	-3.2727167388
H73	0.3804843550	2.0814988128	-5.4634610866
H74	-0.8815406085	0.9084739604	-7.2328825003
C71	-3.7470316270	5.0906876545	-0.1268370608
C72	-3.6784724261	5.5401221862	-1.4571373826
C73	-2.6746550227	5.0616100548	-2.3120424190
C74	-1.7187488463	4.1256474806	-1.8494332578
C75	-1.7981341288	3.6773825389	-0.5163296378
C76	-2.8082876712	4.1570149237	0.3364883427
H77	-4.5315482249	5.4651593137	0.5410455634
H78	-4.4087174328	6.2671146056	-1.8320220659
H79	-2.6320628294	5.4196027360	-3.3468790766
H80	-1.0822576405	2.9253251760	-0.1641178473
H81	-2.8606144073	3.7901265842	1.3682853499
C81	0.3607751462	1.2378962647	-0.9078641876
C82	-0.2334604621	0.4325742254	-0.1668711487
C119	-2.2884123353	-2.3171284578	2.3809633696
C120	-1.8811805530	-2.7081580684	1.0937904708
C121	-1.2081191971	-1.8118383668	0.2554272481
C122	-0.9206258885	-0.4859179711	0.6828709069
C123	-1.3389242185	-0.1088184075	1.9893094734
C124	-2.0116182403	-1.0113347858	2.8210723424
H125	-2.8150628915	-3.0224742285	3.0347143139
H126	-2.0906054705	-3.7252672562	0.7390424881
H127	-0.8962724673	-2.1182597703	-0.7490654854
H128	-1.1207382770	0.9072687876	2.3382099449
H129	-2.3227157029	-0.6936076988	3.8242650685

Additional Complexes for Binding Energies

$[Au(PPh_3)(C_6H_6)]^+$

E = -1403.924078 Hartree

Au1	2.5146011799	-3.5825300752	-2.4876248206
P70	2.1919954784	-3.2767157319	-4.7513745947
C71	1.5684078116	-7.2609263973	-7.0507778639
C72	0.9210302958	-7.0419805126	-5.8221771702
C73	1.1361039898	-5.8503708232	-5.1163886335
C74	1.9983574381	-4.8643444892	-5.6451303337
C75	2.6491667876	-5.0855723764	-6.8773508042
C76	2.4308789238	-6.2848243072	-7.5740855393
H77	1.4012385621	-8.1943445160	-7.5985402889
H78	0.2487159808	-7.8027243814	-5.4113525136
H79	0.6281341921	-5.6811098818	-4.1589941472
H80	3.3213845006	-4.3266698267	-7.2912239371
H81	2.9381926492	-6.4535100771	-8.5300005884
C82	5.8237211439	-1.1164233050	-6.6667244872
C83	6.0239875140	-2.1448888202	-5.7300634450
C84	4.9235714684	-2.7821860799	-5.1419145873
C85	3.6123238963	-2.3949362483	-5.4973104311
C86	3.4129822854	-1.3620200167	-6.4374502627
C87	4.5218187745	-0.7269862429	-7.0180050832
H88	6.6856928380	-0.6157346774	-7.1204880506
H89	7.0393259439	-2.4479971051	-5.4532502893
H90	5.0819016831	-3.5840565015	-4.4100819804
H91	2.3993326462	-1.0533098014	-6.7133518736
H92	4.3646062231	0.0762137261	-7.7458609653
C93	-1.5252929270	-0.6504462883	-5.6611717910
C94	-1.2563510898	-1.7734839025	-6.4591002290
C95	-0.1499673031	-2.5909187271	-6.1797755559
C96	0.6929339118	-2.2796264676	-5.0914116004
C97	0.4169119424	-1.1520993417	-4.2867311542
C98	-0.6881707279	-0.3399130364	-4.5759551202
H99	-2.3907436267	-0.0166992706	-5.8828058391
H100	-1.9099302823	-2.0179965262	-7.3032994814
H101	0.0543814675	-3.4669146329	-6.8041889489
H102	1.0689294736	-0.9096544657	-3.4385471061
H103	-0.8989041378	0.5347829207	-3.9513544003
C36	0.7358549836	-4.5144837383	0.2467893245
C37	0.4628613946	-3.1921395440	0.6347164613
C38	1.4597893893	-2.2002803968	0.5568143156
C39	2.7490086840	-2.5302185815	0.1140460697
C40	3.0528913445	-3.8734671775	-0.2705836301
C41	2.0249452768	-4.8659553623	-0.1958673302
H42	-0.0440780751	-5.2799672466	0.3114118374
H43	-0.5345303458	-2.9301606252	1.0037792954
H44	1.2361769658	-1.1734430270	0.8639227120
H45	3.5410856779	-1.7741000092	0.0947065004
H46	4.1007129548	-4.1812871623	-0.3891496712
H47	2.2644223035	-5.9084237477	-0.4323485328

$[Au(PPh_3)(CH_2Cl_2)]^+$

E = -2131.418836 Hartree

Au1	2.1933387273	-3.4952805409	-2.4260264752
P70	2.1471024187	-3.2833918233	-4.7037420802
C71	1.7598751154	-7.3226193735	-6.9377203151
C72	1.0362714265	-7.1043415023	-5.7526933342
C73	1.1756829655	-5.8959308198	-5.0567519907
C74	2.0418979190	-4.8971724458	-5.5534578287
C75	2.7723509343	-5.1186727056	-6.7413209332
C76	2.6252593053	-6.3326752717	-7.4290606225
H77	1.6506088586	-8.2692710265	-7.4775705494
H78	0.3645387778	-7.8786396581	-5.3676115105
H79	0.6089526726	-5.7264874740	-4.1331599419
H80	3.4485349595	-4.3491195534	-7.1275569824
H81	3.1912265203	-6.5031575765	-8.3510282624
C82	6.0176209092	-1.2397212118	-6.2234080583
C83	6.0914972386	-2.3159766054	-5.3218110844
C84	4.9179064869	-2.9173224386	-4.8493090903
C85	3.6609395278	-2.4436474373	-5.2881124705
C86	3.5868170273	-1.3624264280	-6.1913027801
C87	4.7693797722	-0.7656632081	-6.6555153543
H88	6.9369001113	-0.7681337236	-6.5867320362
H89	7.0650654153	-2.6848346627	-4.9822877363
H90	4.9780179514	-3.7568550830	-4.1459879601

H91	2.6151131178	-0.9894744716	-6.5306116494
H92	4.7114921191	0.0741405139	-7.3560415685
C93	-1.4487215075	-0.6583358185	-5.9880953233
C94	-1.1560490392	-1.8308176152	-6.7020002943
C95	-0.0808434726	-2.6455672541	-6.3146076782
C96	0.7058541184	-2.2774422946	-5.2027032054
C97	0.4085345541	-1.0987023061	-4.4825996521
C98	-0.6656201966	-0.2918262606	-4.8797656755
H99	-2.2912396861	-0.0286600161	-6.2932933109
H100	-1.7672556385	-2.1171571249	-7.5643821254
H101	0.1424003180	-3.5604240638	-6.8729623847
H102	1.0196332182	-0.8115438572	-3.6182652380
H103	-0.8940876604	0.6220428943	-4.3213075589
Cl36	2.3021719101	-3.7095331182	0.0797952942
H38	1.5245432373	-2.3482148901	1.8638583523
H40	0.2444519103	-2.5704610627	0.5755416872
C39	1.2896073276	-2.3159581846	0.7915754840
Cl40	1.7041661237	-0.7460086149	0.1118804856

$[Au(PPh_3)_2]^+$

E = -2208.020058 Hartree

Au1	2.3456014525	-3.2067898963	-2.7825179862
P70	2.5004589934	-2.8541388469	-5.1065422856
C71	2.8504096497	-6.8568426121	-7.4430098082
C72	2.0067750229	-6.7545666113	-6.3231953206
C73	1.9190375821	-5.5467534261	-5.6166055573
C74	2.6706216991	-4.4262651953	-6.0344771635
C75	3.5198940668	-4.5322666029	-7.1562825605
C76	3.6055050473	-5.7466047050	-7.8555525712
H77	2.9224371597	-7.8027514372	-7.9904203883
H78	1.4198927231	-7.6192407903	-5.9945056712
H79	1.2639131601	-5.4708162761	-4.7394436475
H80	4.1162392132	-3.6719229038	-7.4790723086
H81	4.2682844171	-5.8244184398	-8.7243249267
C82	6.2786768397	-0.3417606631	-6.1193590117
C83	6.3484028096	-1.4007674612	-5.1973599424
C84	5.1994663564	-2.1423435833	-4.8892735667
C85	3.9692493040	-1.8328015319	-5.5128671176
C86	3.9013238515	-0.7706285834	-6.4376195178
C87	5.0561599163	-0.0291616289	-6.7352922061
H88	7.1760577425	0.2408713081	-6.3533798526
H89	7.2993126716	-1.6475701501	-4.7121993360
H90	5.2583867805	-2.9658621961	-4.1663310148
H91	2.9502938750	-0.5195990812	-6.9188027683
H92	4.9972430755	0.7977091767	-7.4514882905
C93	-1.2016469790	-0.5646137990	-6.7335550892
C94	-0.6396263972	-1.6006412190	-7.4969420296
C95	0.4726447391	-2.3116689110	-7.0181891060
C96	1.0277092088	-1.9833911776	-5.7641260753
C97	0.4552944257	-0.9462611877	-4.9941290169
C98	-0.6519419959	-0.2379689299	-5.4818294675
H99	-2.0703101212	-0.0146621498	-7.1110805818
H100	-1.0678157897	-1.8607651683	-8.4711073710
H101	0.9038861819	-3.1211043263	-7.6170446110
H102	0.8783754125	-0.6927430044	-4.0138592104
H103	-1.0893998992	0.5662709237	-4.8801582950
P36	2.2872798771	-3.5273821294	-0.4495574891
C39	2.3634496098	0.5205394854	1.8327858785
C39	2.3634496098	0.5205394854	1.8327858785
C40	1.5657163951	-0.5287944191	2.3157192395
C41	1.5202875148	-1.7560157278	1.6349040731
C42	2.2811451363	-1.9361532079	0.4610593798
C43	3.0765714692	-0.8748426250	-0.0277258753
C44	3.1191319262	0.3456303534	0.6605031976
H45	2.3936587076	1.4763167337	2.3667468857
H46	0.9723535307	-0.3948556341	3.2266365035
H47	0.8958582846	-2.5711184217	2.0159195451
H48	3.6630128274	-1.0071696192	-0.9456424272
H49	3.7398460772	1.1634497456	0.2786873588
C49	-1.4644401560	-5.8836117938	0.9635818217
C50	-1.5653050959	-4.9413891199	-0.0738645494
C51	-0.4275011515	-4.2458036132	-0.5070279831
C52	0.8234962044	-4.4848257061	0.1042834155
C53	0.9222932619	-5.4342166285	1.1446301797
C54	-0.2217375675	-6.1279710666	1.5703629163
H55	-2.3534276995	-6.4315131892	1.2937150349
H56	-2.5318553146	-4.7534171433	-0.5537428705
H57	-0.5101750707	-3.5140343066	-1.3202789110
H58	1.8899554111	-5.6348926110	1.6169907827
H59	-0.1375503985	-6.8659575903	2.3755104604
C59	6.0020649536	-5.9736034540	0.8913028746
C60	5.6180447762	-4.8468593118	1.6344769460
C61	4.5027321899	-4.0882893680	1.2438299528
C62	3.7674648686	-4.4615230084	0.1000087972
C63	4.1628055469	-5.5916812140	-0.6512459442
C64	5.2733027583	-6.3464155747	-0.2509784234
H65	6.8741561138	-6.5607132960	1.1993358724
H66	6.1889451065	-4.5533215540	2.5220441312
H67	4.2077724486	-3.2078039798	1.8242219920
H68	3.5973781045	-5.8815461411	-1.5457529127
H69	5.5746731325	-7.2231092778	-0.8345480839

$[Au(PPh_3)(\eta^2\text{-}HC{\equiv}CH)]^+$

E = -1249.011992 Hartree

Au1	-0.2116081381	-0.7542466463	0.0379040769
C1	0.3822318684	1.4284824483	0.0276854997
C2	-0.8480522913	1.4100914277	0.1927939642
H3	-1.8991199444	1.6142336244	0.3475014470
H4	1.4296652176	1.6599376047	-0.1121645031
P7	-0.1575340548	-3.0809364449	-0.0203242737
C10	-2.4176660203	-4.9648474807	3.5622458619
C11	-2.9796430791	-3.8847270950	2.8597981648
C12	-2.2826951047	-3.3036052194	1.7921659530
C13	-1.0169095160	-3.8092473685	1.4200013002
C14	-0.4535686617	-4.8931684964	2.1261620629
C15	-1.1589095180	-5.4661276162	3.1961383635
H16	-2.9632010537	-5.4152009133	4.3983408697
H17	-3.9615674455	-3.4932145006	3.1457299386
H18	-2.7269160965	-2.4654533676	1.2409451011
H19	0.5288097549	-5.2865662722	1.8446993589
H20	-0.7204704239	-6.3070274146	3.7439012668
C20	4.2543940402	-4.4980218298	0.1703994533
C21	3.7665855939	-3.5697714832	1.1069423365
C22	2.4361175077	-3.1360143013	1.0373233991
C23	1.5838541095	-3.6431456204	0.0298041142
C24	2.0748949324	-4.5710727539	-0.9114206495
C25	3.4106198888	-4.9959937327	-0.8344406826
H26	5.2961424200	-4.8317079632	0.2245266192
H27	4.4243169477	-3.1821276014	1.8920956989
H28	2.0551443126	-2.4177066537	1.7739168386
H29	1.4191109771	-4.9631531270	-1.6955848452
H30	3.7902909217	-5.7194282700	-1.5637129569
C30	-1.9946401334	-4.8331094529	-3.8969747376
C31	-2.1807835565	-5.4983933213	-2.6744186615
C32	-1.6496036754	-4.9634866369	-1.4914241752
C33	-0.9256429064	-3.7520152031	-1.5363686512
C34	-0.7473292891	-3.0798413662	-2.7651163297
C35	-1.2773357542	-3.6256926076	-3.9422826077
H36	-2.4148092284	-5.2535176316	-4.8169171816
H37	-2.7461819980	-6.4356248947	-2.6384070022
H38	-1.8029080833	-5.4811658464	-0.5387723743
H39	-0.1858543677	-2.1381013222	-2.8025565975
H40	-1.1368303120	-3.1032204322	-4.8943450421

$[Au(PPh_3)(\eta^2\text{-}HC{\equiv}CPh)]^+$

E = -1480.081698 Hartree

Au1	0.0690456345	-0.9590349863	-0.6108726462
C1	1.0019898808	1.5483859349	-0.3319479481
C2	0.1436030385	1.0940214480	-1.1415635608
H3	-0.5027848149	1.4394500387	-1.9471070791
P7	-0.1808950762	-3.2283437136	-0.1579834353
C10	-1.7273352629	-3.9551212410	4.1585049321
C11	-2.2640063509	-2.9175841899	3.3771278852
C12	-1.7779405096	-2.6895998555	2.0823948320
C13	-0.7537966101	-3.5099079893	1.5599449113
C14	-0.2149555059	-4.5501646507	2.3465722790
C15	-0.7051214003	-4.7676000993	3.6436841729
H16	-2.1047370084	-4.1279256304	5.1722196556
H17	-3.0594693593	-2.2806356482	3.7785043767
H18	-2.1950413945	-1.8765538432	1.4755872242
H19	0.5850424271	-5.1844198555	1.9507441550
H20	-0.2833092151	-5.5743549109	4.2528646211

C20	3.8589807641	-5.4928331169	-0.4887640839
C21	3.7856775129	-4.2603231007	0.1831392965
C22	2.5669557008	-3.5728867867	0.2571992376
C23	1.4082382748	-4.1256154976	-0.3332498808
C24	1.4847589205	-5.3603573247	-1.0091954375
C25	2.7114788479	-6.0387944375	-1.0838653965
H26	4.8135181727	-6.0268151675	-0.5490049986
H27	4.6809584203	-3.8326045241	0.6472990538
H28	2.5117973616	-2.6114297451	0.7825123844
H29	0.5911385081	-5.7921265248	-1.4715181298
H30	2.7675398152	-6.9982762293	-1.6091395004
C30	-3.1581234014	-5.3298354018	-3.0335206962
C31	-3.1478408054	-5.6710284987	-1.6713806742
C32	-2.2672944980	-5.0284152269	-0.7874529187
C33	-1.3884816273	-4.0358397996	-1.2717448440
C34	-1.4054948381	-3.6890609059	-2.6405214016
C35	-2.2861024942	-4.3390745794	-3.5165019735
H36	-3.8478438565	-5.8333132632	-3.7191319920
H37	-3.8285688185	-6.4402274629	-1.2911278417
H38	-2.2660644802	-5.2972200126	0.2740513075
H39	-0.7276708807	-2.9143271724	-3.0200693019
H40	-2.2950858244	-4.0671600178	-4.5773705072
C40	3.8671117458	2.7959313881	2.4903459140
C41	4.2880048321	2.3634618729	1.2180351725
C42	3.3473867403	1.9433926913	0.2765933581
C43	1.9622767047	1.9563001573	0.6129615344
C44	1.5451268985	2.4004267403	1.9022360244
C45	2.5007470111	2.8150327808	2.8308407414
H46	4.6121447869	3.1232497257	3.2237736875
H47	5.3532653047	2.3572000685	0.9657891976
H48	3.6547077797	1.6031846709	-0.7172151397
H49	0.4784361877	2.4088355262	2.1466820079
H50	2.1872429706	3.1547722867	3.8230324657

$[Au(PPh_3)((\eta^2\text{-}PhC{\equiv}CPh)]^+$

E = -1711.137604 Hartree

Au1	-0.1546262157	-0.9062798857	-0.0051135709
C1	0.4409158565	1.2960327771	-0.0302120508
C2	-0.8098055398	1.2855272857	0.0950890639
P7	-0.1332608530	-3.2203866737	-0.0208464698
C10	-2.6846929179	-5.0282314280	3.4071929970
C11	-3.1511845161	-3.9171157225	2.6847388850
C12	-2.3639923728	-3.3599468878	1.6680960107
C13	-1.1046944533	-3.9218860847	1.3643774015
C14	-0.6364630300	-5.0361356830	2.0919923169
C15	-1.4301625901	-5.5845262511	3.1115405775
H16	-3.2997315068	-5.4590172227	4.2046145831
H17	-4.1286062116	-3.4805280527	2.9163202552
H18	-2.7288051320	-2.4906741306	1.1072099151
H19	0.3422684612	-5.4724490495	1.8659761505
H20	-1.0639511321	-6.4490819935	3.6756270782
C20	4.1690337441	-4.8954780699	0.4567698024
C21	3.7361779198	-3.8157163648	1.2454302913
C22	2.4432003030	-3.3001141753	1.0817180912
C23	1.5724112007	-3.8727933162	0.1280811804
C24	2.0089837760	-4.9552601207	-0.6635641162
C25	3.3071692374	-5.4617473046	-0.4952445125
H26	5.1815220204	-5.2938509066	0.5836287552
H27	4.4085089849	-3.3708669273	1.9869213639
H28	2.1081333901	-2.4562969682	1.6972894863
H29	1.3398334539	-5.4007991156	-1.4068627310
H30	3.6439806180	-6.3017022617	-1.1123437061
C30	-1.8029278701	-5.0159514305	-3.9631458959
C31	-2.1190120601	-5.6185505395	-2.7356742435
C32	-1.6371386195	-5.0729898090	-1.5358600035
C33	-0.8333205141	-3.9136746034	-1.5652138651
C34	-0.5215310263	-3.3070185849	-2.8023591032
C35	-1.0034477463	-3.8608958383	-3.9958192196
H36	-2.1825418653	-5.4448957018	-4.8967684587
H37	-2.7440684424	-6.5176090062	-2.7079619568
H38	-1.8875123985	-5.5463358765	-0.5805844512
H39	0.1003668702	-2.4038419644	-2.8300722814
H40	-0.7584532595	-3.3877154733	-4.9527933050
C40	4.5861138484	2.1913425564	-0.2817240042
C41	3.8862534334	1.7934945919	-1.4342101539
C42	2.5228470633	1.4897206020	-1.3602610699
C43	1.8458196383	1.5923445784	-0.1184803870
C44	2.5563171580	1.9891810665	1.0426006606
C45	3.9192009023	2.2897841005	0.9516914821
H46	5.6539454970	2.4261402943	-0.3452491615
H47	4.4058970471	1.7199364331	-2.3953405863
H48	1.9691352677	1.1805004919	-2.2527811518
H49	2.0297396039	2.0638994741	1.9990214575
H50	4.4642373977	2.6035173489	1.8481316315
C50	-4.9847837575	1.9932557515	0.3967905997
C51	-4.2012898384	1.9146342870	1.5613759416
C52	-2.8262030829	1.6732451188	1.4714350249
C53	-2.2232050767	1.5190194618	0.1977914638
C54	-3.0166641011	1.5956469469	-0.9745614256
C55	-4.3904785767	1.8342619236	-0.8674601909
H56	-6.0611617278	2.1799989808	0.4742971081
H57	-4.6649013982	2.0423922540	2.5452052602
H58	-2.2085924003	1.6096138970	2.3730252259
H59	-2.5448542502	1.4729490580	-1.9544866399
H60	-5.0006786668	1.8985285915	-1.7745487604

CNC complex tautomers

A) H/Me

alkyne

E = -1275.64173 Hartree

Au1	1.0514693689	-1.1522594453	-0.1794991435
C1	0.7702219813	1.7192929876	0.2344003169
C2	0.0682995653	2.9098141497	0.4923463159
C3	-1.3221518691	2.8640590941	0.6666882821
C4	-2.0221333063	1.6522775770	0.5875742266
C5	-1.3177383841	0.4624090858	0.3300329236
N6	0.0403398520	0.5600211589	0.1693965435
H7	0.6089501466	3.8573844187	0.5546901850
H8	-1.8705461443	3.7903801738	0.8677390580
H9	-3.1055224789	1.6238168453	0.7249082914
C10	4.9692814140	1.0790899523	-0.5079980909
C11	4.0318435983	0.0071376878	-0.4875154908
C12	2.6776360864	0.2141536396	-0.2270796533
C13	2.2077223875	1.5439145608	0.0148220921
C14	3.1249235315	2.6108315328	0.0048434304
C15	4.4823214933	2.3755333685	-0.2481784873
H17	4.3915566859	-1.0074967302	-0.7006912858
H18	2.7891604156	3.6383825696	0.1865266386
H19	5.1672700261	3.2278645394	-0.2497463219
C20	-2.7551526949	-3.5878037318	-0.0207820438
C21	-1.3753451703	-3.2609587066	-0.1522188112
C22	-0.9115898326	-1.9500060092	-0.0462246271
C23	-1.8476251254	-0.8980568810	0.2132196010
C24	-3.2129673413	-1.2084606729	0.3514874216
C25	-3.6536437129	-2.5325385440	0.2331344864
H27	-0.6615964784	-4.0724209210	-0.3404467947
H29	-3.9479130192	-0.4205782740	0.5530596249
H30	-4.7219494068	-2.7380961069	0.3434441244
C31	2.4980753159	-3.0295236789	0.1986147646
C32	1.9360986878	-3.0148478192	-0.9176126732
H33	1.6475161737	-3.3533383564	-1.9046439672
C35	3.2057036414	-3.1321052002	1.4684395783
H36	2.5046048212	-3.2272712921	2.3160375830
H37	3.8415598571	-4.0383452132	1.4392781420
H38	3.8548412920	-2.2540266061	1.6312922430
X	2.2142233242#	-3.0299819122#	-0.3946590594#
C38	-3.2158904245	-5.0507388305	-0.1598313056
C41	-4.7432935738	-5.2033742680	0.0109049605
H42	-5.0834250978	-4.8731432031	1.0091460795
H43	-5.3040090996	-4.6381723075	-0.7555135526
H44	-5.0201296922	-6.2669298450	-0.0960839234
C44	-2.5147522300	-5.9097347935	0.9253437813
H45	-2.7806783453	-5.5612254844	1.9393013244
H46	-2.8306068148	-6.9646591613	0.8325902829
H47	-1.4144232799	-5.8807781189	0.8315417161
C47	-2.8279796843	-5.5726121250	-1.5689530484
H48	-3.1476295989	-6.6243846563	-1.6823765030
H49	-3.3189348416	-4.9788419626	-2.3606253943
H50	-1.7373387385	-5.5346586609	-1.7404913534
C50	6.4518429972	0.7981784641	-0.8144860647
C53	7.3149351276	2.0777593131	-0.7539868852
H54	6.9895690399	2.8307864321	-1.4942947434

H55	7.2981558764	2.5417861134	0.2488773011
H56	8.3650043972	1.8241933594	-0.9825612377
C56	6.5670639516	0.1968083100	-2.2400625559
H57	6.1832498308	0.9018160157	-2.9986657955
H58	7.6256616872	-0.0158430728	-2.4752699499
H59	6.0051484959	-0.7490258525	-2.3392739694
C59	7.0051327217	-0.2135184280	0.2234956741
H60	8.0685719913	-0.4266035975	0.0122243036
H61	6.9351609159	0.1910446186	1.2492235348
H62	6.4618204936	-1.1753699248	0.1950289567

vinylidene
E = -1275.63686 Hartree

Au1	1.0758420909	-1.3180183709	-0.1087035717
C1	0.8418130805	1.6260447061	0.0704930867
C2	0.1766301018	2.8592517946	0.1755856468
C3	-1.2237671611	2.8799850217	0.2215523011
C4	-1.9593832526	1.6890204465	0.1625947073
C5	-1.2766467208	0.4650028335	0.0574341076
N6	0.0904542973	0.4838828618	0.0151448559
H7	0.7498723453	3.7880206356	0.2217673098
H8	-1.7486818649	3.8373559721	0.3041990520
H9	-3.0512373824	1.7047744741	0.1994360665
C10	5.0660171453	0.7845394882	-0.1526510056
C11	4.0891277004	-0.2489312741	-0.1698298691
C12	2.7250088064	0.0367757384	-0.0899266725
C13	2.2835438157	1.3881192032	0.0063870336
C14	3.2465658443	2.4141692618	0.0247599722
C15	4.6114248034	2.1134573196	-0.0524292064
H17	4.4263407623	-1.2856902831	-0.2490936700
H18	2.9352938092	3.4624039149	0.0967470239
H19	5.3290050314	2.9382765207	-0.0357689353
C20	-2.8586802232	-3.5401365102	-0.1892592282
C21	-1.4596164608	-3.2814764008	-0.1924323587
C22	-0.9591207988	-1.9818989093	-0.1090935160
C23	-1.8543201766	-0.8765845061	-0.0175763796
C24	-3.2389954304	-1.1276495911	-0.0117576073
C25	-3.7276782041	-2.4361518107	-0.0959955581
H27	-0.7742541687	-4.1310653232	-0.2657277255
H29	-3.9503194186	-0.2968907685	0.0561349939
H30	-4.8101176173	-2.5899144400	-0.0903276444
C31	1.9518940259	-2.9960344772	-0.1906980193
C32	2.4944064438	-4.1826235643	-0.2155302809
C33	3.9676573749	-4.5528178087	-0.2315764657
H34	4.1928213040	-5.1163930119	-1.1539489649
H35	4.6138393955	-3.6644518062	-0.1862556183
H36	4.1887178185	-5.2027966933	0.6328136646
H37	1.7661661523	-5.0164027293	-0.2332633005
C37	-3.3664412551	-4.9919768011	-0.2853931062
C40	-4.9087846797	-5.0731607978	-0.2551674898
H41	-5.3263904274	-4.6732821969	0.6864748369
H42	-5.3683831547	-4.5314793614	-1.1016388393
H43	-5.2215917206	-6.1293275031	-0.3311933514
C43	-2.8098987083	-5.8037518123	0.9137224238
H44	-3.1545085672	-5.3801701892	1.8736577371
H45	-3.1611350805	-6.8497816086	0.8551383732
H46	-1.7053066044	-5.8221793254	0.9274146227
C46	-2.8712744604	-5.6181613558	-1.6155065455
H47	-3.2254736245	-6.6618853108	-1.6939604499
H48	-3.2587778778	-5.0591095454	-2.4855597055
H49	-1.7688934810	-5.6339234737	-1.6849506169
C49	6.5607542489	0.4195917980	-0.2454934522
C52	7.4669784919	1.6704773872	-0.2258949953
H53	7.2680630316	2.3388701125	-1.0829533428
H54	7.3510139935	2.2509348853	0.7071935617
H55	8.5240658424	1.3581827924	-0.2906193830
C55	6.8149202585	-0.3486017743	-1.5691255056
H56	6.5566179323	0.2727213599	-2.4447874258
H57	7.8828472195	-0.6218181308	-1.6462276177
H58	6.2260263618	-1.2815168233	-1.6296149162
C58	6.9430125796	-0.4781156009	0.9603753351
H59	8.0119197696	-0.7517841749	0.9012300204
H60	6.7769084639	0.0488754062	1.9165549155
H61	6.3595282446	-1.4160922074	0.9839710618

B) H/Ph

alkyne
E = -1467.3848 Hartree

Au1	1.0708976390	-1.0776112816	-0.1271059571
C2	0.7880828078	1.8070270581	0.2703756581
C3	0.1098425177	2.9960216931	0.5970937643
C4	-1.2408646309	2.9347131517	0.9670650705
C5	-1.9235336064	1.7109211156	1.0138268271
C6	-1.2370131021	0.5272677766	0.6858865457
N7	0.0788145056	0.6398873787	0.3318354298
H8	0.6374794995	3.9523638542	0.5625722712
H9	-1.7715339117	3.8574898079	1.2246859728
H10	-2.9762438880	1.6694870888	1.3032339508
C11	4.8871528499	1.2106574103	-0.9344661390
C12	3.9736212506	0.1277478739	-0.8025847616
C13	2.6467513348	0.3144772222	-0.4121364900
C14	2.1880258728	1.6438698186	-0.1389916166
C15	3.0799349795	2.7244565568	-0.2701350136
C16	4.4068902284	2.5075442559	-0.6619926436
H18	4.3314550245	-0.8885128884	-1.0079732916
H19	2.7488169825	3.7495960305	-0.0664976894
H20	5.0720603172	3.3703539205	-0.7513831091
C21	-2.6317857625	-3.5576751798	0.6196669866
C22	-1.2919606760	-3.2098747231	0.2918363888
C23	-0.8377854725	-1.8904447514	0.3090443862
C24	-1.7508449333	-0.8480795508	0.6704747407
C25	-3.0801759098	-1.1770901027	0.9938021612
C26	-3.5093328538	-2.5102249799	0.9658334893
H28	-0.5909078299	-4.0103051622	0.0254331868
H29	-3.7971492843	-0.3958235923	1.2723995569
H30	-4.5495609836	-2.7274015109	1.2228944651
C31	2.1324269349	-2.8311225585	-0.4890188396
C32	2.0249548674	-3.2278459904	-1.6951314591
X33	2.1950559061#	-3.0514665354#	-0.4678297136#
C34	1.5008895117	-4.2382883062	-5.7328151016
C35	2.5907054196	-3.4251820812	-5.3590340757
C36	2.7729576840	-3.0830243892	-4.0215305966
C37	1.8530365453	-3.5633400529	-3.0368996936
C38	0.7522237815	-4.3887831395	-3.4312832265
C39	0.5850088460	-4.7182284365	-4.7740348600
H40	1.3623178091	-4.5003277314	-6.7878924054
H41	3.2901876681	-3.0627905299	-6.1188907245
H42	3.6057568525	-2.4463997044	-3.7078885280
H43	0.0503945775	-4.7423818915	-2.6693536568
H44	-0.2557843832	-5.3460367429	-5.0854138191
H45	2.6623961663	-3.2436745522	0.3738809917
C45	6.3462739903	0.9397715317	-1.3536500512
C48	7.1776312238	2.2376319502	-1.4649503843
H49	6.7679028747	2.9278036564	-2.2246600950
H50	7.2351431700	2.7745039905	-0.5008133596
H51	8.2111142576	1.9903547107	-1.7656380860
C51	7.0132432623	0.0203409632	-0.2945663922
H52	7.0218185478	0.5025210865	0.6991718843
H53	6.4878812998	-0.9463809313	-0.1972574753
H54	8.0596039556	-0.1922772467	-0.5801191763
C54	6.3598144275	0.2339255074	-2.7367524345
H55	7.4002007365	0.0288294358	-3.0480322728
H56	5.8234514642	-0.7322599965	-2.7098418123
H57	5.8887472534	0.8662814819	-3.5109076543
C57	-3.0744921460	-5.0342047472	0.5919310681
C60	-4.5684645485	-5.2074719782	0.9467953937
H61	-4.7949929513	-4.8450679749	1.9656532124
H62	-5.2275904161	-4.6793975883	0.2339449761
H63	-4.8345153709	-6.2787009023	0.9117162584
C63	-2.2306731790	-5.8380343331	1.6184022628
H64	-2.3812637267	-5.4527461678	2.6424456777
H65	-2.5303064434	-6.9017848713	1.6059044110
H66	-1.1501101928	-5.7906350631	1.3942361499
C66	-2.8453028167	-5.6088487681	-0.8324773641
H67	-3.1596364457	-6.6676294805	-0.8717902042
H68	-3.4290858717	-5.0499435043	-1.5861900356
H69	-1.7793074283	-5.5678512706	-1.1232958257

vinylidene
E = -1467.36952 Hartree

Au1	0.1407365795	-0.2484617932	2.0038444199
C2	1.1110391731	0.4841863694	4.6952774621

C3	1.0333926111	0.6635355236	6.0869543079
C4	-0.1624248250	0.3589863304	6.7509203620
C5	-1.2737915663	-0.1167126705	6.0422951988
C6	-1.1790937717	-0.2867335431	4.6504312556
N7	0.0058530741	0.0173415086	4.0372994829
H8	1.8994971194	1.0359836127	6.6391233347
H9	-0.2294756872	0.4952069308	7.8352758215
H10	-2.2068856391	-0.3529689657	6.5593226940
C11	4.4366331750	1.1508497171	2.0243552088
C12	3.1790001134	0.6745701765	1.5607399086
C13	2.1090510277	0.4723781845	2.4322932595
C14	2.2602904465	0.7354217535	3.8243302490
C15	3.5021377410	1.2075817083	4.2887970487
C16	4.5660940505	1.4124599669	3.4025377588
H18	3.0663422655	0.4594750994	0.4937530064
H19	3.6496157948	1.4174287158	5.3541471241
H20	5.5137411393	1.7809699655	3.8033725039
C21	-4.1863704704	-1.5198698889	1.8162657931
C22	-2.8574299044	-1.2040335474	1.4157510849
C23	-1.8876421512	-0.8304254835	2.3472200918
C24	-2.2195583645	-0.7477175604	3.7311430002
C25	-3.5288866836	-1.0742978975	4.1338646103
C26	-4.4908421148	-1.4567163597	3.1909491678
H28	-2.6061599110	-1.2453363549	0.3521325014
H29	-3.8104573808	-1.0206010860	5.1917354756
H30	-5.4971974678	-1.6994119743	3.5410825345
C31	0.3346092274	-0.4881478199	0.1356746357
C32	0.5772972372	-0.5679165662	-1.1521062909
H33	1.5151238910	-0.0413684646	-1.4247580187
C34	-1.5547402732	-2.3842769576	-4.3961777361
C35	-0.6431099230	-1.3444155012	-4.6391174208
C36	0.0549820585	-0.7578459451	-3.5758480181
C37	-0.1664224198	-1.2070708475	-2.2554139414
C38	-1.0767549248	-2.2616860749	-2.0137277046
C39	-1.7651084787	-2.8436604288	-3.0840817752
H40	-2.0914218622	-2.8472005717	-5.2308808353
H41	-0.4665016051	-0.9931314030	-5.6611249644
H42	0.7668475979	0.0534086079	-3.7663345875
H43	-1.2058340457	-2.6474231552	-0.9961686573
H44	-2.4591559904	-3.6696100766	-2.8958456806
C44	-5.2296343402	-1.9063547257	0.7472908492
C47	-6.6113008892	-2.2178808617	1.3666512714
H48	-6.5679478248	-3.0692104923	2.0699975283
H49	-7.0336328629	-1.3456635135	1.8974365376
H50	-7.3204675836	-2.4890372350	0.5649568480
C50	-4.7408989063	-3.1701880764	-0.0129923471
H51	-4.6017775950	-4.0237148530	0.6744576630
H52	-5.4866280052	-3.4625902399	-0.7741342303
H53	-3.7845366212	-2.9922965515	-0.5359443331
C53	-5.3908370504	-0.7259243837	-0.2513421114
H54	-6.1327051260	-0.9876596546	-1.0272988801
H55	-5.7432332529	0.1862944364	0.2622865292
H56	-4.4433520142	-0.4819013075	-0.7642029666
C56	5.5925000742	1.3581162753	1.0230071979
C59	6.8695681952	1.8930722619	1.7113603197
H60	6.7013028613	2.8735881167	2.1926129197
H61	7.2555840767	1.1910552238	2.4724308873
H62	7.6644644724	2.0288696957	0.9572287142
C62	5.1558931804	2.3856594133	-0.0592509789
H63	4.9098792180	3.3632150042	0.3929356508
H64	5.9758863050	2.5420337388	-0.7831724988
H65	4.2723021792	2.0438360392	-0.6275899709
C65	5.9302389222	-0.0021099366	0.3498135246
H66	6.7528909540	0.1305404850	-0.3759248028
H67	6.2526584622	-0.7490413951	1.0972580889
H68	5.0673489410	-0.4226388244	-0.1973565121

C) Ph/Ph
alkyne
E = -1698.437154 Hartree

Au1	1.1492388845	-1.2897780251	-0.2437557131
C1	0.9647570326	1.5686369303	0.3075339677
C2	0.3282299566	2.7548901229	0.7157167753
C3	-1.0077582994	2.7072969591	1.1369062169
C4	-1.7170302983	1.4984295879	1.1579743284
C5	-1.0758901747	0.3150680920	0.7492908353
N6	0.2293444198	0.4140267973	0.3465535409
H7	0.8765528502	3.6999642005	0.7012917014
H8	-1.5058325294	3.6294253848	1.4547268728
H9	-2.7581720386	1.4681336296	1.4873496759
C10	4.9980871294	0.9395596801	-1.0833723834
C11	4.0638945467	-0.1292985293	-0.9661719886
C12	2.7564513084	0.0711100501	-0.5202375970
C13	2.3414077791	1.3952894208	-0.1648039579
C14	3.2539364459	2.4604298150	-0.2749384121
C15	4.5587496632	2.2307954628	-0.7283774409
H17	4.3872487614	-1.1431946863	-1.2331848182
H18	2.9567348232	3.4814200566	-0.0071530949
H19	5.2411015766	3.0817873920	-0.8030094166
C20	-2.5843312757	-3.7194467607	0.5459781592
C21	-1.2512242177	-3.3909270747	0.1685904470
C22	-0.7604914674	-2.0863745973	0.2330171081
C23	-1.6257106881	-1.0426012977	0.6948775006
C24	-2.9454414982	-1.3531723927	1.0707110714
C25	-3.4116002676	-2.6714772886	0.9963211242
H27	-0.5922301214	-4.1916536734	-0.1891629181
H29	-3.6250829093	-0.5698350383	1.4259868075
H30	-4.4423620342	-2.8772743754	1.2973482124
C31	2.3149859214	-3.2710502348	-0.2821587387
C32	1.9855591387	-3.0328590240	-1.4763014290
X	2.1950559061#	-3.0514665354#	-0.4678297136#
C38	1.0251978945	-3.2631858328	-5.6016003708
C39	1.5773713436	-2.0786030330	-5.0834952764
C40	1.8938036606	-1.9852510473	-3.7245706997
C41	1.6519748625	-3.0914607466	-2.8707952666
C42	1.0906259348	-4.2834506891	-3.3959092438
C43	0.7870390145	-4.3625333887	-4.7585801726
H44	0.7776563813	-3.3295258204	-6.6664707192
H45	1.7612462491	-1.2235462598	-5.7424677192
H46	2.3256902980	-1.0689691447	-3.3082191420
H47	0.9060596005	-5.1330559780	-2.7310701490
H48	0.3578119321	-5.2843873027	-5.1647110556
C45	4.1520720772	-4.6532573365	3.2815047088
C46	2.7879747538	-4.3135143197	3.2920708550
C47	2.1687672730	-3.8516801165	2.1263636709
C48	2.9258637152	-3.7224962335	0.9342807083
C49	4.3027065142	-4.0626371403	0.9278013549
C50	4.9041445384	-4.5311474647	2.1001557297
H51	4.6317232005	-5.0134824853	4.1979291520
H52	2.2049482056	-4.4091931560	4.2140486069
H53	1.1064254157	-3.5857995627	2.1199664266
H54	4.8803438805	-3.9624399638	0.0035153655
H55	5.9661610748	-4.7977974519	2.0938971546
C55	-3.0745044429	-5.1771482691	0.4513698146
C58	-4.5446996412	-5.3334235851	0.9013638034
H59	-4.6898444316	-5.0320819336	1.9546616264
H60	-5.2356096431	-4.7440543451	0.2717150874
H61	-4.8457622057	-6.3924798938	0.8172853317
C61	-2.9614988341	-5.6538830224	-1.0223704761
H62	-3.5939009030	-5.0394010354	-1.6878641534
H63	-1.9235487845	-5.5992609106	-1.3962373216
H64	-3.2948731393	-6.7041230110	-1.1076392653
C64	-2.1878715729	-6.0719953287	1.3592178883
H65	-2.5227213642	-7.1231848732	1.2969990932
H66	-1.1243800915	-6.0420428794	1.0622900688
H67	-2.2553804078	-5.7553998672	2.4156870087
C67	6.4291277080	0.6627513103	-1.5825985795
C70	7.2815108120	1.9494502008	-1.6638759543
H71	6.8499605549	2.6881871977	-2.3633940309
H72	7.3994594750	2.4317732722	-0.6766379066
H73	8.2926683333	1.7000091683	-2.0307675571
C73	7.1245319825	-0.3239225525	-0.6057210428
H74	7.1959972161	0.1066827972	0.4091277476
H75	6.5808127780	-1.2823334446	-0.5294264228
H76	8.1490483628	-0.5452339067	-0.9561463755
C76	6.3603675864	0.0329990253	-3.0005963601
H77	7.3799969637	-0.1771534732	-3.3710135766
H78	5.7999081428	-0.9188251817	-3.0068995535
H79	5.8733434927	0.7196206335	-3.7163820450

vinylidene
E = -1698.41947 Hartree

Au1	-0.0011215319	-0.0532801412	1.8904183758
C2	1.0131624454	0.4076562498	4.6110773897
C3	0.9554649964	0.4474355089	6.0151552379
C4	-0.2041293451	0.0026714930	6.6653451661
C5	-1.2976331852	-0.4821215072	5.9345351489
C6	-1.2255120775	-0.5121717988	4.5309006710
N7	-0.0787013600	-0.0637143389	3.9342840862
H8	1.8075260401	0.8224473371	6.5871836775
H9	-0.2556484799	0.0324550587	7.7588215282
H10	-2.1983021013	-0.8341494161	6.4434936392
C11	4.2984458127	1.3212405880	1.9654069698
C12	3.0165708039	0.9528793759	1.4738732531
C13	1.9494575504	0.6926194691	2.3339664674
C14	2.1317874359	0.7935323341	3.7460792197
C15	3.3908108453	1.1876208307	4.2376567613
C16	4.4508384813	1.4470290515	3.3601012030
H18	2.8780390859	0.8570849320	0.3921360519
H19	3.5627314358	1.2717298848	5.3167740201
H20	5.4168426637	1.7377528463	3.7818900425
C21	-4.1072573862	-1.9008475448	1.6373815234
C22	-2.8437136071	-1.3735631583	1.2492787938
C23	-1.9226059500	-0.9182658261	2.1927510311
C24	-2.2392658512	-0.9820192741	3.5842853319
C25	-3.4905556486	-1.4942809772	3.9750707310
C26	-4.4044423958	-1.9437755161	3.0139491479
H28	-2.5936757780	-1.3299129323	0.1840371475
H29	-3.7632771159	-1.5477692243	5.0351704976
H30	-5.3662490504	-2.3374220823	3.3540758800
C31	0.1647496154	0.1533790785	0.0002452308
C32	0.3021077944	0.3700437799	-1.2880646993
C33	-1.7995419679	-2.7630693082	-3.3880899923
C34	-2.2496911164	-1.4304435787	-3.4767221864
C35	-1.6073695913	-0.4202386748	-2.7527993592
C36	-0.4790674712	-0.7438299396	-1.9606561071
C37	-0.0391563290	-2.0825529792	-1.8569405330
C38	-0.7016826976	-3.0884641109	-2.5763551783
H39	-2.3103800358	-3.5482306043	-3.9559680615
H40	-3.1053962658	-1.1812209709	-4.1134246599
H41	-1.9456876513	0.6190385898	-2.8203485984
H42	0.8333793098	-2.3164944818	-1.2386668814
H43	-0.3541814292	-4.1246543918	-2.5077535488
C44	2.1523930161	3.5415358477	-3.4981637198
C45	1.8467637529	2.3271129255	-4.1332722115
C46	1.2536654562	1.2834227616	-3.4104398595
C47	0.9634919927	1.4542115112	-2.0397672715
C48	1.2781499138	2.6765700703	-1.3992252339
C49	1.8676649072	3.7127217508	-2.1311899525
H50	2.6066672341	4.3586041301	-4.0688491324
H51	2.0677526676	2.1908451519	-5.1973252343
H52	1.0155539911	0.3359524613	-3.9053181445
H53	1.0294772894	2.8171781441	-0.3417272349
H54	2.0940584587	4.6639089793	-1.6375970674
C54	-5.0879917338	-2.4113893251	0.5633719162
C57	-6.4200743897	-2.9001334361	1.1755013798
H58	-6.2720095472	-3.7425836846	1.8749598332
H59	-6.9520705673	-2.0921040306	1.7092222355
H60	-7.0854645795	-3.2564886285	0.3698226748
C60	-4.4320953705	-3.5966056167	-0.1965582975
H61	-4.2064429673	-4.4320812897	0.4897089744
H62	-5.1216364236	-3.9719930248	-0.9745941717
H63	-3.4917951188	-3.3006630978	-0.6943073900
C63	-5.4003000839	-1.2631971154	-0.4336352701
H64	-6.1078845995	-1.6174057392	-1.2049422595
H65	-5.8617447770	-0.4023902709	0.0819000178
H66	-4.4932755081	-0.9045337359	-0.9514310205
C66	5.4558764301	1.5557478098	0.9761927027
C69	6.7808246117	1.8889176042	1.6974615400
H70	6.7063457380	2.8149509619	2.2956723555
H71	7.1095472377	1.0692133229	2.3614526161
H72	7.5764672836	2.0460570605	0.9485198162
C72	5.0923798920	2.7402002050	0.0405681403
H73	4.9482876759	3.6710351747	0.6175825912
H74	5.9086092104	2.9117300475	-0.6843128451
H75	4.1692902193	2.5493665661	-0.5345330530
C75	5.6678479074	0.2703901574	0.1298735697
H76	6.4939025662	0.4248087568	-0.5874105847
H77	5.9290788571	-0.5905064287	0.7707641980
H78	4.7687317365	0.0010925996	-0.4519440185

D) F/F

alkyne

E = -1434.72887 Hartree

Au1	-0.0270378961	0.0162250808	1.9677108710
C2	1.1363331652	-0.0603610503	4.6894092431
C3	1.1184022141	-0.1555746566	6.0911959070
C4	-0.1105358551	-0.2291168927	6.7593605882
C5	-1.3139903982	-0.2088090555	6.0434325476
C6	-1.2823815827	-0.1190346606	4.6408833839
N7	-0.0614718731	-0.0492832816	4.0248274271
H8	2.0589121696	-0.1713562087	6.6469702738
H9	-0.1304231722	-0.3023532218	7.8515752227
H10	-2.2736812774	-0.2638880411	6.5626120821
C11	4.4890246951	0.4879304111	2.0433747567
C12	3.1584573500	0.3498990520	1.5568048392
C13	2.0869501432	0.1193224569	2.4167390838
C14	2.3035588979	0.0578476843	3.8233443134
C15	3.6183852339	0.1922359604	4.3100167369
C16	4.6900249782	0.3931818371	3.4332822677
H18	3.0036394048	0.4263978435	0.4782686856
H19	3.8104748370	0.1610107600	5.3885693082
H20	5.6962789099	0.4890207381	3.8499351187
C21	-4.5597003536	-0.1328142696	1.8479363168
C22	-3.2057117964	-0.0304124272	1.4206008909
C23	-2.1484329535	-0.0048977867	2.3292512803
C24	-2.4190316472	-0.0976683102	3.7267885307
C25	-3.7562155576	-0.1905656195	4.1572028485
C26	-4.8058154601	-0.2041374141	3.2321121046
H28	-3.0167688306	0.0300859811	0.3474071568
H29	-3.9874250763	-0.2627960321	5.2260453498
H30	-5.8310938581	-0.2772700701	3.6046444647
C31	0.5804790426	-0.5316283361	-0.0492497158
C32	-0.3611667493	0.3197332286	-0.1278827153
F33	1.6085670474	-1.1885034613	-0.5003195502
F34	-1.3098724857	0.9150973031	-0.8001293145
X	0.1095441438#	-0.1687471679#	-0.1043038538#
C35	-5.6851232951	-0.1639618286	0.7964786754
C38	-7.0834045186	-0.2704930219	1.4441592218
H39	-7.1980931421	-1.1988389985	2.0324577685
H40	-7.3029147395	0.5914747299	2.0998719929
H41	-7.8528530084	-0.2862599392	0.6525823895
C41	-5.4778753148	-1.3940690705	-0.1269149308
H42	-5.5176793376	-2.3354025717	0.4495559636
H43	-6.2749906770	-1.4273746774	-0.8913241108
H44	-4.5092632488	-1.3592467689	-0.6569251027
C44	-5.6351159936	1.1371555041	-0.0483704853
H45	-6.4367577283	1.1198932331	-0.8085700135
H46	-5.7845547556	2.0292628060	0.5854984166
H47	-4.6746740102	1.2539072821	-0.5810097965
C47	5.6379151835	0.7182743448	1.0433631556
C50	7.0000841583	0.8815927545	1.7529263795
H51	7.0084039523	1.7484262151	2.4381150249
H52	7.2811181721	-0.0217801343	2.3239098073
H53	7.7874073251	1.0509963436	0.9978027399
C53	5.3520630570	2.0060630811	0.2264084536
H54	5.2878959140	2.8898570484	0.8855995283
H55	6.1685512204	2.1780691124	-0.4977517376
H56	4.4098073221	1.9379436053	-0.3461548039
C56	5.7279135201	-0.4993185970	0.0843230423
H57	6.5446379923	-0.3433241630	-0.6432681955
H58	5.9395232009	-1.4294705576	0.6412268632
H59	4.7956553534	-0.6494347189	-0.4888276997

vinylidene

E = -1434.75957 Hartree

Au1	0.0179840920	0.0003525203	1.9108033420
C2	1.1387660735	0.0098037392	4.6630179362
C3	1.1066088146	-0.0333768462	6.0666671426
C4	-0.1288828745	-0.1301052092	6.7205718542
C5	-1.3216090732	-0.1831849486	5.9873303578
C6	-1.2674561996	-0.1384027834	4.5842333546
N7	-0.0447220645	-0.0428676008	3.9768757021
H8	2.0386414848	0.0077602219	6.6354634667

H9	-0.1625793541	-0.1656141590	7.8142982818
H10	-2.2864699242	-0.2607672879	6.4941962560
C11	4.5012392983	0.2986428094	1.9736876096
C12	3.1610520284	0.2245990586	1.4994556661
C13	2.0992954124	0.1319065621	2.3979409428
C14	2.3140101676	0.1083748783	3.8007440980
C15	3.6412382078	0.1825198934	4.2669704779
C16	4.7101096076	0.2752329731	3.3671531916
H18	2.9784375213	0.2416891920	0.4231559051
H19	3.8455488491	0.1670601010	5.3437006479
H20	5.7254866504	0.3308340916	3.7681836412
C21	-4.4697400231	-0.2606543589	1.6938065324
C22	-3.1045598586	-0.1761776693	1.3000508429
C23	-2.0943675726	-0.1405119219	2.2605613828
C24	-2.3887161953	-0.1845929465	3.6486588770
C25	-3.7408474027	-0.2676145317	4.0344421926
C26	-4.7566244883	-0.3039549926	3.0721518062
H28	-2.8620863497	-0.1426822058	0.2360937800
H29	-4.0069776066	-0.3008768190	5.0971342675
H30	-5.7937552389	-0.3676052709	3.4120375834
C31	0.0540233450	0.0287133741	0.0353569999
C32	0.0585724815	0.0327444432	-1.2923361422
F33	1.1638463158	0.1318685018	-2.0181791130
F34	-1.0449678593	-0.0574003096	-2.0239975518
C34	-5.5641667149	-0.3041656109	0.6073038834
C37	-6.9807710975	-0.3891705361	1.2186227663
H38	-7.1186256682	-1.3056434840	1.8202402782
H39	-7.2125861181	0.4867981278	1.8510121305
H40	-7.7267727358	-0.4146804521	0.4051261973
C40	-5.3405587525	-1.5516731055	-0.2882127384
H41	-5.4021671537	-2.4826593820	0.3028812327
H42	-6.1180974675	-1.5926383106	-1.0721610078
H43	-4.3587556770	-1.5323994478	-0.7938939071
C43	-5.4793355931	0.9827387365	-0.2560861311
H44	-6.2597893254	0.9590237885	-1.0378403582
H45	-5.6391304292	1.8863743096	0.3586441691
H46	-4.5036979884	1.0829545133	-0.7640045037
C46	5.6520313971	0.4006589197	0.9519260127
C49	7.0320173884	0.4723636508	1.6429397492
H50	7.1247339280	1.3617386156	2.2920028257
H51	7.2400343676	-0.4291656984	2.2470278890
H52	7.8207561604	0.5427431430	0.8736435739
C52	5.4612480549	1.6833342751	0.0998841785
H53	5.4784956018	2.5882343663	0.7328635666
H54	6.2792194266	1.7665558664	-0.6381522291
H55	4.5084990414	1.6755830586	-0.4589182848
C55	5.6282415197	-0.8483590249	0.0309067420
H56	6.4487131376	-0.7840485146	-0.7062873152
H57	5.7649604118	-1.7761819826	0.6143475343
H58	4.6820150462	-0.9351787595	-0.5322077277

E) Me/CO_2Me

alkyne

E = -1503.5189 Hartree

Au1	0.0103631881	0.0571186927	2.0679916621
C2	1.1341548613	0.1415412830	4.7530816464
C3	1.0886417581	0.1335644595	6.1590592742
C4	-0.1528860646	0.0315003289	6.8028941070
C5	-1.3457036995	-0.0636337620	6.0716037228
C6	-1.2971061422	-0.0554438587	4.6664994040
N7	-0.0594920750	0.0490094137	4.0837937624
H8	2.0142556375	0.2058174132	6.7347764208
H9	-0.1928088137	0.0248281545	7.8973162507
H10	-2.3087955065	-0.1443232765	6.5816880990
C11	4.5225782120	0.3589828796	2.0941376462
C12	3.1850213206	0.2774975171	1.6103829099
C13	2.0896950122	0.2145035338	2.4711355788
C14	2.3111715341	0.2304710268	3.8853971862
C15	3.6267149776	0.3161766949	4.3766083651
C16	4.7097346097	0.3801272280	3.4909864734
H18	3.0207896855	0.2557821859	0.5256599380
H19	3.8207631549	0.3305095649	5.4557242999
H20	5.7187101108	0.4442712131	3.9068540326
C21	-4.4792719278	-0.3584005508	1.7698389970
C22	-3.1138521242	-0.2256151746	1.3848678590
C23	-2.0878670156	-0.1208288184	2.3229619607
C24	-2.4098730329	-0.1492682003	3.7178437775
C25	-3.7549114169	-0.2755532840	4.1114572362
C26	-4.7686744924	-0.3768357931	3.1497124980
H28	-2.8696078551	-0.2109716580	0.3151955963
H29	-4.0264843780	-0.2992472440	5.1736280540
H30	-5.8026357854	-0.4759107779	3.4905144203
C31	0.1382260718	-0.4971625724	-0.0893891701
C32	0.0314379261	0.7529038642	-0.1341130758
C33	-0.0941440902	2.1746294349	-0.4476321920
H34	-1.0473146110	2.5804662248	-0.0648544405
H35	0.7372675734	2.7516819557	-0.0054713031
H36	-0.0692203001	2.2962665021	-1.5469199372
C37	0.3141756694	-1.8815680293	-0.5754558042
O38	0.4100065892	-2.1180295038	-1.7688008257
O39	0.3514240192	-2.7593201366	0.4405611526
C40	0.5362979335	-4.1525945379	0.0384615141
H41	0.5608819970	-4.7144330140	0.9804880638
H42	-0.3038117397	-4.4749339260	-0.5957602339
H43	1.4829830547	-4.2601196350	-0.5137266268
X44	-0.0069837728#	-0.0000126621#	0.0000154084#
C44	-5.5716762409	-0.4782163639	0.6898508157
C47	-6.9881835894	-0.5908857084	1.2966407121
H48	-7.0940696101	-1.4853580211	1.9369653984
H49	-7.2557562082	0.2999334111	1.8933669377
H50	-7.7312841985	-0.6777268343	0.4844783023
C50	-5.5262903663	0.7810125052	-0.2191033834
H51	-5.7172836974	1.6999465164	0.3636848967
H52	-4.5496092441	0.8931150262	-0.7231659702
H53	-6.3001991460	0.7081651308	-1.0043668329
C53	-5.3026875330	-1.7462124758	-0.1661808387
H54	-6.0779697627	-1.8444141765	-0.9473662724
H55	-4.3220992278	-1.7060656204	-0.6733578745
H56	-5.3274774165	-2.6589524880	0.4558067565
C56	5.6996239561	0.4123988748	1.1008290163
C59	7.0655890329	0.5285204173	1.8143365701
H60	7.1374993159	1.4477686639	2.4234306135
H61	7.2680299552	-0.3399734164	2.4670904159
H62	7.8726034977	0.5680678462	1.0617952152
C62	5.5287302214	1.6450777795	0.1716964699
H63	5.5250191473	2.5843173423	0.7535743699
H64	6.3656210595	1.6933737720	-0.5480748405
H65	4.5913097517	1.6003696521	-0.4109684020
C65	5.6999223833	-0.8864315248	0.2487394725
H66	6.5361087828	-0.8639966187	-0.4733242452
H67	5.8239636777	-1.7798948373	0.8867635721
H68	4.7643654622	-1.0053183629	-0.3265387725

vinylidene

E = -1503.51197 Hartree

Au1	-0.1135952648	0.1474757226	1.9489531983
C2	1.1161803227	0.0715304297	4.6468080401
C3	1.1495182007	-0.0938084554	6.0426135140
C4	-0.0208451809	-0.4604438966	6.7176407308
C5	-1.2155399468	-0.6646726587	6.0141981533
C6	-1.2283577628	-0.4981512183	4.6195879131
N7	-0.0674662008	-0.1372386852	3.9915053258
H8	2.0832578534	0.0643062295	6.5873693802
H9	-0.0024149685	-0.5898486449	7.8047089281
H10	-2.1298359853	-0.9525563616	6.5382740664
C11	4.2928210664	1.1455149461	1.9427591028
C12	2.9677956999	0.8938411359	1.4816705741
C13	1.9532099320	0.5568035049	2.3753183308
C14	2.2198085167	0.4464579816	3.7701407952
C15	3.5285992857	0.6969123162	4.2254492050
C16	4.5429018011	1.0412339828	3.3246393675
H18	2.7559340162	0.9624212487	0.4119899199
H19	3.7647144336	0.6224262391	5.2928274203
H20	5.5465091215	1.2275559435	3.7161129013
C21	-4.4537794251	-1.1519247271	1.8352952470
C22	-3.1685856775	-0.7115589320	1.4110550363
C23	-2.1407350528	-0.4691496710	2.3235677879
C24	-2.3599029754	-0.6861118000	3.7135229143
C25	-3.6311382724	-1.1135362580	4.1399242024
C26	-4.6583691547	-1.3348019174	3.2160067386
H28	-2.9927884945	-0.5804669293	0.3409325733
H29	-3.8245377419	-1.2892488010	5.2042584647

H30	-5.6313499989	-1.6667813250	3.5872469993
C31	-0.1834223454	0.4957865550	0.0879112589
C32	-0.3021478751	0.7793326323	-1.1915727670
C33	0.9374288814	1.0208536586	-2.0409924606
O34	2.0907761255	0.9778472597	-1.6341165745
O35	0.5661393429	1.2806686395	-3.3081770987
H36	2.2457746383	2.4024140016	-3.9040378075
H37	2.3212789228	0.6432515484	-4.2821054831
C38	1.6661293869	1.5268302892	-4.2351555797
H39	1.1814524214	1.7142112292	-5.2020504971
C40	-1.6829703988	0.8718181235	-1.8435093076
H41	-1.7925720922	0.0672169398	-2.5901110886
H42	-2.4932295127	0.8007070323	-1.1036345558
H43	-1.7592784806	1.8426680655	-2.3605252748
C43	-5.5576358779	-1.4085948472	0.7880536459
C46	-6.8803997492	-1.8731323795	1.4404152273
H47	-6.7590795254	-2.8226986090	1.9920327418
H48	-7.2900879313	-1.1152851502	2.1322523663
H49	-7.6367919197	-2.0435035205	0.6545778461
C49	-5.0825971880	-2.5136108518	-0.1957323000
H50	-4.8833539313	-3.4617124394	0.3347096929
H51	-5.8641819744	-2.7043915783	-0.9530987577
H52	-4.1613340986	-2.2270339102	-0.7338655396
C52	-5.8352797570	-0.0950536509	0.0063520522
H53	-6.6246787160	-0.2644832498	-0.7479134150
H54	-6.1760539167	0.7089596602	0.6826679864
H55	-4.9388136066	0.2686112562	-0.5277151605
C55	5.3888973178	1.5145721287	0.9227933633
C58	6.7579295316	1.7508262324	1.6003927416
H59	6.7239516933	2.5821623215	2.3278097642
H60	7.1269044250	0.8469686049	2.1183521573
H61	7.5053679063	2.0163721453	0.8324001566
C61	4.9759951801	2.8151248748	0.1784841234
H62	4.8492284819	3.6561430180	0.8836530811
H63	5.7620365065	3.0947140154	-0.5464639612
H64	4.0339293391	2.6879833627	-0.3820578544
C64	5.5372193807	0.3557810572	-0.1027470034
H65	6.3253852317	0.6061032765	-0.8361736671
H66	5.8259957420	-0.5856517636	0.3981638763
H67	4.6026861424	0.1774868450	-0.6618037135

F) Ph/C(O)Ph
alkyne
E = -1811.764042 Hartree

Au1	0.8275800984	-0.9223534033	-0.0993873574
C1	0.6050487533	1.9343617482	0.5065821093
C2	-0.0560529636	3.1167419872	0.8848119158
C3	-1.4203613309	3.0668219557	1.2052869517
C4	-2.1294969338	1.8598837172	1.1548364639
C5	-1.4591532835	0.6812567769	0.7746911953
N6	-0.1286119047	0.7814569588	0.4733026418
H7	0.4934872787	4.0604436642	0.9259067239
H8	-1.9394874359	3.9855787176	1.4984575084
H9	-3.1929786465	1.8247134467	1.4039883854
C10	4.7363413654	1.3414429036	-0.5948883653
C11	3.8032147919	0.2670794850	-0.5500382491
C12	2.4608166635	0.4481779874	-0.2041532625
C13	2.0156548607	1.7663161742	0.1361456975
C14	2.9274945199	2.8372714831	0.1041384859
C15	4.2626672478	2.6251432745	-0.2593513990
H17	4.1541639917	-0.7412203348	-0.8061496561
H18	2.6042139026	3.8535014879	0.3580706767
H19	4.9391177818	3.4839413219	-0.2805734989
C20	-2.9621322283	-3.3408381824	0.3890376797
C21	-1.6043332998	-3.0126098904	0.1139212391
C22	-1.1157294795	-1.7120263472	0.2325335014
C23	-2.0065785529	-0.6722507539	0.6552242852
C24	-3.3501327957	-0.9860019398	0.9360733977
C25	-3.8172037840	-2.2996222747	0.8038387214
H27	-0.9313109982	-3.8100331506	-0.2207509875
H29	-4.0481983125	-0.2054507100	1.2607844463
H30	-4.8673028519	-2.5063336492	1.0276966318
C31	2.5602934243	-3.1496747540	0.0801852317
C32	1.7294532173	-2.6887243013	-0.7725958508
X	2.2407998489#	-3.0514464196#	-0.4204320988#
C35	4.9751853912	-4.8124114568	3.0862288021
C36	5.5761814255	-4.0485933532	2.0652689123
C37	4.7875291947	-3.4866018575	1.0642190649
C38	3.3737401021	-3.6940195189	1.0745895010
C39	2.7789018580	-4.4814926542	2.1107000730
C40	3.5824517280	-5.0278356140	3.1090166913
H41	5.6012473832	-5.2462963251	3.8736814748
H42	6.6598440545	-3.8948124865	2.0611447812
H43	5.2325414132	-2.8891731661	0.2630732803
H44	1.6957558576	-4.6370547965	2.1036689499
H45	3.1327735261	-5.6252843973	3.9082741253
C45	1.1826278021	-3.3506537249	-2.0633542164
O46	0.5195554087	-4.3737751085	-1.9272249804
C47	2.0100029587	-1.5965320220	-5.8783579577
C48	1.2727471482	-2.7915732724	-5.7816798113
C49	1.0132882266	-3.3521391123	-4.5294946742
C50	1.4909761276	-2.7132372605	-3.3593168525
C51	2.2338313259	-1.5173545976	-3.4603037029
C52	2.4879718718	-0.9611562910	-4.7198353803
H53	2.2101121811	-1.1581039848	-6.8624468369
H54	0.8997138944	-3.2818049673	-6.6871469265
H55	0.4399980111	-4.2789556763	-4.4285605253
H56	2.6024483691	-1.0166463789	-2.5590208000
H57	3.0593214170	-0.0303777381	-4.7987197688
C57	-3.4448615679	-4.7931568150	0.2140974299
C60	-4.9349596135	-4.9649998330	0.5833053142
H61	-5.1338526723	-4.6986367578	1.6373973731
H62	-5.5939807938	-4.3551596427	-0.0609053987
H63	-5.2294237692	-6.0207273558	0.4481220637
C63	-2.6043408270	-5.7250166319	1.1283426718
H64	-2.7160985671	-5.4450070011	2.1913712182
H65	-2.9419337753	-6.7709091265	1.0131016190
H66	-1.5300636291	-5.6920151161	0.8747394220
C66	-3.2519349175	-5.2116824008	-1.2694909809
H67	-3.5773854778	-6.2585721012	-1.4114475890
H68	-3.8541797512	-4.5738189885	-1.9412755599
H69	-2.1966812553	-5.1393864263	-1.5852844361
C69	6.2013968399	1.0864550029	-1.0069804219
C72	7.0380068773	2.3858465090	-1.0328392424
H73	6.6373059644	3.1193234090	-1.7555528630
H74	7.0880047638	2.8673853854	-0.0395830551
H75	8.0734358067	2.1533541659	-1.3385933758
C75	6.2332687274	0.4625850761	-2.4284025003
H76	5.7839129750	1.1479818930	-3.1694785828
H77	7.2769953301	0.2681879243	-2.7354052451
H78	5.6866940670	-0.4961365682	-2.4771670636
C78	6.8551826540	0.1095600628	0.0061728650
H79	7.9030746868	-0.0938153746	-0.2807048346
H80	6.8544085943	0.5348788072	1.0256965630
H81	6.3227406195	-0.8580146693	0.0436237078

vinylidene
E = -1811.748719 Hartree

Au1	-0.1678878946	-0.0752768036	1.9005554574
C2	0.6348075320	1.1690675992	4.4558425892
C3	0.5479134794	1.4572888307	5.8290507575
C4	-0.4544874794	0.8466223157	6.5940860192
C5	-1.3605350339	-0.0457205486	6.0060564110
C6	-1.2576363572	-0.3225950557	4.6316946125
N7	-0.2707526558	0.2977612436	3.9165803755
H8	1.2566750656	2.1505844328	6.2881795608
H9	-0.5295302301	1.0676162777	7.6639853965
H10	-2.1403349273	-0.5242336413	6.6033955245
C11	3.4773092585	2.5794960872	1.5363053709
C12	2.4053342853	1.7111044266	1.1856324391
C13	1.4814978208	1.2654801689	2.1330982659
C14	1.6042953232	1.6887022866	3.4909796156
C15	2.6543737045	2.5571041127	3.8429462115
C16	3.5724757435	2.9907917270	2.8799950833
H18	2.3192321968	1.3848146062	0.1454854072
H19	2.7698542946	2.8946274807	4.8795017316
H20	4.3798310218	3.6583000247	3.1931574396
C21	-3.5778845188	-3.0348389828	2.2133128842
C22	-2.5452925062	-2.2286896233	1.6560192554
C23	-1.8084963466	-1.3399913015	2.4426840130
C24	-2.0887372813	-1.2276203545	3.8374280915
C25	-3.1194351842	-2.0105153289	4.3893638027

C26	-3.8480471587	-2.8959967425	3.5882281280
H28	-2.3254994349	-2.3203431455	0.5878965982
H29	-3.3533572648	-1.9435127746	5.4582433488
H30	-4.6358390767	-3.4932962130	4.0550556844
C31	-0.1499281170	-0.4081753128	0.0220493075
C32	-0.0748849789	-0.6223167859	-1.2541048980
C33	1.1556061799	0.0464748018	-2.0309411013
O34	2.1693804117	-0.6197306663	-2.1496120751
C35	-2.6450965776	-2.7410093699	-3.9737600769
C36	-1.2598035411	-2.9679803304	-3.9963121618
C37	-0.4156570113	-2.2869281983	-3.1075613475
C38	-0.9707309730	-1.3860687395	-2.1764513882
C39	-2.3632758288	-1.1590744569	-2.1455062932
C40	-3.1936055333	-1.8366172986	-3.0495032518
H41	-3.2977178508	-3.2653121905	-4.6798713393
H42	-0.8278172732	-3.6727065282	-4.7147489713
H43	0.6653544358	-2.4586603163	-3.1269722147
H44	-2.7829985938	-0.4399780232	-1.4339489313
H45	-4.2730120599	-1.6509897386	-3.0336083114
C46	0.4746981605	3.8189984129	-3.9277519071
C47	-0.4546591140	3.3596852887	-2.9784815149
C48	-0.2563231555	2.1289115930	-2.3427848276
C49	0.8882253681	1.3583314272	-2.6499706971
C50	1.8262400939	1.8275083793	-3.6042206207
C51	1.6136168304	3.0527814685	-4.2397172475
H52	0.3106686216	4.7789440736	-4.4294585299
H53	-1.3376495229	3.9609782307	-2.7386162574
H54	-0.9810515971	1.7651830414	-1.6083006493
H55	2.7017914082	1.2125105796	-3.8340213750
H56	2.3338456537	3.4148839111	-4.9808432495
C56	-4.3555642563	-4.0179954424	1.3158780152
C59	-5.4107594108	-4.8210241148	2.1100150569
H60	-4.9530557869	-5.4294988722	2.9105582108
H61	-6.1768246721	-4.1661378222	2.5632067111
H62	-5.9340165598	-5.5140480036	1.4282720047
C62	-3.3576872178	-5.0195084345	0.6718411921
H63	-2.8240724837	-5.6020129546	1.4436696959
H64	-3.9032674361	-5.7302317790	0.0253023268
H65	-2.6024138082	-4.5125246982	0.0462843820
C65	-5.0854436311	-3.2191532444	0.2025839775
H66	-5.6490286622	-3.9111536215	-0.4491094748
H67	-5.8014825344	-2.4965042456	0.6331273820
H68	-4.3766192982	-2.6629866884	-0.4349339604
C68	4.4804553325	3.0351832897	0.4581099353
C71	5.5962751312	3.9296291586	1.0446406390
H72	5.1963584831	4.8645542068	1.4770467465
H73	6.1796328840	3.4063292601	1.8234894916
H74	6.2990525203	4.2144021868	0.2422382533
C74	5.1429892062	1.7865523062	-0.1874177610
H75	5.6868507055	1.1900469954	0.5664650559
H76	4.4073393728	1.1234477180	-0.6754056339
H77	5.8692579733	2.1029439291	-0.9577624649
C77	3.7204506280	3.8471877909	-0.6262544960
H78	4.4252261885	4.1802253212	-1.4095019885
H79	2.9327695036	3.2488813193	-1.1167130487
H80	3.2450019401	4.7446797584	-0.1919402020

[**6**]$^{+}$ conformer closer to XRD
E = -3069.423351 Hartree

Au1	6.4089106482	5.6332162695	6.4437524357
Au2	6.5398319833	5.6508219166	1.5686972668
Au3	8.4129198000	4.0646084986	4.0879309367
C4	4.2565631999	3.1491122135	-2.0203687287
C5	8.3992267342	8.6071318644	9.8345820741
C6	5.5298508397	2.6540269549	-1.6710701914
C7	2.4342190703	7.9643852398	0.8238240656
C8	7.1883539265	8.8632846321	9.1805330503
C9	9.1451053948	7.4427444405	9.5585535542
C10	6.8736413261	9.7853316759	4.2144431539
C11	3.9465136706	7.1257861902	5.9053447785
C12	2.5499596479	4.4274973027	3.6214738489
C13	10.4676971432	7.1216044298	10.2822747128
C14	7.6484430630	4.1055833305	6.1475041000
C15	3.7091622687	4.2622040690	-1.3710394463
C16	9.5050279707	4.5095510458	2.1625855449
C17	3.3469768140	2.0186400196	3.1336406331
C18	6.2276561816	3.3040756632	-0.6147593137
C19	4.5618596109	7.7787440636	1.9683392694
C20	3.0280192227	8.1826249351	6.0452152894
C21	4.4197561141	4.9107811523	-0.3427298557
C22	9.3983606462	9.5220162762	4.7177775478
C23	11.4213555388	4.0621163066	0.6863380876
C24	5.7047268642	4.4141289632	0.0552404796
C25	6.6913254386	7.9643926634	8.2182366905
C26	4.8642655299	4.9516964050	5.1530117188
C27	3.5360946077	3.4251903739	3.7355241225
C28	5.6816545828	8.1686700055	2.8327594202
C29	6.1728897269	1.4542489464	-2.3949542287
C30	2.7069279073	6.7957035057	0.0991358365
C31	3.8153642880	5.9220209551	5.0764732423
N32	4.7845978580	6.6375796454	1.2484929035
C33	9.0467267105	1.3535839534	7.7168728573
C34	8.0545891610	9.0164592096	4.1577748881
C35	7.4398896395	6.7849516927	7.8963133408
C36	10.9188355125	4.3072375679	1.9890136318
C37	3.9221051256	6.1193748756	0.3240896135
C38	6.8412814519	7.3312655284	2.8265114466
N39	5.0898071243	7.1685371297	6.6537179589
C40	2.6802658090	5.6523736830	4.2880884822
C41	3.3150854667	9.2250499328	6.9372162889
C42	8.2168661766	2.9738717122	6.0687110394
C43	4.5019527725	9.2294096098	7.6816987041
C44	5.4116613541	8.1658956743	7.5292594135
C45	5.7036814038	9.3725686484	3.5633315831
C46	8.7764712209	1.6834927763	6.3648576849
C47	11.8161648177	4.3807332805	3.0812064400
C48	9.5500844930	0.0881248010	8.0357997785
C49	9.0279313913	0.7324212524	5.3479989369
C50	12.7972006062	3.9056291036	0.4887224876
C51	9.5412577981	-0.5259291235	5.6799896396
C52	8.2726940719	4.7599974231	1.9842791328
C53	13.1890896134	4.2128700678	2.8714000193
X54	8.1697595000#	3.9983050000#	6.1974750000#
X55	8.6241420000#	4.3226030000#	1.8992395000#
H56	3.6813060467	2.6743786692	-2.8198890388
H57	8.7521628412	9.3239792650	10.5809036598
H58	1.4947145521	8.5002133974	0.6473990879
H59	6.6284381308	9.7704032779	9.4373919363
H60	6.8665064169	10.7425254061	4.7439225386
H61	1.6475421550	4.2470596850	3.0305416566
H62	1.2013768954	2.1796796030	2.6106955573
H63	2.3170385738	2.6759239150	1.2952475875
H64	9.4125613946	8.1736126364	6.4625116165
H65	10.2688764276	7.5090463324	5.0452397316
H66	2.7256389880	4.6311984103	-1.6872367045
H67	7.2125287455	2.9251767650	-0.3182587269
H68	2.0962427730	8.1769766110	5.4736205631
H69	10.7261583022	4.0053398152	-0.1570909102
H70	1.9956670085	6.4171447125	-0.6392208300
H71	8.8485543172	2.0916327992	8.5010620216
H72	1.8721561741	6.3890829782	4.2058314280
H73	2.5987133962	10.0452844029	7.0587055622
H74	4.7190421483	10.0408041216	8.3810884806
H75	5.5022760919	1.4938450740	3.0716363442
H76	4.8887477341	2.2510084806	1.5759987644
H77	4.8213188506	10.0225152909	3.5947611429
H78	11.4216871707	4.5732228758	4.0856108283
H79	10.5058547879	8.9430059491	2.8899264658
H80	9.8897273765	10.6189658523	2.8645423792
H81	9.7502032389	-0.1650430738	9.0826363846
H82	8.8131038691	0.9936352715	4.3053387505
H83	13.1799868401	3.7230897566	-0.5213404120
H84	9.7345085964	-1.2578722531	4.8882963211
H85	13.8777680512	4.2706527974	3.7212255317
C86	9.8013847592	-0.8517097854	7.0216113380
H87	10.1989674983	-1.8398136053	7.2776218569
C88	13.6827830056	3.9768554886	1.5773455026
H89	14.7588362185	3.8491420013	1.4166884221
C90	6.4527517038	0.3227601249	-1.3695181659
H91	7.1310196672	0.6525325270	-0.5626949234
H92	5.5151524115	-0.0280440933	-0.9014604078
H93	6.9250878324	-0.5395089501	-1.8749861624

C94	7.5097492085	1.9137022365	-3.0390599422
H95	8.2213326174	2.2933100518	-2.2845270752
H96	7.9916458037	1.0660985096	-3.5602774915
H97	7.3389648113	2.7170552132	-3.7783450686
C98	5.2673678495	0.8870125556	-3.5115531486
H99	5.7702810081	0.0324292235	-3.9982285965
H100	4.3022484256	0.5210679518	-3.1161644388
H101	5.0596114455	1.6371388230	-4.2963378622
C102	3.3499907926	8.4654122704	1.7607621560
H103	3.1422337991	9.3883007137	2.3080569136
C104	4.6312130366	1.5608518045	2.3965309696
H105	4.4738956690	0.5548666735	1.9652853298
C106	2.1730328067	1.9653502357	2.1296841961
H107	2.1026052118	0.9515375285	1.6969683413
C108	3.0462521187	1.0378063826	4.3014785529
H109	2.9061620019	0.0125873898	3.9111260154
H110	3.8731190760	1.0148232152	5.0336419659
H111	2.1252691976	1.3284585050	4.8384697268
C112	4.6988044574	3.7285129062	4.4973289070
H113	5.4812675827	2.9686634564	4.5952403833
C114	8.6401073506	6.5494358645	8.5725316671
H115	9.2125342791	5.6461836427	8.3318893986
C116	10.8683847678	8.2244782802	11.2878212254
H117	11.0189571847	9.2005139079	10.7912019094
H118	10.1133752219	8.3525244618	12.0847056640
H119	11.8206397025	7.9524000516	11.7768707324
C120	10.3025703157	5.7863217681	11.0580649644
H121	11.2413781721	5.5325361224	11.5839222204
H122	9.4983516478	5.8630231071	11.8119844293
H123	10.0558020304	4.9471019179	10.3837316108
C124	11.6071035939	6.9796098992	9.2372913493
H125	12.5589413466	6.7370287998	9.7445869842
H126	11.4029561050	6.1771932341	8.5063291858
H127	11.7495990797	7.9207467630	8.6757548984
C128	7.9953255547	7.7682503434	3.4800209825
H129	8.8958916976	7.1462751724	3.4322020604
C130	9.2354885367	10.8050143811	5.5624601943
H131	8.5572444732	10.6464899371	6.4207187319
H132	10.2178817265	11.1107684612	5.9642629074
H133	8.8523290260	11.6507012559	4.9632918818
C134	10.3284240780	9.8383089373	3.5121885339
H135	11.3083056490	10.2032331347	3.8723103545
C136	10.0571482390	8.4361600996	5.6064728767
H137	11.0205881629	8.8098260191	6.0000049727

[**6**]$^{+}$ perpendicular
E = -3069.43213 Hartree

Au1	-2.9610215341	-0.4601996254	0.8945289050
Au2	2.9998429566	-0.4662541582	-0.9887980680
Au3	0.0217340692	1.2130990000	-0.0496480794
C4	6.4026799094	2.4610105066	1.0441740754
C5	-6.3947555272	2.4535405672	-1.0996128324
C6	5.2462378115	3.1279772488	0.5875794351
C7	6.5724497826	-3.3766917248	0.2346849203
C8	-6.5228687852	1.0613553295	-0.9804337364
C9	-5.2427661338	3.1259224453	-0.6375164465
C10	1.4962213074	-4.9723887999	-2.3057832324
C11	-4.3387016691	-3.0417369498	0.6918281314
C12	-1.4802585837	-4.9299563446	2.3510961362
C13	-5.0887233502	4.6601967898	-0.7113154090
C14	-1.4855618141	0.7566318835	1.4260887948
C15	6.5442308321	1.0737581836	0.9066508986
C16	0.7262681064	1.5055268598	-2.1718080070
C17	0.7915505319	-4.1195824770	3.3002317234
C18	4.2242466656	2.3419371270	-0.0131118985
C19	4.3733370049	-3.0454849886	-0.7255047966
C20	-5.3913564213	-3.9141459131	0.3536238344
C21	5.5262193879	0.3062678839	0.3091349225
C22	-0.7795375511	-4.1794553438	-3.2632058878
C23	0.6957159002	3.4410339942	-3.7126427544
C24	4.3373634156	0.9566199027	-0.1599217200
C25	-5.4947928042	0.2950722512	-0.3953847034
C26	-2.1514733247	-2.2917559669	1.5901360926
C27	-0.5680534916	-3.8856161427	2.6112114432
C28	3.0961583041	-3.3880465440	-1.3647738884
C29	5.0675030478	4.6552931491	0.7116762114
C30	6.6807470185	-2.0028932100	0.4923559513
C31	-3.0631234391	-3.3707365957	1.3435024544
N32	4.5207759823	-1.7131675583	-0.4553784203
C33	-0.6080424334	3.2496755358	3.7891012066
C34	0.5870824894	-3.9321694425	-2.5929362597
C35	-4.3056149909	0.9507732285	0.0649196160
C36	0.0434407466	2.3154447775	-3.1505408254
C37	5.6191584142	-1.1507578448	0.1338032775
C38	2.1908954776	-2.3130286696	-1.6452787620
N39	-4.4851949779	-1.7144361665	0.3918410784
C40	-2.7109595033	-4.6805405331	1.7287813082
C41	-6.5350060484	-3.3905851881	-0.2687632174
C42	-0.6631850442	1.4763692334	2.0712884191
C43	-6.6448084921	-2.0204012859	-0.5531435558
C44	-5.5836514266	-1.1614140933	-0.2066146723
C45	2.7357960970	-4.7078901368	-1.7046573947
C46	0.0506871427	2.2138279545	3.0811379754
C47	-1.2585569870	1.9738612840	-3.5889209385
C48	0.0568399894	3.9212521103	4.8212883872
C49	1.3871743657	1.8809675172	3.4086554564
C50	0.0584280326	4.1954300507	-4.7049091143
C51	2.0421522037	2.5623121429	4.4402184643
C52	1.5323532611	0.7577628327	-1.5367046815
C53	-1.8862036819	2.7374273444	-4.5797414607
H54	7.2141140349	3.0240012377	1.5134155812
H55	-7.2157341561	3.0168512115	-1.5525013060
H56	7.3979564549	-4.0423356054	0.5098026349
H57	-7.4395847403	0.5790276546	-1.3423205438
H58	1.2436777343	-6.0078965254	-2.5520226287
H59	-1.2391171013	-5.9574408792	2.6399241784
H60	0.2915470925	-6.0245472262	4.3047773931
H61	1.0445106181	-6.2301119853	2.6931618067
H62	-1.9094386025	-4.0767332376	-1.3685705121
H63	-1.7888606071	-2.5094819444	-2.2038822667
H64	7.4619535504	0.5964418470	1.2713095906
H65	3.3161774663	2.8392613664	-0.3745597536
H66	-5.3155934077	-4.9805612111	0.5784895042
H67	1.7026582246	3.7040795799	-3.3724643635
H68	7.5783456433	-1.5949256167	0.9630049038
H69	-1.6398626134	3.5062301523	3.5295741297
H70	-3.3946706523	-5.5190746362	1.5513465800
H71	-7.3582544783	-4.0629235553	-0.5339471381
H72	-7.5409233193	-1.6200454742	-1.0324825401
H73	1.8306880759	-2.5331199625	2.1483020431
H74	1.9221834320	-4.1521214578	1.4059867043
H75	3.4197313575	-5.5417738417	-1.5038218678
H76	-1.7632890804	1.1078696497	-3.1484258715
H77	-0.6330449731	-2.3841058981	-4.5526562675
H78	-0.0094011912	-3.8762534408	-5.3094156944
H79	-0.4599108986	4.7144027497	5.3722901604
H80	1.8952866197	1.0852152020	2.8534154153
H81	0.5719984646	5.0593270807	-5.1402109756
H82	3.0725451800	2.2947677651	4.6964713310
H83	-2.8903713561	2.4622355012	-4.9191347127
C84	1.3795805359	3.5800793195	5.1490708288
H85	1.8943576859	4.1071673403	5.9598509711
C86	-1.2315515065	3.8482442064	-5.1405918966
H87	-1.7248982585	4.4408232355	-5.9182675395
C88	3.7832352355	4.9591428630	1.5282043508
H89	2.8797885716	4.5385102280	1.0540280589
H90	3.8506760814	4.5395558060	2.5485833857
H91	3.6385633520	6.0518347657	1.6140484113
C92	4.9329582120	5.2668037630	-0.7104961574
H93	4.0665524933	4.8519318292	-1.2549551649
H94	4.7957550684	6.3621490499	-0.6445956900
H95	5.8378817098	5.0727498863	-1.3132146657
C96	6.2664362976	5.3294096495	1.4149670962
H97	6.0885677191	6.4170697798	1.4895713502
H98	6.4114940381	4.9439806781	2.4412869704
H99	7.2078606466	5.1885959229	0.8542968810
C100	5.4264027584	-3.9110823549	-0.3721287890
H101	5.3484004434	-4.9815251701	-0.5742005976
C102	1.9262641439	-3.6114033794	2.3695073231
H103	2.9090091566	-3.7712910939	2.8527592100
C104	1.0448048509	-5.6126903642	3.6092754899
H105	2.0320672137	-5.7307625671	4.0896922439

C106	0.8264267562	-3.3332605109	4.6391474746
H107	1.8005079187	-3.4804589614	5.1420505799
H108	0.6875171689	-2.2479869429	4.4852882195
H109	0.0333040447	-3.6815730816	5.3243274812
C110	-0.9355137727	-2.5690416789	2.2176422861
H111	-0.2416921108	-1.7427756782	2.4122267227
C112	-4.2048814671	2.3393782556	-0.0639059030
H113	-3.2978563907	2.8386720635	0.2980905190
C114	-6.2929010306	5.3420032448	-1.4005963757
H115	-6.4244204669	4.9934834191	-2.4418621018
H116	-7.2362321305	5.1659036062	-0.8534836070
H117	-6.1321300727	6.4347588948	-1.4341881341
C118	-4.9693167704	5.2206502511	0.7332815565
H119	-4.8513356524	6.3200507021	0.7081258909
H120	-5.8713503786	4.9875805835	1.3257322157
H121	-4.0972850445	4.8005660963	1.2651140055
C122	-3.8045003276	5.0186216291	-1.5047928117
H123	-3.6836787082	6.1168348853	-1.5539311866
H124	-2.8964289120	4.6041155698	-1.0325944752
H125	-3.8524210959	4.6326839742	-2.5388731011
C126	0.9690465219	-2.6050580691	-2.2547935724
H127	0.2805784857	-1.7816935146	-2.4750146129
C128	-1.0637030725	-5.6835103600	-3.4774645348
H129	-1.0616544573	-6.2423218216	-2.5233414982
H130	-2.0596275255	-5.8129409911	-3.9384444168
H131	-0.3268340215	-6.1523117086	-4.1556887414
C132	-0.7965089922	-3.4728156006	-4.6464980035
H133	-1.7721580420	-3.6284095033	-5.1430860046
C134	-1.9035572989	-3.5949454647	-2.3622800443
H135	-2.8893833813	-3.7638980127	-2.8324629720

S5.2. B3LYP (Jaguar)

M^1 = $[CpRu(PPh_3)_2]^+$, M^2 = $[Au(PPh_3)]^+$

Ru Conformer D

E = -3839.48713 Hartree

Ru1	1.4090747439	2.7545575283	-1.9253281160
Au2	1.4488811065	1.6931879021	1.6893132274
C2	3.2325624786	3.3531396946	-0.7015376399
C3	2.2156859708	4.3446978866	-0.4922394278
C4	1.9413354906	4.9704878718	-1.7303637186
C5	2.7837517995	4.3718535523	-2.7297183286
C6	3.5857240182	3.3896301898	-2.0787507978
H7	1.7393590945	4.5666125737	0.4525892908
H8	1.2347182451	5.7708537411	-1.9008265884
H9	2.8435166726	4.6774267641	-3.7633934792
H10	4.3429500383	2.7745471600	-2.5453925609
H11	3.6792614043	2.7268869034	0.0551465568
P40	-0.5639838929	3.4172248207	-3.1834895802
P41	1.9887735563	0.6037529163	-2.8532035178
C36	0.6806418441	6.5876315589	-6.4067428390
C37	-0.2142766648	6.9453536117	-5.3998558239
C38	-0.6057029913	6.0144622491	-4.4335522710
C39	-0.0980834307	4.7061368571	-4.4494511645
C40	0.8222109450	4.3671593263	-5.4578147057
C41	1.1969968487	5.2912506704	-6.4324067086
H42	0.9766625217	7.3111090948	-7.1620359240
H43	-0.6190847731	7.9528011191	-5.3630058217
H44	-1.3110067083	6.3205929175	-3.6698332227
H45	1.2601528520	3.3747306507	-5.4812958302
H46	1.8951926634	4.9967447019	-7.2106673555
C43	3.3649806967	0.4521215458	-7.3193959307
C44	2.7385518930	-0.6571126120	-6.7515699970
C45	2.3029633114	-0.6238280868	-5.4261082561
C46	2.4721724540	0.5335996954	-4.6474813177
C47	3.1067997713	1.6408584563	-5.2304527481
C48	3.5550069340	1.6009949706	-6.5516136139
H49	3.7064127818	0.4206549586	-8.3506440263
H50	2.5918681756	-1.5590248253	-7.3392009092
H51	1.8354213761	-1.5054638337	-5.0043140191
H52	3.2547946510	2.5419213444	-4.6461097619
H53	4.0506292338	2.4683901128	-6.9794823482
C50	5.8690856371	-0.9519804447	-0.7265946177
C51	5.8706007230	-0.7515058427	-2.1059024873
C52	4.7208062501	-0.2970977960	-2.7609377874
C53	3.5499711051	-0.0140442005	-2.0418255203
C54	3.5630906122	-0.2134994753	-0.6502157577
C55	4.7038520337	-0.6881323127	-0.0014144083
H56	6.7599464916	-1.3182034976	-0.2231027037
H57	6.7664500384	-0.9592632228	-2.6860468758
H58	4.7456605301	-0.1690205310	-3.8386552395
H59	2.6701880856	-0.0058600920	-0.0680376939
H60	4.6763386278	-0.8625955855	1.0722622412
C57	-0.7286629145	-3.1922063801	-2.8989048223
C58	0.4298696842	-3.1945652049	-2.1225530418
C59	1.2386161636	-2.0573876988	-2.0546222073
C60	0.8927772513	-0.8919356783	-2.7555448329
C61	-0.2859691674	-0.8965154831	-3.5200409050
C62	-1.0849490454	-2.0360976340	-3.5957873987
H63	-1.3445042542	-4.0853761910	-2.9669970686
H64	0.7230372231	-4.0907018919	-1.5800678332
H65	2.1526662228	-2.0986903067	-1.4715761849
H66	-0.5705189437	-0.0187400428	-4.0884243457
H67	-1.9831960019	-2.0148843200	-4.2073650419
C64	-3.3814809769	0.5491619934	-5.6123919517
C65	-3.5763102295	0.7675936086	-4.2473475992
C66	-2.7360745951	1.6288665713	-3.5410165367
C67	-1.6838154773	2.3040652484	-4.1836845210
C68	-1.5069993000	2.0867090598	-5.5607584553
C69	-2.3437104147	1.2165769881	-6.2639088501
H70	-4.0384255227	-0.1174223010	-6.1645094362
H71	-4.3855323039	0.2682621200	-3.7225583881
H72	-2.9183029705	1.7823956631	-2.4843112180
H73	-0.7274269086	2.6064004184	-6.1069870305
H74	-2.1852859246	1.0728434326	-7.3297383384
C71	-3.6706231354	5.8850521834	-0.6960875584
C72	-3.9868495483	5.4589420002	-1.9891312204
C73	-3.0754336330	4.6991586313	-2.7224529498
C74	-1.8279717225	4.3425984297	-2.1769777255
C75	-1.5267669671	4.7687534402	-0.8759435771
C76	-2.4375910972	5.5373189385	-0.1433874210
H77	-4.3792441944	6.4820497574	-0.1279608603
H78	-4.9436582108	5.7228959462	-2.4324099878
H79	-3.3369585118	4.3863636333	-3.7288684696
H80	-0.5832692503	4.4792279833	-0.4267999786
H81	-2.1807654718	5.8603803891	0.8627414817
C82	-0.7323513115	1.3353722980	-0.2026475828
P86	2.5437444953	1.4304532008	3.7430742864
C89	6.4379085701	3.9386757912	3.9822139029
C90	5.4803397148	4.0638792973	4.9879893480
C91	4.3057441691	3.3085479145	4.9437027272
C92	4.0813616385	2.4187725630	3.8849947645
C93	5.0472376107	2.3009723146	2.8700857762
C94	6.2182537733	3.0530221071	2.9229937947
H95	7.3483453353	4.5293825091	4.0195534597
H96	5.6422757407	4.7529421350	5.8122729927
H97	3.5676988874	3.4167875240	5.7333382454
H98	4.8885564676	1.6150748169	2.0413155411
H99	6.9570156690	2.9529693827	2.1305972254
C99	-0.1733866728	2.6434992934	7.2871708577
C100	-0.3159298041	3.2567635984	6.0413418415
C101	0.5030592584	2.8770452566	4.9788411555
C102	1.4791557448	1.8857228248	5.1596157297
C103	1.6153005691	1.2700173862	6.4130367426
C104	0.7903683475	1.6508643786	7.4710389324
H105	-0.8173211796	2.9334633249	8.1128542742
H106	-1.0702382448	4.0240779237	5.8933411977
H107	0.3808544620	3.3440951759	4.0043425752
H108	2.3556176539	0.4894258340	6.5622686080
H109	0.8976503034	1.1665967632	8.4386929492
C109	3.6765290130	-3.0120583287	4.4479908687
C110	4.5556224705	-2.0074374172	4.8568891174
C111	4.2394143993	-0.6636703219	4.6450215674
C112	3.0353189751	-0.3150779415	4.0163158984
C113	2.1559951416	-1.3302039167	3.6027393197
C114	2.4752606060	-2.6693271438	3.8215066957
H115	3.9273951372	-4.0561230674	4.6119555807
H116	5.4921869960	-2.2670324555	5.3418352982
H117	4.9326054543	0.1091891889	4.9645479466
H118	1.2230282601	-1.0705782809	3.1071950405

H119	1.7879190652	-3.4458066851	3.4970345158
C119	-4.5944124548	-0.3529565706	0.0413911288
C120	-3.5085596752	-1.1488134887	-0.3341030942
C121	-2.2378470450	-0.5927996131	-0.4392686087
C122	-2.0393108695	0.7775825068	-0.1679397443
C123	-3.1436355910	1.5723214561	0.2120212465
C124	-4.4097260986	1.0061236466	0.3145859718
H125	-5.5856811216	-0.7918006723	0.1250306136
H126	-3.6532857078	-2.2046141491	-0.5441948248
H127	-1.3901158899	-1.2035439017	-0.7280708960
H128	-2.9892977802	2.6267980842	0.4192035296
H129	-5.2544323843	1.6228818548	0.6085189750

Ru Conformer E

E = -3839.505741 Hartree

Ru1	1.4435271888	2.7377849280	-1.8777860938
Au2	0.9929644195	1.3526199504	1.5894140011
C2	3.2653990805	3.1095965115	-0.5371475162
C3	2.2514220251	4.0463889494	-0.1632176750
C4	1.9980677113	4.8942228155	-1.2679903365
C5	2.8803641880	4.5124520770	-2.3386063396
C6	3.6571755092	3.4210831022	-1.8779948156
H7	1.7582104679	4.0941169891	0.7983701834
H8	1.2973205996	5.7158373952	-1.2874906447
H9	2.9483648250	4.9986603825	-3.3017317298
H10	4.4242767626	2.9038306782	-2.4382398030
H11	3.7051563107	2.3535599616	0.0943733674
P40	-0.4119841394	3.5475547580	-3.1671152856
P41	2.0143682651	0.6968532131	-2.9770525030
C36	0.9291093596	7.1782680438	-5.8235641328
C37	0.4721746279	7.3705554484	-4.5200502799
C38	0.0524337991	6.2830099258	-3.7533215938
C39	0.0822737355	4.9748895034	-4.2687351378
C40	0.5427729389	4.7983637421	-5.5823857146
C41	0.9589662999	5.8878341595	-6.3502213646
H42	1.2497402184	8.0251896215	-6.4245459351
H43	0.4305004904	8.3709025922	-4.0969391522
H44	-0.3258018572	6.4667251650	-2.7529425170
H45	0.5678979880	3.8147580568	-6.0323811158
H46	1.2989695767	5.7221103148	-7.3693470596
C43	3.5997164578	1.1200107914	-7.3554013584
C44	3.1037576957	-0.1092420540	-6.9184759203
C45	2.6116611126	-0.2516312951	-5.6201599861
C46	2.6031956439	0.8380230548	-4.7346199330
C47	3.0919684009	2.0722758754	-5.1907725377
C48	3.5924018906	2.2113764091	-6.4871971279
H49	3.9837346006	1.2267318141	-8.3668556325
H50	3.0986227322	-0.9641981478	-7.5897159053
H51	2.2255978510	-1.2148226806	-5.3049486827
H52	3.0631559376	2.9335619509	-4.5326345937
H53	3.9686370989	3.1761893864	-6.8178077560
C50	5.6841929640	-1.0968525383	-0.7112310079
C51	5.8692788374	-0.5282241941	-1.9706125144
C52	4.7822033853	0.0028433157	-2.6729705585
C53	3.4967864096	-0.0173854006	-2.1166586426
C54	3.3220050749	-0.5840053788	-0.8418850169
C55	4.4035841839	-1.1256931216	-0.1494766092
H56	6.5274694797	-1.5253296103	-0.1745485343
H57	6.8588704945	-0.5086594696	-2.4206007733
H58	4.9424802869	0.4181983324	-3.6638710331
H59	2.3321827451	-0.6150135109	-0.3945136441
H60	4.2436776409	-1.5842974063	0.8242853389
C57	-0.7608565513	-3.0577735778	-3.2154458636
C58	0.6275414399	-3.2079100051	-3.1864504204
C59	1.4545093082	-2.0886629228	-3.0824236058
C60	0.9090339507	-0.7930395587	-3.0093082233
C61	-0.4852824848	-0.6586537373	-3.0214065919
C62	-1.3116896423	-1.7803376303	-3.1272076500
H63	-1.4049185760	-3.9295621040	-3.2986959966
H64	1.0725530826	-4.1979255831	-3.2444314992
H65	2.5305504136	-2.2304215387	-3.0520993747
H66	-0.9368120613	0.3209040607	-2.9438413727
H67	-2.3898938072	-1.6470799694	-3.1346270083
C64	-2.8240305524	0.7575325316	-6.0610848894
C65	-3.4718571739	1.3763659211	-4.9921707563
C66	-2.7677966132	2.2117295386	-4.1201199553
C67	-1.3952221932	2.4468538723	-4.3000946013
C68	-0.7476905633	1.7825923467	-5.3570547932
C69	-1.4541335230	0.9605430683	-6.2341389769
H70	-3.3760825922	0.1149341852	-6.7420768449
H71	-4.5346083210	1.2143306069	-4.8303114935
H72	-3.3005616727	2.6748575970	-3.2976811710
H73	0.3240654031	1.8752213393	-5.4870742901
H74	-0.9241607477	0.4668713949	-7.0443759321
C71	-3.6830862536	5.7119368884	-0.6335449583
C72	-3.7394024331	5.7418861534	-2.0296287006
C73	-2.7674294603	5.0870749140	-2.7828064032
C74	-1.7244889256	4.3799152756	-2.1546484559
C75	-1.6765363559	4.3619789013	-0.7553716317
C76	-2.6491703992	5.0249499517	-0.0003772245
H77	-4.4396617541	6.2262799739	-0.0463696129
H78	-4.5380326350	6.2808146087	-2.5329924286
H79	-2.8163900532	5.1322721721	-3.8672267213
H80	-0.8802294108	3.8226985561	-0.2564743887
H81	-2.5940589183	5.0032644288	1.0856833949
C82	-0.5131775990	0.9510691779	0.0190096271
P86	2.2618933142	1.4536677908	3.5463154855
C89	6.3027328206	3.6708597249	2.9746158879
C90	5.3303586986	4.2099485337	3.8191046824
C91	4.1137908717	3.5495521573	4.0117973835
C92	3.8572452734	2.3406707920	3.3513357405
C93	4.8358003818	1.8068197368	2.4914173904
C94	6.0517743645	2.4660928362	2.3126243213
H95	7.2493103414	4.1849539156	2.8316439537
H96	5.5166860729	5.1464163496	4.3379046207
H97	3.3717128672	3.9765418002	4.6809167596
H98	4.6547159127	0.8726243919	1.9645742864
H99	6.8024666259	2.0387778181	1.6516485482
C99	0.0099532422	3.6273167934	6.9583249065
C100	-0.2718043980	3.9292675073	5.6266682379
C101	0.3960332617	3.2584001862	4.6017638916
C102	1.3606071414	2.2848594370	4.9041968792
C103	1.6379723158	1.9839528515	6.2457473886
C104	0.9625260575	2.6533819601	7.2657922102
H105	-0.5157060617	4.1456692634	7.7560042295
H106	-1.0177042266	4.6816117452	5.3849801015
H107	0.1646687065	3.4848495780	3.5644803456
H108	2.3733127038	1.2243459095	6.4946178322
H109	1.1793893464	2.4111480380	8.3019641960
C109	3.1975336011	-2.7525232676	5.2421798537
C110	4.1662075117	-1.7530714853	5.3219448645
C111	3.9129711606	-0.4840814069	4.7963308802
C112	2.6840586535	-0.2107724732	4.1791239591
C113	1.7157511514	-1.2242713953	4.0933184605
C114	1.9723117348	-2.4865279525	4.6277576716
H115	3.3984807862	-3.7381281431	5.6548470199
H116	5.1229178127	-1.9578728174	5.7942344376
H117	4.6733241634	0.2873647211	4.8652524340
H118	0.7624017812	-1.0261733508	3.6082001679
H119	1.2160736375	-3.2632653218	4.5622655932
C119	-3.8639635986	-1.3264055582	1.3401566679
C120	-2.6869651604	-1.9703822454	0.9527575211
C121	-1.5911587993	-1.2283284188	0.5175284035
C122	-1.6603628511	0.1758712757	0.4585491365
C123	-2.8511504896	0.8161070134	0.8471251227
C124	-3.9426309493	0.0669976459	1.2825940812
H125	-4.7155259916	-1.9073163861	1.6846795705
H126	-2.6215914404	-3.0552632436	0.9887951612
H127	-0.6775492601	-1.7273725417	0.2075165072
H128	-2.9123488674	1.9000281480	0.7987103430
H129	-4.8573743189	0.5732576090	1.5805177662

Ru Conformer F

E = -3839.510512 Hartree

Ru1	1.2172887990	2.4694814548	-1.5530785805
Au2	-0.4734105710	0.6137402634	1.6724319905
C2	2.6839942710	2.4465633500	0.2102399456
C3	1.7361686608	3.4901652870	0.4444845707
C4	1.8808544982	4.4607822462	-0.5757334201
C5	2.9628577273	4.0441438491	-1.4335493855
C6	3.4529030625	2.8156520196	-0.9435024591
H7	1.0103707020	3.5125479089	1.2452360028

H8	1.3113818866	5.3758218762	-0.6592989771
H9	3.3350045879	4.5861669874	-2.2912650993
H10	4.2646634961	2.2385176524	-1.3655414715
H11	2.8412101603	1.5744051150	0.8268884976
P40	-0.0531790200	3.6403811745	-3.2592190917
P41	1.7525039217	0.3872520856	-2.6067216152
C36	2.4847374113	6.4920433299	-5.9735691933
C37	2.2923099174	6.7643441576	-4.6171475542
C38	1.5328020558	5.9015029957	-3.8306251564
C39	0.9494395357	4.7449159658	-4.3777783553
C40	1.1418917149	4.4904432644	-5.7428615698
C41	1.9039338577	5.3565885515	-6.5311660183
H42	3.0714928819	7.1673955316	-6.5900830292
H43	2.7229180076	7.6571824507	-4.1718488003
H44	1.3687376186	6.1523102901	-2.7874140659
H45	0.6820790068	3.6304181242	-6.2134745130
H46	2.0290278129	5.1423773932	-7.5897435707
C43	3.8292370565	0.6664444492	-6.7733572549
C44	3.1104908008	-0.4812322121	-6.4394307540
C45	2.4707475190	-0.5763902089	-5.2032577169
C46	2.5338227229	0.4827700123	-4.2841836445
C47	3.2514993584	1.6351018884	-4.6345071077
C48	3.8994494531	1.7241692272	-5.8676677485
H49	4.3272154256	0.7369091550	-7.7366886199
H50	3.0473453003	-1.3079147034	-7.1418011834
H51	1.9172905750	-1.4763085165	-4.9597076154
H52	3.2901567961	2.4723494897	-3.9446183663
H53	4.4474927748	2.6261073251	-6.1224469863
C50	4.9957189695	-1.8002707488	-0.0449691683
C51	5.3232290571	-1.3411591755	-1.3195403339
C52	4.3663693229	-0.6919141329	-2.1071685200
C53	3.0665224479	-0.4868438063	-1.6251389455
C54	2.7460740114	-0.9528845980	-0.3382549215
C55	3.6991535741	-1.6057323762	0.4415824633
H56	5.7394768472	-2.3087047366	0.5623051382
H57	6.3253805522	-1.4912301300	-1.7133326070
H58	4.6402854328	-0.3556651734	-3.1022435928
H59	1.7407071697	-0.8090245478	0.0514494855
H60	3.4281942568	-1.9648374729	1.4315909061
C57	-1.4176199132	-3.0060936696	-3.1065653161
C58	-0.0759586438	-3.3263346741	-2.8851134515
C59	0.8708177590	-2.3149010313	-2.7190661753
C60	0.4938199648	-0.9599310483	-2.7782931660
C61	-0.8565402328	-0.6523111320	-2.9982641311
C62	-1.8029301883	-1.6659834402	-3.1611361421
H63	-2.1550608009	-3.7945896061	-3.2303358778
H64	0.2385221662	-4.3663068706	-2.8392282478
H65	1.9065323407	-2.5866912904	-2.5384008353
H66	-1.1808596923	0.3793646220	-3.0380096363
H67	-2.8443928648	-1.3993807165	-3.3204281700
C64	-2.7697890474	1.4108316554	-6.3352140734
C65	-3.3281947653	2.3572605780	-5.4783589876
C66	-2.5310505144	3.0283040986	-4.5495050294
C67	-1.1581174314	2.7538333785	-4.4543421513
C68	-0.6115974125	1.7847145847	-5.3125577032
C69	-1.4067598279	1.1272134125	-6.2494259148
H70	-3.3918077303	0.8952460910	-7.0615411774
H71	-4.3897371323	2.5833564763	-5.5324501874
H72	-2.9875221416	3.7725184131	-3.9072206323
H73	0.4410009473	1.5336265988	-5.2524416230
H74	-0.9577830678	0.3859679002	-6.9049187308
C71	-2.9285840989	6.8110336830	-1.3920631881
C72	-2.5370021690	6.9127236507	-2.7290100259
C73	-1.6751212980	5.9673196440	-3.2815462344
C74	-1.1884873792	4.9004572870	-2.5061543014
C75	-1.5930846257	4.8065969587	-1.1671992672
C76	-2.4576308803	5.7559691608	-0.6154032676
H77	-3.5980319904	7.5511616807	-0.9615285260
H78	-2.9009475294	7.7309970143	-3.3438018309
H79	-1.3774281522	6.0631141652	-4.3215098348
H80	-1.2394143272	3.9853322392	-0.5548755376
H81	-2.7623783844	5.6644663636	0.4241554715
C81	-1.3716490333	1.1141879684	-0.1987735116
C82	-0.3858592074	1.6608404857	-0.8148542244
C84	-5.5422301662	0.2405586078	-0.7049912922
C85	-4.9606911795	1.3198337755	-1.3726347437
C86	-3.6078980858	1.6095021551	-1.2078553173
C87	-2.7983155753	0.8183373254	-0.3717703337
C88	-3.3987194753	-0.2688014114	0.2922457799
C89	-4.7525677531	-0.5529717322	0.1277058284
H90	-6.5988807442	0.0203473841	-0.8321890056
H91	-5.5653295510	1.9464875123	-2.0236164054
H92	-3.1733267324	2.4608009399	-1.7197147535
H93	-2.7876178735	-0.9066870435	0.9258872640
H94	-5.1899582977	-1.4011288306	0.6492681091
P95	0.2084749723	-0.0223092544	3.8260973041
C98	-2.7187056356	1.3551954953	7.1449067074
C99	-1.3481656076	1.3132142245	7.4091355347
C100	-0.4512166753	0.9209446453	6.4145461728
C101	-0.9237001320	0.5662108310	5.1419329821
C102	-2.3015684641	0.6194566641	4.8784466970
C103	-3.1924731058	1.0089526337	5.8779291905
H104	-3.4140768025	1.6625486525	7.9211487979
H105	-0.9728465947	1.5877756523	8.3910931854
H106	0.6134188326	0.8976575409	6.6295486951
H107	-2.6774637574	0.3616953056	3.8911854325
H108	-4.2572158482	1.0473933153	5.6640978699
C108	4.3636285561	1.7444260126	4.8686252238
C109	3.2982728457	2.5782195807	4.5161383375
C110	2.0547206167	2.0301506381	4.2111024451
C111	1.8596906411	0.6393628835	4.2679429757
C112	2.9313792692	-0.1909933231	4.6230143802
C113	4.1780378435	0.3635368221	4.9202765458
H114	5.3348736791	2.1721787200	5.1012475982
H115	3.4377342551	3.6552090725	4.4755937113
H116	1.2302705171	2.6852741440	3.9378364252
H117	2.7968777929	-1.2673506344	4.6738261293
H118	5.0031280406	-0.2883612997	5.1955854127
C118	0.5429341832	-4.6230625930	4.2605293538
C119	0.3155819916	-3.8375968057	5.3925510223
C120	0.1996996313	-2.4529400150	5.2743225593
C121	0.3130576734	-1.8409643241	4.0155079585
C122	0.5311689666	-2.6381536801	2.8802955437
C123	0.6489981805	-4.0225962683	3.0048763177
H124	0.6286120881	-5.7022607615	4.3565923624
H125	0.2241051468	-4.3035924800	6.3700894739
H126	0.0132973087	-1.8524800341	6.1601631162
H127	0.5993621077	-2.1773378626	1.8977738619
H128	0.8158804839	-4.6307175050	2.1197554913

M^1 = [Au(^{t}BuC^N^C^{t}Bu)]$^+$, M^2 = [Au(PPh_3)]$^+$

Au(III), Conformer D

E = -2638.582591 Hartree

Au1	1.0443966506	-2.2131241581	1.3829775273
Au2	1.2319512987	-1.5798629924	-2.1456653690
C3	0.6719820975	-0.8333915806	3.9325765566
C4	0.0766076893	-0.5778914647	5.1774912845
C5	-0.9948320603	-1.3787769156	5.5924875596
C6	-1.4744943799	-2.4206504104	4.7939256311
C7	-0.8664412022	-2.6624747353	3.5531275361
N8	0.1691622386	-1.8557996940	3.1885553444
H9	0.4446135762	0.2268079370	5.8058590962
H10	-1.4647184429	-1.1878637394	6.5573075231
H11	-2.3059420235	-3.0368194962	5.1275605516
C12	3.9813141388	1.1450420847	2.0089060455
C13	3.2970755046	0.0636234059	1.4064955908
C14	2.2275863739	-0.5806251574	2.0212452245
C15	1.7999274247	-0.1254194054	3.3043525220
C16	2.4610399046	0.9545950377	3.9097509604
C17	3.5354947161	1.5772247442	3.2679903327
H18	3.6200561834	-0.2861327167	0.4266081946
H19	2.1510886723	1.3208757542	4.8868877808
H20	4.0269756398	2.4071086769	3.7681430560
C21	-1.7358164896	-5.6761544101	0.5844035931
C22	-0.7058811356	-4.7135236761	0.4075357856
C23	-0.4230448852	-3.7362410678	1.3633422792
C24	-1.2033692808	-3.6979608589	2.5622929551
C25	-2.2363140367	-4.6333466959	2.7464609598
C26	-2.4953351697	-5.6047242434	1.7713055761
H27	-0.1078240599	-4.7411546131	-0.5063246925
H28	-2.8477725443	-4.6199665484	3.6513717882
H29	-3.3006770519	-6.3120452140	1.9521282625

C30	-1.9854734798	-6.7487356073	-0.5105727677
C31	-3.1170780265	-7.7203920094	-0.1481506495
H32	-2.8778007579	-8.2807108451	0.7621671638
H33	-4.0750553332	-7.2043413765	0.0148328136
H34	-3.2589477008	-8.4448512755	-0.9740573678
C35	-0.6949472578	-7.5729133471	-0.7185191081
H36	-0.3843296264	-8.0594415435	0.2113255656
H37	-0.8645640768	-8.3504432256	-1.4767834933
H38	0.1323844089	-6.9601287743	-1.0638470129
C39	-2.3595415023	-6.0816728600	-1.8564719039
H40	-2.5426269506	-6.8344612538	-2.6385647773
H41	-3.2659837755	-5.4844418759	-1.7465573714
H42	-1.5610062080	-5.4415564147	-2.2156015846
C43	5.1686729283	1.7980231439	1.2760813377
C44	5.7454403096	2.9979624055	2.0452111995
H45	4.9963969234	3.7822249602	2.1797308766
H46	6.1253175134	2.7188692384	3.0442055647
H47	6.5838553858	3.4285832736	1.4809980900
C48	4.7001558061	2.2832664634	-0.1205902160
H49	3.9004831822	3.0190329429	-0.0251642734
H50	5.5363107939	2.7541697127	-0.6599815091
H51	4.3220219298	1.4613879353	-0.7432836839
C52	6.3045179247	0.7709945082	1.1004094113
H53	7.1682288997	1.2255989675	0.5895338565
H54	6.6434921860	0.4098482999	2.0679402746
H55	5.9850714410	-0.0851414460	0.5034664471
C56	1.9300199658	-2.5624320264	-0.4418665496
C57	2.8904007317	-3.3808461825	-0.5325009396
C58	6.0567557563	-6.1309230151	-0.8189791148
C60	4.7432827132	-6.5626132351	-0.9818086732
C61	3.7010991862	-5.6551096171	-0.8960054961
C62	3.9613440082	-4.2941323914	-0.6442583815
C63	5.2971772282	-3.8674624192	-0.4807509805
C64	6.3345090627	-4.7865969412	-0.5690740644
H65	6.8684241599	-6.8483281071	-0.8861994917
H66	4.5373146586	-7.6086559810	-1.1734849616
H67	2.6757527781	-5.9739041340	-1.0140395770
H68	5.4950279276	-2.8217344593	-0.2816468850
H70	7.3590109302	-4.4636782774	-0.4411749888
P71	0.3771930672	-0.4749062396	-4.0318366065
C72	-3.2332047906	-2.7400754409	-5.8510644065
C73	-3.1080084933	-2.5907360171	-4.4762468074
C74	-2.0086586924	-1.9226088170	-3.9475466889
C75	-1.0278784474	-1.3853768183	-4.7915302598
C76	-1.1572993035	-1.5397338903	-6.1675245018
C77	-2.2561400399	-2.2161563793	-6.6891230789
H78	-4.0880458660	-3.2638782530	-6.2619144977
H79	-3.8659497763	-2.9980105583	-3.8138032245
H80	-1.9138996498	-1.8168080911	-2.8765001098
H81	-0.4060687756	-1.1328329488	-6.8264721356
H82	-2.3444277173	-2.3295137536	-7.7577360351
C83	3.5525608909	-0.0036447852	-7.3806990129
C84	3.5468497204	-1.1280616775	-6.5652876676
C85	2.5994170348	-1.2514411189	-5.5497526404
C86	1.6384827025	-0.2525747993	-5.3428257978
C87	1.6487639720	0.8797926990	-6.1583498250
C88	2.6036743975	1.0002925856	-7.1702956417
H89	4.2941032340	0.0908236208	-8.1732810815
H90	4.2848959760	-1.9096513900	-6.7164859273
H91	2.6046905610	-2.1259804821	-4.9102725041
H92	0.9159710439	1.6650473705	-6.0009024883
H93	2.6079254477	1.8812667067	-7.7957858251
C94	-1.2129202114	3.7008764954	-2.8967319506
C95	-1.8591629033	2.9697473197	-3.9035759131
C96	-1.3982645306	1.7116092383	-4.2561454804
C97	-0.2802244539	1.1747791385	-3.5989658831
C98	0.3658870319	1.9091365035	-2.5839345622
C99	-0.0997630734	3.1641310988	-2.2362524940
H100	-1.5758539162	4.6824948973	-2.6226968609
H101	-2.7274300195	3.3773047410	-4.4176069560
H102	-1.9128181969	1.1530283603	-5.0394523868
H103	1.2261797690	1.4918933569	-2.0581100064
H104	0.3979428880	3.7219126993	-1.4421599275

Au(III), Conformer E
E = -2638.589837 Hartree

Au1	0.9533771303	-1.3386524189	-0.0762626039
Au2	2.3801931318	-3.2092410563	-2.6001805860
C2	0.3724829633	1.4988101172	0.2582198411
C3	-0.4285950178	2.6154193804	0.5150479812
C4	-1.7873755843	2.4309424985	0.7696580431
C5	-2.3551137426	1.1577293348	0.7655006238
C6	-1.5391102146	0.0527495645	0.5057177128
N7	-0.2207394812	0.2780971951	0.2724877558
H8	0.0023445331	3.6091353623	0.5176596155
H9	-2.4144855269	3.2945418961	0.9725284428
H10	-3.4125990949	1.0225640065	0.9594245591
C11	4.5705856620	1.2850910332	-0.6617676558
C12	3.7647513252	0.1282718958	-0.5526109347
C13	2.4094115412	0.1900936524	-0.2513020096
C14	1.8110890503	1.4656347772	-0.0447328451
C15	2.5965881583	2.6182910411	-0.1470820149
C16	3.9541254832	2.5266382420	-0.4529374787
H17	4.2211778461	-0.8456008664	-0.7036764280
H18	2.1595537225	3.6018219554	0.0080672346
H19	4.5287758896	3.4428387180	-0.5243267754
C20	-2.5805492235	-4.1054705888	0.1836969869
C21	-1.2488834800	-3.6525659926	0.0441574688
C22	-0.9061804825	-2.3116926028	0.1601934176
C23	-1.9301451272	-1.3611280837	0.4324094375
C24	-3.2489689343	-1.7981330886	0.5873506512
C25	-3.5653728291	-3.1491322482	0.4623772701
H26	-0.4648862616	-4.3741690285	-0.1651594399
H27	-4.0473839398	-1.0913545403	0.7979853168
H28	-4.6006368556	-3.4472046834	0.5814108377
C29	-2.9033127854	-5.6009692550	0.0148067786
C30	-4.4046703063	-5.9017198412	0.1886877371
H31	-4.7630272545	-5.6324269958	1.1884779316
H32	-5.0162338068	-5.3710096767	-0.5499325144
H33	-4.5838681716	-6.9743134909	0.0544237069
C34	-2.1197773550	-6.4196371283	1.0690280007
H35	-2.4061478939	-6.1270079035	2.0854093094
H36	-2.3311936938	-7.4894062336	0.9529105723
H37	-1.0373303421	-6.2803134112	0.9747620772
C38	-2.4863926931	-6.0545079056	-1.4062675065
H39	-2.7091565238	-7.1193711924	-1.5446914325
H40	-3.0332422184	-5.4913356284	-2.1719943117
H41	-1.4144015981	-5.9126821943	-1.5839787270
C42	6.0662567336	1.1462716473	-0.9979027600
C43	6.7780336786	2.5109255887	-1.0750387476
H44	6.3476044657	3.1540356695	-1.8517068602
H45	6.7349132303	3.0487228369	-0.1208605844
H46	7.8357130241	2.3623428394	-1.3198430565
C47	6.2205147022	0.4435429874	-2.3688907531
H48	5.7450841821	1.0280610038	-3.1654751139
H49	7.2822001143	0.3326884811	-2.6198556529
H50	5.7719176219	-0.5560682505	-2.3712783020
C51	6.7602008428	0.2990828686	0.0961606075
H52	7.8269468500	0.1870153541	-0.1316944112
H53	6.6723758467	0.7781255069	1.0778766894
H54	6.3277069557	-0.7045144865	0.1738358158
C55	2.0898095068	-2.9458820469	-0.4074953012
C56	2.7761499897	-3.9813830644	-0.3466069517
X57	2.4834136084#	-3.4494366013#	-0.4006262824#
C58	4.9931812253	-7.5181017624	0.3376842478
C59	3.6059788749	-7.5837219955	0.1778295647
C60	2.8744142685	-6.4240384780	-0.0586128034
C61	3.5318502221	-5.1813867376	-0.1360182896
C62	4.9298544482	-5.1227608707	0.0254963279
C63	5.6522168387	-6.2885703593	0.2622695155
H64	5.5610444015	-8.4258388170	0.5238025435
H65	3.0946872700	-8.5398688746	0.2404207418
H66	1.7955444595	-6.4655822120	-0.1800407394
H67	5.4325957649	-4.1615971131	-0.0264989547
H68	6.7300782883	-6.2391722676	0.3923509222
P70	2.3175723619	-3.0499645534	-4.9196205235
C71	0.1764219047	-6.6594194655	-6.8585401538
C72	-0.3210709591	-6.0850360513	-5.6862968268
C73	0.3423420803	-5.0099892688	-5.0999343204
C74	1.5071681063	-4.4947370273	-5.6919582371
C75	2.0045009552	-5.0749035830	-6.8670878774

C76	1.3376900248	-6.1562410289	-7.4447509590
H77	-0.3392730093	-7.5014444175	-7.3116256903
H78	-1.2233113719	-6.4779792590	-5.2260468416
H79	-0.0449346728	-4.5697675988	-4.1838966572
H80	2.9076047152	-4.6890874932	-7.3300529225
H81	1.7287564033	-6.6046122233	-8.3536816902
C82	6.5291916357	-2.7870001092	-6.8032649484
C83	6.3036421828	-3.5909505379	-5.6833276089
C84	5.0355329593	-3.6483142708	-5.1096506050
C85	3.9793776310	-2.9063862279	-5.6612760965
C86	4.2102706401	-2.0993806333	-6.7858122042
C87	5.4842387235	-2.0418573331	-7.3510232305
H88	7.5198102952	-2.7378793691	-7.2459181685
H89	7.1168535600	-4.1682844326	-5.2528751151
H90	4.8652612181	-4.2701834201	-4.2336136281
H91	3.4033783373	-1.5127928796	-7.2151376123
H92	5.6593100629	-1.4121260516	-8.2190643490
C93	0.0187987009	0.7477035084	-6.2219064963
C94	-0.2113971916	-0.4549862525	-6.8896619039
C95	0.4636289651	-1.6140546180	-6.5024935165
C96	1.3750469290	-1.5694634316	-5.4385105872
C97	1.5967587884	-0.3589488030	-4.7618758304
C98	0.9232722842	0.7946494735	-5.1585423830
H99	-0.5088086108	1.6475788603	-6.5266374943
H100	-0.9175310409	-0.4949998258	-7.7142910670
H101	0.2785054269	-2.5463704530	-7.0273860451
H102	2.2916262072	-0.3169724147	-3.9268466898
H103	1.1017625906	1.7288781244	-4.6338286575

Au(III) Conformer F

E = -2638.565983 Hartree

Au1	1.0700335686	-1.2814188770	0.0888975966
Au2	2.4050236648	-4.7585622055	-2.5924038742
C2	0.4641805343	1.4210956125	1.0194990743
C3	-0.3565141412	2.4966709936	1.3700090394
C4	-1.7403927685	2.3490351369	1.2891441851
C5	-2.3149877067	1.1503223409	0.8671737623
C6	-1.4777032205	0.0856748935	0.5240028139
N7	-0.1358535392	0.2712769584	0.6167455023
H8	0.0798050220	3.4315165502	1.6997670222
H9	-2.3817473341	3.1828756753	1.5598303006
H10	-3.3910883161	1.0427092144	0.8063845637
C11	4.7566987284	1.1435506773	0.9524298775
C12	3.9282823930	0.0545447537	0.5987635651
C13	2.5431499490	0.1433349721	0.6262217213
C14	1.9310364610	1.3637060114	1.0238153945
C15	2.7421433899	2.4452774671	1.3812792715
C16	4.1313408057	2.3343132141	1.3449331896
H17	4.3931500511	-0.8770873809	0.2948900650
H18	2.3003889258	3.3900293759	1.6870313498
H19	4.7243662401	3.1967938442	1.6263370553
C20	-2.4945982436	-3.9204815222	-0.6543040048
C21	-1.1541594925	-3.4766765004	-0.5855090474
C22	-0.8255532685	-2.1761965199	-0.2285925495
C23	-1.8664533133	-1.2572813582	0.0762542591
C24	-3.1970935586	-1.6758885209	-0.0183192413
C25	-3.5013386099	-2.9873608360	-0.3784784855
H26	-0.3561702662	-4.1815251226	-0.7972039501
H27	-4.0105528684	-0.9913423496	0.2049965070
H28	-4.5444048104	-3.2781398656	-0.4265328869
C29	2.2405580809	-2.7305934493	-0.4529813052
C30	2.9955476661	-3.6482378008	-0.9064592537
C31	-2.7967756983	-5.3901365993	-0.9976112990
C32	-4.3092075943	-5.6838164096	-1.0377192237
H33	-4.7887927267	-5.4914495661	-0.0705724431
H34	-4.8230574790	-5.0878487107	-1.8014406700
H35	-4.4724054279	-6.7398688037	-1.2802106058
C36	-2.1551374239	-6.3013311334	0.0782815252
H37	-2.5620291256	-6.0826291722	1.0722104632
H38	-2.3605009793	-7.3543545292	-0.1476980023
H39	-1.0678952907	-6.1763416140	0.1272593212
C40	-2.2006069781	-5.7311414944	-2.3847280255
H41	-2.4077426061	-6.7768930861	-2.6418013798
H42	-2.6350081456	-5.0986372952	-3.1680296739
H43	-1.1135701947	-5.5975481385	-2.4041170177
C44	6.2865009786	0.9839570205	0.8960116264
C45	7.0224236900	2.2846645504	1.2685238590
H46	6.7850496348	3.1005554753	0.5779386598
H47	6.7826213476	2.6121049353	2.2859913314
H48	8.1052390207	2.1220339829	1.2240604780
C49	6.7101577629	0.5833681555	-0.5391665351
H50	6.4060860178	1.3445541545	-1.2664619289
H51	7.8004811891	0.4807024329	-0.5940211098
H52	6.2726052634	-0.3719475068	-0.8472331103
C53	6.7216796946	-0.1205574116	1.8897962845
H54	7.8115735977	-0.2423910827	1.8606881197
H55	6.4381601220	0.1411541741	2.9166221196
H56	6.2725601172	-1.0904014822	1.6517513607
C57	6.7845346011	-4.4680945779	0.9730484508
C58	5.6396016578	-4.2841267118	1.7497761638
C59	4.4115416388	-4.0130994940	1.1448584417
C60	4.3196412630	-3.9218310539	-0.2538469400
C61	5.4710603545	-4.1196795258	-1.0290671397
C62	6.6956484363	-4.3828205641	-0.4167770024
H63	7.7378710729	-4.6842795687	1.4474109741
H64	5.6977872210	-4.3556593352	2.8323590029
H65	3.5191323842	-3.8927993215	1.7513659392
H66	5.4052198926	-4.0649803581	-2.1115533037
H67	7.5796219136	-4.5329055038	-1.0293641728
P69	2.0698266275	-6.1251350099	-4.4648724598
C70	-0.4081673619	-4.0767912289	-7.7937543224
C71	0.5837882169	-4.9977431396	-8.1373723407
C72	1.3451820147	-5.6129784577	-7.1442702365
C73	1.1143463976	-5.3102243012	-5.7927184361
C74	0.1217584081	-4.3771606855	-5.4530133227
C75	-0.6369180308	-3.7678114433	-6.4506911551
H76	-0.9952795087	-3.5960114272	-8.5706184864
H77	0.7711310561	-5.2354523483	-9.1812394615
H78	2.1211190426	-6.3202192507	-7.4225868562
H79	-0.0551989671	-4.1237272870	-4.4105928603
H80	-1.4004668641	-3.0445591632	-6.1784707357
C81	6.1698500673	-7.2332876305	-6.3156997079
C82	5.8541442839	-5.9042555427	-6.0186972875
C83	4.6194907446	-5.5870624458	-5.4579894479
C84	3.6796973300	-6.5989865511	-5.1991473005
C85	3.9995972313	-7.9303160347	-5.4998202816
C86	5.2423990042	-8.2414672545	-6.0551377406
H87	7.1358435238	-7.4800317666	-6.7461113217
H88	6.5725292783	-5.1146198437	-6.2196534422
H89	4.3833606494	-4.5509783181	-5.2272388782
H90	3.2865415119	-8.7245463013	-5.3016465410
H91	5.4828264108	-9.2761451365	-6.2821207203
C92	-0.0184656606	-10.0996187125	-3.3314863023
C93	-0.3608366213	-9.4598134156	-4.5244791882
C94	0.2486365908	-8.2551438964	-4.8785508319
C95	1.2092606651	-7.6809067720	-4.0331644464
C96	1.5438036852	-8.3236914613	-2.8286789487
C97	0.9354777992	-9.5288608731	-2.4844009844
H98	-0.4947108315	-11.0372930495	-3.0604188695
H99	-1.1047127881	-9.8973160602	-5.1848821310
H100	-0.0258824081	-7.7669221103	-5.8094036763
H101	2.2802643292	-7.8825218391	-2.1603712312
H102	1.2037082269	-10.0194975707	-1.5522448967

[6]+ closer to XRD

B3LYP

E = -3069.22660529578 Hartrees

Au1	6.2837072249	5.4162773148	6.4136508527
Au2	6.6698793705	5.8960765430	1.6565670252
Au3	8.4025749961	4.0603248387	4.0693309746
C4	4.3379547518	3.1313007957	-1.6770748045
C5	8.4826535193	8.5114425126	9.5357884979
C6	5.6210299150	2.6784941815	-1.3393230822
C7	2.4960067122	8.0363103617	0.9165265544
C8	7.2320618357	8.7332336609	8.9642758722
C9	9.2087408306	7.3446239956	9.2594120276
C10	6.8305419163	10.0960850463	4.2138118611
C11	3.8575146065	6.9501749231	5.8999284876
C12	2.3957900481	4.3117890833	3.6203647413
C13	10.5820129809	7.0637516544	9.8922047493
C14	7.4944297334	3.8593989806	6.0898511443
C15	3.8000963249	4.2770282059	-1.0960076730

C16	9.6199344602	4.6993551771	2.2318782492
C17	3.1364337027	1.9179586568	3.0606174971
C18	6.3465355030	3.4155296393	-0.3717300343
C19	4.6262420801	7.9502552488	2.0305914592
C20	2.9687541354	8.0214554636	6.0322761904
C21	4.5348907779	5.0039768324	-0.1536781786
C22	9.3491289893	9.9812013720	4.7232680957
C23	11.6137173780	4.1903237058	0.8929139791
C24	5.8353229044	4.5616578081	0.2272765815
C25	6.6747779154	7.7940884621	8.0910999263
C26	4.7093962277	4.7605049983	5.1463526203
C27	3.3618736677	3.2973730517	3.7040626929
C28	5.7342391633	8.3995002674	2.8785573532
C29	6.2457335682	1.4281479939	-1.9839689920
C30	2.7956181829	6.8604269306	0.2314667535
C31	3.6932871641	5.7444774329	5.0810205441
N32	4.8801127002	6.8094616677	1.3413786789
C33	8.8768186876	0.9905553193	7.4246790276
C34	8.0419032446	9.3923074637	4.1652072692
C35	7.3906933845	6.6010272770	7.7827444589
C36	11.0351626903	4.4499514545	2.1494216116
C37	4.0253819255	6.2334672903	0.4609707110
C38	6.9231703216	7.6228640602	2.8758488048
N39	5.0048242010	6.9812856893	6.6225951815
C40	2.5522373382	5.5125239617	4.3062957420
C41	3.2951001148	9.0707122722	6.8901923962
C42	8.0373195552	2.7446954604	5.9413704926
C43	4.4922402369	9.0682439790	7.6028234155
C44	5.3685415082	7.9877200737	7.4542636984
C45	5.6923597364	9.6115271145	3.5756240167
C46	8.5815455229	1.4259536206	6.1189575985
C47	11.8503720335	4.4846651085	3.2952622980
C48	9.3438108426	-0.3026342332	7.6348900641
C49	8.7651916014	0.5500623833	5.0347880561
C50	12.9850967043	3.9768008884	0.7919203946
C51	9.2411066685	-0.7384175612	5.2566703901
C52	8.4257261688	5.0248116470	2.0566685575
C53	13.2189399172	4.2623314692	3.1829964440
X54	8.1697595000#	3.9983050000#	6.1974750000#
X55	8.6241420000#	4.3226030000#	1.8992395000#
H56	3.7432982367	2.5971601575	-2.4082768663
H57	8.8841428398	9.2633284218	10.2049194688
H58	1.5461995925	8.5327878958	0.7360316176
H59	6.6982291885	9.6489839895	9.2073896124
H60	6.7719197662	11.0536129018	4.7182782102
H61	1.4942460199	4.1638788423	3.0372886031
H62	1.0699201032	2.2189210715	2.3485318186
H63	2.3184257637	2.6800535222	1.1688846431
H64	9.2995918537	8.8475696065	6.6005433510
H65	10.1992639551	8.0337927343	5.3113555055
H66	2.8075093095	4.6028880179	-1.3975489644
H67	7.3385960812	3.0763740093	-0.0876425989
H68	2.0355185313	8.0274543239	5.4817784096
H69	10.9846178887	4.1626208878	0.0087183186
H70	2.0911984266	6.4388465920	-0.4756881974
H71	8.7272850157	1.6669401020	8.2604249923
H72	1.7666629633	6.2604175850	4.2409287783
H73	2.6062148065	9.9035587261	7.0043816877
H74	4.7426577260	9.8884906668	8.2649956363
H75	5.2213260595	1.2015910301	3.1791755657
H76	4.8355932115	2.0666842813	1.6804262972
H77	4.7853293536	10.2093468841	3.5940791682
H78	11.4033980980	4.6903565462	4.2641728090
H79	10.5648679023	9.2532457229	3.0328698164
H80	9.9148621932	10.8845845602	2.8038259668
H81	9.5631128611	-0.6354582501	8.6455072750
H82	8.5261695840	0.8851843631	4.0290381622
H83	13.4264656560	3.7808398729	-0.1811643889
H84	9.3814485172	-1.4114162896	4.4156214490
H85	13.8422499755	4.2895940037	4.0723095223
C86	9.5292236847	-1.1677695053	6.5540834590
H87	9.8952294426	-2.1764673643	6.7233635886
C88	13.7891168550	4.0088377200	1.9336689988
H89	14.8584119139	3.8361866369	1.8495959891
C90	6.5552992508	0.3853974148	-0.8824466672
H91	7.2536801006	0.7751792003	-0.1337226543
H92	5.6401223982	0.0805819371	-0.3615823043
H93	7.0065854928	-0.5103436249	-1.3259327858
C94	7.5565465115	1.8279108828	-2.7041684719
H95	8.2887935308	2.2593445196	-2.0131999568
H96	8.0155942158	0.9475850535	-3.1698640140
H97	7.3631327596	2.5652293180	-3.4920823380
C98	5.3097970450	0.7741485826	-3.0197062593
H99	5.7974731663	-0.1066995074	-3.4516470817
H100	4.3683942866	0.4389903887	-2.5687493051
H101	5.0719213384	1.4552265748	-3.8450142104
C102	3.3988391611	8.5888438523	1.8234710742
H103	3.1650831444	9.5097155310	2.3429330538
C104	4.4397009901	1.3764052055	2.4323943458
H105	4.2423493148	0.4152641370	1.9428301181
C106	2.0599598033	1.9618289246	1.9559228023
H107	1.9713881572	0.9739740938	1.4906238076
C108	2.6621929657	0.9504710032	4.1737852312
H109	2.4879635024	-0.0500296683	3.7596811110
H110	3.4077388719	0.8627941967	4.9721093375
H111	1.7262003087	1.2986632724	4.6254867926
C112	4.5216407253	3.5593594748	4.4698573063
H113	5.2845449082	2.7926743220	4.5496910474
C114	8.6315510885	6.4018787630	8.3756150955
H115	9.1796090575	5.4927806348	8.1459022221
C116	11.0663031684	8.2293329752	10.7770753333
H117	11.1679547803	9.1604037092	10.2071314467
H118	10.3892779129	8.4144443865	11.6190133060
H119	12.0503352552	7.9907459307	11.1953258470
C120	10.4749119664	5.7949974394	10.7734925313
H121	11.4430850656	5.5708758076	11.2370225493
H122	9.7401389117	5.9352127393	11.5747259173
H123	10.1714854105	4.9188457024	10.1901964827
C124	11.6314106339	6.8359100883	8.7776443469
H125	12.6128900992	6.6302038014	9.2210467338
H126	11.3723160207	5.9869657353	8.1355153045
H127	11.7274940512	7.7224172276	8.1399620689
C128	8.0474447937	8.1329602015	3.5173200954
H129	8.9712088640	7.5629936335	3.4862798317
C130	9.1320385947	11.3401426845	5.4176081891
H131	8.4448055973	11.2588250737	6.2681415110
H132	10.0879142848	11.7147047543	5.8000623161
H133	8.7390456028	12.0961202427	4.7277273227
C134	10.3324386847	10.1932119926	3.5450479743
H135	11.2748349451	10.6179749769	3.9110783260
C136	9.9722732962	9.0102221133	5.7521992132
H137	10.9122751888	9.4250281212	6.1368092504

[6]+ perpendicular

E = -3069.233881

Au1	-2.8593463638	-0.4777246600	1.0060490772
Au2	2.9018576196	-0.4413715044	-1.0398162273
Au3	0.0122983081	1.3184120899	-0.0178887318
C4	6.4352356859	2.1047036511	1.2212218777
C5	-6.3532689619	2.1092572504	-1.2673416503
C6	5.3593511325	2.8763373021	0.7639311086
C7	6.2169364163	-3.6404962768	0.0835644295
C8	-6.4154920459	0.7343297086	-1.0526216150
C9	-5.2659317151	2.8665216045	-0.8118310390
C10	1.1465626744	-4.7364712856	-2.6492344958
C11	-4.0686782528	-3.1297761384	0.8489319742
C12	-1.1219398108	-4.8065065691	2.5402808200
C13	-5.1796127364	4.3905410223	-1.0062050491
C14	-1.4591668132	0.8429622543	1.5269891425
C15	6.4735967162	0.7271216059	1.0168565551
C16	0.7025109987	1.6007546703	-2.1953604631
C17	1.1107722101	-3.8664128103	3.4262128050
C18	4.3026853512	2.2061804607	0.1037992520
C19	4.0904197004	-3.1042565803	-0.9070576005
C20	-5.0514796292	-4.0684599792	0.5210699444
C21	5.4293428389	0.0781799986	0.3516577994
C22	-1.0779573836	-3.7710545646	-3.5314153035
C23	0.5909763205	3.4646067673	-3.7951998084
C24	4.3135069986	0.8335027323	-0.1094841230
C25	-5.3825162384	0.0724352206	-0.3821317350
C26	-1.9441329751	-2.2396721002	1.7478520506
C27	-0.2736447758	-3.7164188185	2.7723719717

C28	2.8102832552	-3.3219797183	-1.5938272909
C29	5.3057963131	4.4026968839	0.9466626255
C30	6.4098770840	-2.3028679629	0.4268274145
C31	-2.7844324938	-3.3664251668	1.5210916556
N32	4.3193897497	-1.8139765135	-0.5535161390
C33	-0.7222809904	3.4464910217	3.7891018310
C34	0.3056731406	-3.6377272649	-2.8700183978
C35	-4.2572830398	0.8136659633	0.0788712825
C36	-0.0130455264	2.3443638222	-3.1973880071
C37	5.4255365325	-1.3674696110	0.0929025651
C38	1.9810913687	-2.1855479859	-1.8140590593
N39	-4.2894436139	-1.8339152298	0.5119334985
C40	-2.3612278999	-4.6359380684	1.9274444284
C41	-6.2052754473	-3.6394514871	-0.1326640595
C42	-0.6950293409	1.6141143879	2.1464196775
C43	-6.3878516863	-2.2980336041	-0.4647409716
C44	-5.3937754527	-1.3741523937	-0.1281542872
C45	2.3817155778	-4.5826877367	-2.0225972017
C46	-0.0208478853	2.4211463020	3.1285055850
C47	-1.2837841254	1.9232637265	-3.6278837024
C48	-0.1004920741	4.1677746206	4.8042373337
C49	1.3095146950	2.1395485783	3.4906615720
C50	-0.0644759227	4.1417431067	-4.8181874705
C51	1.9202780164	2.8662269461	4.5072155996
C52	1.5037046108	0.8828404811	-1.5612591583
C53	-1.9304324121	2.6085701295	-4.6508413048
H54	7.2651171790	2.5722850641	1.7387283880
H55	-7.1733058272	2.5860585845	-1.7913156925
H56	6.9777863293	-4.3730160695	0.3386344411
H57	-7.2808141117	0.1863932242	-1.4161380817
H58	0.8445729843	-5.7313967362	-2.9569478444
H59	-0.8247968084	-5.8067541012	2.8335238222
H60	0.7327893263	-5.7641540054	4.4742049378
H61	1.4593621885	-5.9658349650	2.8662931169
H62	-2.1576986684	-3.8263543402	-1.6218759286
H63	-1.9995921953	-2.1950715651	-2.2857868854
H64	7.3307788924	0.1674259619	1.3816534753
H65	3.4557062522	2.7834400058	-0.2550522595
H66	-4.9139963057	-5.1134274620	0.7726428175
H67	1.5749854708	3.7813623302	-3.4630263370
H68	7.3096645264	-1.9885012473	0.9428581523
H69	-1.7522359380	3.6542520541	3.5139586115
H70	-2.9913517808	-5.5073694003	1.7670918126
H71	-6.9745756962	-4.3626872966	-0.3884111350
H72	-7.2865920922	-1.9720251897	-0.9747544753
H73	2.0377116973	-2.2790077940	2.2020891037
H74	2.1845868247	-3.9013813356	1.5133918271
H75	3.0032856696	-5.4611657068	-1.8685053422
H76	-1.7475335216	1.0572750423	-3.1647683040
H77	-0.9075125847	-1.8764570885	-4.6535525591
H78	-0.3556670971	-3.3009938572	-5.5492471388
H79	-0.6481120358	4.9528090781	5.3178050397
H80	1.8490120781	1.3487858397	2.9768303218
H81	0.4088677439	5.0007237131	-5.2841273866
H82	2.9442041333	2.6379868252	4.7910302525
H83	-2.9075585756	2.2744769405	-4.9879036204
C84	1.2179263260	3.8795180767	5.1655465758
H85	1.6973180018	4.4427590122	5.9616721775
C86	-1.3230087010	3.7159533449	-5.2471285081
H87	-1.8301702775	4.2462289830	-6.0481425008
C88	4.0185529277	4.7870339454	1.7138935907
H89	3.1119847584	4.4732494926	1.1840825960
H90	3.9980226816	4.3258579358	2.7078903941
H91	3.9673182720	5.8750497979	1.8441900571
C92	5.2979338500	5.0745343918	-0.4489149171
H93	4.4401496603	4.7535423145	-1.0509078831
H94	5.2468815785	6.1652132606	-0.3457664251
H95	6.2085009209	4.8303793052	-1.0071604266
C96	6.5169053396	4.9393767380	1.7355649832
H97	6.4332129459	6.0256227339	1.8472273513
H98	6.5722547636	4.5080158899	2.7422503672
H99	7.4635430559	4.7369363707	1.2233510609
C100	5.0641873577	-4.0537527239	-0.5830146798
H101	4.9215550205	-5.0951015021	-0.8480435453
C102	2.1909996501	-3.3343688458	2.4518778950
H103	3.1850631165	-3.4325360658	2.9055445469
C104	1.4460136579	-5.3335623656	3.7621976643
H105	2.4391128230	-5.3908984707	4.2214991546
C106	1.1488930132	-3.0510480513	4.7417072248
H107	2.1305547744	-3.1484395081	5.2212240235
H108	0.9631674650	-1.9847736284	4.5697855538
H109	0.3939750752	-3.4133856070	5.4484773513
C110	-0.7192597552	-2.4368222314	2.3699864241
H111	-0.0786053311	-1.5780497948	2.5460104549
C112	-4.2255452193	2.1847751654	-0.1392950879
H113	-3.3724742006	2.7519360345	0.2211784347
C114	-6.3641126736	4.9438180950	-1.8215631700
H115	-6.4111616375	4.5017077335	-2.8244376735
H116	-7.3230096783	4.7665247264	-1.3234334156
H117	-6.2543309846	6.0271993524	-1.9440630407
C118	-5.1825963973	5.0724529169	0.3848431847
H119	-5.1177739853	6.1617843808	0.2746195377
H120	-6.1017333718	4.8415050292	0.9341176215
H121	-4.3356364753	4.7473050028	0.9991301991
C122	-3.8731874212	4.7485220978	-1.7519225790
H123	-3.8043182789	5.8343367499	-1.8912550448
H124	-2.9824802890	4.4289604469	-1.2001557653
H125	-3.8400559510	4.2774161288	-2.7411354400
C126	0.7586643378	-2.3661538316	-2.4475874427
H127	0.1271030811	-1.4995258649	-2.6185443562
C128	-1.4203700764	-5.2326898268	-3.8869190428
H129	-1.4356003783	-5.8783474982	-2.9999934043
H130	-2.4147349484	-5.2799800603	-4.3466524424
H131	-0.7092012795	-5.6565930251	-4.6056841396
C132	-1.1065620833	-2.9384098921	-4.8372414981
H133	-2.0906958274	-3.0169496751	-5.3170315598
C134	-2.1582984075	-3.2456572145	-2.5521340994
H135	-3.1529222996	-3.3295594432	-3.0082811898

S5.3. BP86 (Gaussian)

C_6H_6

E = -232.2333854 H.

C	-0.1711785425	2.5825987789	0.0000001473
C	-0.8735689361	3.7994390132	-0.000000142
C	-2.2785553989	3.7993891	-0.0000004249
C	-2.9809790041	2.5825262091	-0.0000001524
C	-2.2786009395	1.3656955808	-0.0000001055
C	-0.8735948854	1.3657458019	-0.0000005032
H	0.9249722503	2.5825501814	-0.0000000687
H	-0.325381034	4.7486562968	-0.0000002445
H	-2.826728841	4.7486114411	-0.0000000182
H	-4.0771312134	2.5825579804	-0.0000000726
H	-2.8267578191	0.4164636769	-0.0000000881
H	-0.3254396238	0.4165153348	-0.0000001507

CH_2Cl_2

E = -959.7460564 H

Cl	2.3360953437	-3.7732874685	-0.0907008689
H	1.2892402456	-2.5534200741	1.6600763184
H	0.252474505	-2.6610494811	0.1750355766
C	1.2641225716	-2.4893743293	0.5646458587
Cl	1.763828994	-0.8282213797	0.0953623132

G

$[Au(PPh_3)(C_6H_6]^+$

E= -1404.2549281 H

Au	2.3953151073	-3.6878294956	-2.5122837776
P	2.1193271038	-3.3171177717	-4.7773085447
C	1.5398353921	-7.3032319667	-7.0826909139
C	0.9133962302	-7.1062366161	-5.8393337185
C	1.1064502264	-5.9078882364	-5.1382889515
C	1.9241840817	-4.8946506241	-5.6876570147
C	2.5520052073	-5.0935151184	-6.9355996095
C	2.3562254095	-6.299558619	-7.6279195553
H	1.3939690178	-8.2436030075	-7.6244988523
H	0.2795310498	-7.8901470213	-5.411860094
H	0.6219066945	-5.7565765166	-4.1659983909
H	3.1919548605	-4.3143284569	-7.3625003621
H	2.8468587489	-6.4535533155	-8.5945966411
C	5.8265702517	-1.1945458239	-6.5927029669

C	5.9902566232	-2.2366822185	-5.6630954399
C	4.8668575823	-2.8611619988	-5.1041772598
C	3.5694431722	-2.4478412058	-5.4834328091
C	3.4065688545	-1.4014651028	-6.4154620712
C	4.5386609866	-0.7786990515	-6.9660218691
H	6.7056854329	-0.7034897012	-7.0229354041
H	6.9942301261	-2.5596113809	-5.3684906786
H	4.9963045617	-3.6711303123	-4.3760728684
H	2.404002625	-1.0718553553	-6.7069925516
H	4.4102795538	0.0350973493	-7.6872758841
C	-1.5836656689	-0.6561444623	-5.6413901324
C	-1.2979594157	-1.7425046113	-6.4837814307
C	-0.1889890789	-2.5643416392	-6.2259428703
C	0.6375322907	-2.2947328433	-5.114398863
C	0.3453251643	-1.2041131416	-4.26476841
C	-0.7610501735	-0.3863139812	-4.5335278974
H	-2.4514923869	-0.0200787176	-5.8448992845
H	-1.9400737948	-1.9557624232	-7.3446671532
H	0.0285862566	-3.4132860181	-6.8824593803
H	0.9829654495	-0.9974292111	-3.3966641916
H	-0.9854738038	0.4586770903	-3.8741708649
C	0.9427052183	-4.4768442345	0.1080744874
C	0.5487253741	-3.2311490323	0.6075280374
C	1.4676984761	-2.158715379	0.6686623944
C	2.7855450282	-2.3261802249	0.2302904873
C	3.2118324048	-3.5884206614	-0.2700364228
C	2.2812881293	-4.673740765	-0.3315668824
H	0.2383462644	-5.314322181	0.0822659006
H	-0.4757107728	-3.0885086593	0.9667646099
H	1.1487707207	-1.1940324243	1.0768435785
H	3.5048571263	-1.5039959311	0.29942715
H	4.2764976874	-3.7694439586	-0.4593176667
H	2.6343300661	-5.6838398475	-0.5706955321

$[Au(PPh_3)(CH_2C_{l2})]^+$

E= -2131.7505911 H

Au	2.0518650573	-3.5582938873	-2.4666621074
P	2.0759132388	-3.2647150509	-4.7383489645
C	1.7662669517	-7.3469688732	-6.9136612904
C	0.9776149851	-7.0903637833	-5.7780801381
C	1.0865381476	-5.8630171194	-5.1102573296
C	1.9863046555	-4.8820557396	-5.5860507327
C	2.7790387073	-5.1407729608	-6.7250702622
C	2.6638730655	-6.37508413	-7.3841959485
H	1.6840229267	-8.3097462882	-7.428697529
H	0.281915249	-7.8501849357	-5.4073268367
H	0.4751317204	-5.6669582849	-4.2211504836
H	3.4830705853	-4.3872936071	-7.0929496993
H	3.2814669432	-6.5759482236	-8.2656765793
C	5.9849240436	-1.1920628119	-6.1185217065
C	6.0167543106	-2.1303802965	-5.0719649182
C	4.8310883593	-2.7413418178	-4.6411759552
C	3.6059320196	-2.4157909168	-5.2658513837
C	3.5743403429	-1.4726871616	-6.3161017941
C	4.7675961894	-0.8652570667	-6.7379816661
H	6.911578357	-0.7105977083	-6.4479736039
H	6.9647683606	-2.3812386915	-4.585067861
H	4.8552693425	-3.4676101742	-3.8196624732
H	2.6260137814	-1.2116490886	-6.7971123384
H	4.7426041611	-0.1316359525	-7.5503921154
C	-1.4900604563	-0.6286099775	-6.0940462755
C	-1.2010238743	-1.8132253773	-6.7897876834
C	-0.1322093022	-2.6291199253	-6.3844108593
C	0.650202461	-2.2508589414	-5.27298865
C	0.356697382	-1.0592618032	-4.5710655567
C	-0.7098148116	-0.2509202252	-4.9864527721
H	-2.3271222771	0.0015683632	-6.4121923049
H	-1.8088448845	-2.1082860216	-7.6513498185
H	0.0892819201	-3.5528987593	-6.9282713723
H	0.9623482407	-0.7646307705	-3.7055210187
H	-0.9360845129	0.6718883829	-4.4422363064
Cl	2.0503236617	-3.9983241678	-0.0049085765
H	1.8006556676	-2.6168669884	1.9102289256
H	0.5195103828	-2.2660993678	0.6529163517
C	1.588241269	-2.4111935928	0.8528349708
Cl	2.5179434271	-1.0267903723	0.2910329052

$[Au(PPh_3)_2]^+$

E= -2208.3514851 H

Au	2.4484337841	-3.1966132294	-2.7721852507
P	2.5386270129	-2.8454222333	-5.1024828814
C	2.7256033761	-6.8597536726	-7.4364403836
C	1.9361690504	-6.7444675967	-6.2791534252
C	1.8980131539	-5.5337313177	-5.5727826062
C	2.6461239434	-4.4252904931	-6.0296988796
C	3.4392407925	-4.5445460349	-7.1906645801
C	3.4757354847	-5.7622276684	-7.8890936588
H	2.7595792955	-7.8082253663	-7.9828588559
H	1.3545789941	-7.600749161	-5.9214920433
H	1.2869527127	-5.4473377002	-4.6657894565
H	4.0307198748	-3.693225217	-7.5437432512
H	4.0948325769	-5.8517935002	-8.7879965633
C	6.2826939223	-0.3718398417	-6.3128111556
C	6.3671915265	-1.3457782508	-5.3027692259
C	5.2282050891	-2.0758226742	-4.934244515
C	3.9963347893	-1.8394607686	-5.5852650822
C	3.9140390738	-0.8604346745	-6.5977739749
C	5.0585113111	-0.1300900354	-6.9569583332
H	7.1717130558	0.2023159973	-6.5944604507
H	7.3199057429	-1.5326449628	-4.7959965957
H	5.2946292991	-2.831406612	-4.1417590864
H	2.9600977884	-0.6652024219	-7.0988413033
H	4.9902141953	0.6310821897	-7.7413617142
C	-1.2016595041	-0.5333556304	-6.6065487355
C	-0.6674931783	-1.5671610351	-7.3927083163
C	0.4563545444	-2.283552959	-6.9502312067
C	1.0490799271	-1.9626284589	-5.7106750891
C	0.5051387901	-0.9262290971	-4.9188515112
C	-0.6140318045	-0.2124350284	-5.370622274
H	-2.0800009725	0.0204549081	-6.9545931981
H	-1.1265949157	-1.8210914372	-8.3539945316
H	0.8659362729	-3.0929205986	-7.5638636104
H	0.95873198	-0.6792303041	-3.9510088197
H	-1.0319175144	0.5902332654	-4.7537842343
P	2.357261967	-3.5373326805	-0.4402472868
C	2.3112085281	0.5011291886	1.8589894704
C	1.519391818	-0.5635308407	2.3189473125
C	1.5126765934	-1.7881935045	1.631693337
C	2.3042689287	-1.9472950147	0.4745421498
C	3.0943163033	-0.8715031525	0.0100483507
C	3.0992146854	0.3461352956	0.7053370429
H	2.3109040476	1.4551086584	2.396813922
H	0.9014457185	-0.4428916224	3.2150022418
H	0.8895949008	-2.6140952576	1.9908050183
H	3.7039205172	-0.9884305827	-0.8944770103
H	3.713119627	1.1770143464	0.341835199
C	-1.4559713703	-5.8860294086	0.8016209129
C	-1.5110909288	-4.9299854094	-0.2273198337
C	-0.3517891434	-4.237657901	-0.6052883138
C	0.8710788355	-4.4939585645	0.0549609821
C	0.9238565873	-5.4552532536	1.0863608699
C	-0.2408105313	-6.147829692	1.4550591126
H	-2.3608682044	-6.4309804885	1.0906332203
H	-2.4566439989	-4.7280824396	-0.7416534846
H	-0.394893194	-3.4968071972	-1.4131498949
H	1.8706620596	-5.6662125383	1.5946023017
H	-0.1954423395	-6.8954207645	2.2540438396
C	6.0293643745	-5.9525593939	1.0689905407
C	5.5324310743	-4.8946785662	1.8474476245
C	4.4296804259	-4.1471457466	1.4033757813
C	3.8206289203	-4.4612608265	0.1700489958
C	4.3271090711	-5.522256251	-0.6140624431
C	5.425406127	-6.2667935271	-0.1607834735
H	6.8915420851	-6.5305231314	1.4182040019
H	6.0043705947	-4.6462166593	2.8039345511
H	4.0491886249	-3.3192433945	2.0109594151
H	3.8608582417	-5.7641486767	-1.5771407241
H	5.8145355573	-7.0882248826	-0.7716808332

HCCPh

E = -308.3751624 H

C	0.5748477034	-0.0001063555	-0.000353669

C	-0.6479247868	0.0000821925	-0.0000626348
H	-1.7222533113	0.0001522026	0.0005975893
C	4.8302854027	-0.0000162879	0.0001063058
C	4.1253374484	-1.2158501494	0.0000341229
C	2.7248894696	-1.2214898812	-0.0001084997
C	2.004833905	-0.0000733831	-0.0001888055
C	2.7248395507	1.2213713482	-0.0001076459
C	4.1252878196	1.2157897205	0.0000339752
H	5.9259222122	0.0000065137	0.0002190146
H	4.6702326751	-2.1665361372	0.0000905398
H	2.1708891851	-2.1656745869	-0.0001660048
H	2.1708023334	2.1655349431	-0.0001631262
H	4.6701434751	2.1664983478	0.0000892803

E (M^1 = H, L = PPh_3)
E = -1480.4130364 H

Au	-0.1231081594	-0.972769114	-0.0950085088
C	0.7852916233	1.5833418386	0.0314614684
C	-0.2934045043	1.1163355993	-0.4335855771
H	-1.2052373274	1.4632344149	-0.9180522163
P	-0.2669403541	-3.2911870593	0.1137412434
C	-2.2278277852	-4.5436344504	4.1309587737
C	-2.6607487983	-3.3858263827	3.4616201568
C	-2.0520096541	-3.0017750344	2.2584284472
C	-1.0089018353	-3.7845564948	1.7150553001
C	-0.573923517	-4.9457093347	2.3897763958
C	-1.1868674862	-5.3201362513	3.5961436401
H	-2.6998119659	-4.8377451263	5.0743488521
H	-3.4684764564	-2.7766741948	3.8806688681
H	-2.3833336999	-2.0931235859	1.7412519429
H	0.2417139478	-5.5496664641	1.978453617
H	-0.846452	-6.2198480091	4.1193763806
C	3.8905077023	-5.352812313	-0.0876995181
C	3.7079840532	-4.1953796364	0.6896762287
C	2.4552287578	-3.5682084716	0.7323709496
C	1.372292014	-4.106035616	0.0005579359
C	1.5576378204	-5.2665456404	-0.7799115746
C	2.8177817766	-5.8850908436	-0.8204343442
H	4.8719639935	-5.8371778505	-0.1244291151
H	4.5445417397	-3.7772922772	1.2594746579
H	2.3160476905	-2.6627513246	1.3354592958
H	0.7246104189	-5.684043705	-1.3545759312
H	2.9586627743	-6.7850602132	-1.4281617665
C	-2.8554083087	-5.0481065282	-3.3179615198
C	-2.9959380652	-5.5557165395	-2.0162731169
C	-2.2281151426	-5.0289952958	-0.9651588895
C	-1.3143792483	-3.9847757538	-1.2212924033
C	-1.1774643492	-3.472817923	-2.5315067919
C	-1.9445600342	-4.0086647512	-3.5754717178
H	-3.4594665321	-5.4595033896	-4.1334734537
H	-3.7073934729	-6.3631691778	-1.8139733084
H	-2.3430701796	-5.425419359	0.0490163185
H	-0.4719204747	-2.6573402604	-2.7323361328
H	-1.8366635625	-3.6092507385	-4.5893498638
C	4.410875734	3.0457560737	1.5991024826
C	4.3427137139	2.6622744281	0.2452263108
C	3.1498462323	2.1618179448	-0.2792992136
C	2.0054634759	2.0419586764	0.5636107333
C	2.0840969121	2.4334429647	1.9329015048
C	3.2857818481	2.9316035359	2.4392412714
H	5.3495402995	3.4397915828	2.0029742353
H	5.2231663645	2.7593203324	-0.3975367672
H	3.0757366089	1.8640379173	-1.3296747766
H	1.1978367621	2.342451423	2.568308087
H	3.3513108591	3.2362762989	3.4883524505

H (M^1 = H)
E = -752.4712878 H

H	8.845115646769	4.229220185872	6.643635529083
H	7.046460681919	5.384754670680	1.895556025093
Au	8.272137737222	3.879970243056	3.920642703069
C	8.439742787890	3.480784130647	5.963926755983
C	8.962276290044	4.362129486471	1.448311504843
C	11.309336296004	4.695049335083	0.819353701217
C	8.290190058685	-0.125159124280	5.854721301702
C	10.118375146449	3.909688994413	0.784689571080
C	7.964190333155	2.305129449690	5.983301974251
C	7.427676346872	1.003770702767	5.986976891644
C	10.083981287745	2.695580956727	0.036015567608
C	7.752365147579	-1.411611824065	5.912447304834
C	6.025915003466	0.814591037271	6.175916335047
C	12.436642679266	4.266444945461	0.117084090385
C	5.507553410354	-0.480051494478	6.229590920955
C	7.930990682004	4.771486467756	2.062640872409
C	11.221500848240	2.284965514464	-0.660434760984
H	11.321998478069	5.627220606443	1.392333456338
H	9.364389706048	0.032389533224	5.717681429945
H	9.162665672606	2.105617145370	0.010897965086
H	8.408569906583	-2.282156321664	5.816567070701
H	5.375152089397	1.687918907287	6.281828315321
H	13.352342684162	4.865293421917	0.137757095139
H	4.433822918427	-0.631960385299	6.376476258671
H	11.200800557813	1.357314715881	-1.240676592327
C	6.366787279573	-1.588907414529	6.098091538915
H	5.952831885249	-2.601814320347	6.143033586968
C	12.393527525859	3.066224860332	-0.619623486301
H	13.281647190509	2.737347301776	-1.169569729368

[**4**] Au(CNC)CCPh
E = -1467.3354325 H

Au	1.0659343318	-1.1457142517	-0.1610716299
C	0.7380452963	1.7567488529	0.1173347784
C	0.0271903546	2.95924157	0.2991570842
C	-1.3663015424	2.9094547968	0.4561443869
C	-2.0572599437	1.6883612728	0.4348744649
C	-1.3311977982	0.495135803	0.2520998038
N	0.0241475685	0.5912139137	0.1033463845
H	0.5573256946	3.914934916	0.3170480088
H	-1.9251002144	3.8411167435	0.5979302534
H	-3.1429415276	1.6589077528	0.557926696
C	4.9663079386	1.0639583574	-0.4291893347
C	4.0242361495	0.0031072735	-0.4080530793
C	2.6555519924	0.2211647021	-0.2316406436
C	2.1873550338	1.5675856464	-0.0659613942
C	3.111338556	2.6304784839	-0.0848196417
C	4.4785116464	2.3780164383	-0.2639096003
H	4.3686866414	-1.0296431573	-0.5334371139
H	2.7738574794	3.6669209211	0.040081901
H	5.1686707288	3.226513951	-0.2734916776
C	-2.6865095296	-3.6020150479	0.0695093235
C	-1.3171510761	-3.2535556648	-0.0600581701
C	-0.8729961507	-1.930187548	-0.0018195226
C	-1.8381879489	-0.8867911218	0.1962711759
C	-3.2009346669	-1.2181502713	0.3264999466
C	-3.6141668994	-2.5561496504	0.2634825617
H	-0.5700063037	-4.040774707	-0.2117212393
H	-3.9545605408	-0.4354388847	0.4785482034
H	-4.6799985981	-2.7783032547	0.3684129639
C	-3.10670895	-5.0838065061	-0.0046141408
C	-4.6310678234	-5.275537296	0.1559062006
H	-4.9923211779	-4.90692576	1.1332138094
H	-5.1976134272	-4.7599724966	-0.6407909012
H	-4.8776375664	-6.3508996635	0.0953613804
C	-2.3954894876	-5.8729890665	1.1275720229
H	-2.6879976367	-5.4887624078	2.1213957353
H	-2.6719265285	-6.9426850955	1.0777979351
H	-1.2968092999	-5.8025747965	1.0499730888
C	-2.6858332077	-5.6651416083	-1.3813529817
H	-2.9638352793	-6.7337220003	-1.4445640702
H	-3.1888878015	-5.1301778314	-2.2069594377
H	-1.5970676279	-5.5876392097	-1.5446353586
C	6.46301553	0.7509290175	-0.6283079888
C	7.3394250591	2.0229698302	-0.6243130329
H	7.0639392667	2.7160171315	-1.4399725462
H	7.2692108283	2.5690091398	0.3340291777
H	8.3984970697	1.7436734959	-0.7700046145
C	6.656850396	0.0311820534	-1.9902511892
H	6.3326452794	0.6752001843	-2.8275131021
H	7.723912721	-0.2173043047	-2.1411720153
H	6.0789373307	-0.9074940027	-2.0448617812
C	6.9471752789	-0.1767127037	0.5186695093
H	8.0157920808	-0.426310101	0.3811789703

H	6.8335163448	0.3165434083	1.5008389313
H	6.3791860927	-1.1224935085	0.5497398959
C	2.0676263414	-2.8157594218	-0.415325393
C	2.6980872391	-3.8668689185	-0.5753739008
C	4.8733556277	-7.4934269329	-1.1275663741
C	3.4771210075	-7.5235944241	-0.9683604145
C	2.7594928931	-6.3350382758	-0.7868407453
C	3.4269652539	-5.0820481901	-0.7603989515
C	4.8375348353	-5.0679223649	-0.9225906441
C	5.5482647378	-6.260682411	-1.1036608987
H	5.4322644388	-8.4252240655	-1.2694465545
H	2.9435515577	-8.4809598337	-0.9858317473
H	1.6718053894	-6.356577449	-0.6626526812
H	5.3615699907	-4.1066832632	-0.903691971
H	6.6369775883	-6.2288381934	-1.2271129652

[**5**]$^{+}$ **E** (M^1 = Au(CNC), L = PPh_3)
E = -2639.3923873 H

Au	0.7958932439	-1.3253588988	-0.1707359507
Au	2.2695866283	-3.1189340991	-2.7889849937
C	0.2126277084	1.5047283047	0.3154431407
C	-0.5891979937	2.6090719553	0.6589871067
C	-1.9358470803	2.3981890919	0.9923446035
C	-2.4906483931	1.1099901037	0.9894718682
C	-1.6771293905	0.0137601356	0.6447533959
N	-0.3718543541	0.2676038523	0.3216068126
H	-0.1630451437	3.6152172698	0.6687318701
H	-2.5635657005	3.2538994306	1.2625144209
H	-3.5391498783	0.9532797135	1.2540732904
C	4.3985080325	1.322542584	-0.7396498504
C	3.5789340869	0.1623145477	-0.6888305828
C	2.2229966311	0.2179420306	-0.3551123523
C	1.6368619563	1.4908822562	-0.0543119426
C	2.4346844323	2.6496178654	-0.1080647947
C	3.792539193	2.5619736387	-0.4464171751
H	4.0260753467	-0.8138209908	-0.9105115744
H	2.0072821583	3.633079958	0.1211443951
H	4.382981102	3.4816867934	-0.4732942358
C	-2.6029000686	-4.2007347507	0.479072482
C	-1.3117916257	-3.6965523656	0.1657327947
C	-1.0118744206	-2.3336921291	0.2114093896
C	-2.0408111674	-1.4096426475	0.5882126739
C	-3.3259589565	-1.8948478466	0.8966481185
C	-3.5979187816	-3.2688980739	0.8407654316
H	-0.5201017119	-4.3998397871	-0.1151515911
H	-4.1274095239	-1.2060495004	1.1888720623
H	-4.6058460308	-3.6108230094	1.0896634201
C	-2.8665699024	-5.7182461585	0.4192145436
C	-4.3230136218	-6.0795497108	0.78645225
H	-4.577692395	-5.7723792594	1.8167217612
H	-5.0507154301	-5.6173208495	0.0950526107
H	-4.4586081789	-7.1737858064	0.7258779728
C	-1.9180325477	-6.4414740859	1.4136754349
H	-2.0965850433	-6.1030460427	2.4497387188
H	-2.0907890434	-7.5326185921	1.3754061827
H	-0.8546075461	-6.2600005714	1.178012944
C	-2.5880613923	-6.228096814	-1.0211455732
H	-2.7613687217	-7.3183393914	-1.0776556712
H	-3.2558740935	-5.7364672739	-1.751300205
H	-1.5449009496	-6.0367119371	-1.3300589737
C	5.892894558	1.1922219104	-1.096025478
C	6.6147780562	2.5579142427	-1.1130764227
H	6.1771482857	3.246189135	-1.8586342392
H	6.5875376604	3.0514140889	-0.1249241314
H	7.676377339	2.4123489696	-1.3799250715
C	6.0328508583	0.5499826678	-2.5027965246
H	5.5617827964	1.1826896414	-3.2766029106
H	7.1011438781	0.4339124398	-2.7616987874
H	5.5660979166	-0.4500333726	-2.5486872967
C	6.5881328135	0.2845675806	-0.0449725381
H	7.6605271471	0.1743364086	-0.2891114797
H	6.5099132964	0.7183121893	0.967782081
H	6.1431052805	-0.7257187343	-0.0159092692
C	1.9360965805	-2.8879306672	-0.6270874508
C	2.6348854389	-3.9376533067	-0.5811563309
C	5.0606666215	-7.3490008651	0.1535872846
C	3.8517774008	-7.4928974522	-0.5505397434
C	3.0471376927	-6.3759712691	-0.802928854
C	3.4565499391	-5.0923417946	-0.3574224461
C	4.6820678429	-4.953340511	0.3449447108
C	5.4702684763	-6.0811456588	0.6029573055
H	5.6835548428	-8.2270867637	0.3544383666
H	3.5328830977	-8.4811590677	-0.8979855226
H	2.1000405815	-6.4796479289	-1.3424116938
H	4.9923050846	-3.9620607725	0.6899379875
H	6.4091908406	-5.9707945457	1.1554611235
P	2.3683815111	-2.9800098461	-5.1006100371
C	-0.0921543227	-6.3536460343	-7.1441810704
C	-0.6127461503	-5.6593485926	-6.0379922198
C	0.1424998896	-4.6519526138	-5.4215374548
C	1.4245117386	-4.3262564087	-5.9191271987
C	1.9443908367	-5.0234480596	-7.0295905682
C	1.1833526497	-6.0360898383	-7.6368592665
H	-0.680926873	-7.1454193657	-7.619469558
H	-1.6064885609	-5.9071290213	-5.6501217827
H	-0.2618330333	-4.1175539453	-4.5533719384
H	2.9400967514	-4.7818619732	-7.4157014077
H	1.5921822344	-6.5775297402	-8.4965799461
C	6.7260734989	-3.3227610367	-6.6798618222
C	6.3163019537	-4.0603370053	-5.555855002
C	5.0047572839	-3.9373892369	-5.0749101738
C	4.0914483742	-3.0787319317	-5.7262000518
C	4.5058450562	-2.3380691996	-6.8535467598
C	5.8224935801	-2.4628320235	-7.3251691014
H	7.7528790085	-3.4144490218	-7.0496232695
H	7.0209078581	-4.726796833	-5.047159917
H	4.6885595899	-4.5035578265	-4.1903433008
H	3.8064758518	-1.6615600256	-7.3562796275
H	6.1418787245	-1.8828107354	-8.197508893
C	0.6587348654	1.0631861939	-6.6238759423
C	0.4693198689	-0.1009477012	-7.3863813255
C	0.9677709605	-1.3318301303	-6.9307003209
C	1.6613145019	-1.397644527	-5.7032160442
C	1.8436732555	-0.22650471	-4.9339887442
C	1.3453220843	0.9992854676	-5.3992963022
H	0.2653006811	2.0207960093	-6.9813102886
H	-0.0709063882	-0.0545442957	-8.3379113363
H	0.8108449216	-2.2389472307	-7.5241116004
H	2.3668286393	-0.2740810966	-3.9710571685
H	1.4878190513	1.9041978118	-4.7991364378

[**6**]$^{+}$ H (M^1 = Au(CNC))
E = -3070.4320366 H

Au	6.5645467649	5.6631746707	7.1859091779
Au	6.6510385884	5.5511877816	0.7604396935
Au	7.986906678	4.5117779861	4.0107835354
C	6.8277982739	1.6052082538	-2.164035338
C	10.3486895447	6.4626848985	10.2183495486
C	7.8328222939	1.6574098592	-1.176174333
C	3.0613893909	6.1495667303	-2.3130410927
C	9.1469937641	7.1824970241	10.2682434533
C	10.5576952756	5.4461919016	9.2635067405
C	4.7730946733	9.9499671298	1.8731903496
C	4.6434196275	7.5854127777	8.2812845162
C	1.8950463884	6.4651760393	5.8949503818
C	11.8582463483	4.6201669643	9.2042416963
C	7.1638155233	4.1895064947	6.0017813982
C	5.8574085858	2.6107663466	-2.273073141
C	9.3330258944	5.4242582158	2.5425537514
C	1.8464708746	4.6321858455	4.0657396904
C	7.8179551984	2.7614290623	-0.2807229791
C	4.3823452007	6.9569319451	-0.44890252
C	4.1956652682	8.603788598	9.1438982604
C	5.8656374451	3.7077630505	-1.3910989466
C	6.485833559	10.4612051643	3.7476030355
C	11.5817143861	5.5293879031	1.5526669007
C	6.8659538081	3.7809450281	-0.3666639743
C	8.1102457308	6.9025477445	9.3582272083
C	4.5952044829	5.889996847	6.4744614737
C	2.5513443422	5.4539340113	5.1628737058
C	4.8420928052	7.8631694918	0.6138404612
C	8.9286270066	0.5799288278	-1.0516486639

C	3.8474497253	4.9899646169	-2.3886177127
C	3.9003295726	6.9042842521	7.2107987632
N	5.1144696965	5.8057158156	-0.5521509861
C	7.7247120734	0.8464029427	6.5596166213
C	5.8814254502	9.5595998371	2.6532469272
C	8.2989857558	5.8849261793	8.3661159604
C	10.752019786	5.6367394913	2.6985067327
C	4.908087278	4.8207466871	-1.4787413424
C	5.961948655	7.4360349683	1.3995298422
N	5.9260797387	7.1362364204	8.4393690709
C	2.5546239834	7.181735601	6.9033692385
C	5.0691019798	9.1038321073	10.121113444
C	7.3528876741	3.0334100513	5.4983994476
C	6.3730228826	8.6033092159	10.2535722114
C	6.8075561464	7.5849217227	9.3843581759
C	4.2579329459	9.1186347687	0.8687466544
C	7.471413657	1.5995636305	5.3842581052
C	11.3259138245	5.973882664	3.9476840393
C	7.8092465011	-0.5491419601	6.4885180487
C	7.3145549926	0.9313368012	4.1463845382
C	12.9571701964	5.7651591344	1.663492267
C	7.407034234	-0.4649530602	4.0891500956
C	8.181618718	5.3331003934	2.0025002668
C	12.7043485002	6.2017217997	4.0449470736
H	6.7961725426	0.7732058896	-2.8722613187
H	11.1279455703	6.7007488226	10.9469778235
H	2.2362070911	6.2869872779	-3.0198376598
H	9.024223152	7.9576335653	11.0339425259
H	4.299716806	10.9216006917	2.038053029
H	0.8476840788	6.701465917	5.6887049327
H	-0.2254277949	4.9133291071	4.7793503348
H	0.291724574	6.1179603145	3.5576121583
H	5.3825287283	9.4865360685	5.3900904551
H	6.9908751507	8.7736050635	5.0929093342
H	5.1005278448	2.5343146051	-3.062687954
H	8.5874009072	2.8240714036	0.4975685312
H	3.1785354209	8.9925311576	9.0526271596
H	11.1358371525	5.2668663521	0.58807027
H	3.6459300857	4.2278226837	-3.1452409882
H	7.8473354007	1.3655464335	7.5154535218
H	2.0029519833	7.9519971771	7.4555072036
H	4.7254557188	9.8948093843	10.7961197424
H	7.0443198665	8.9922619076	11.0230039564
H	3.6484475059	4.4872932233	2.7832689704
H	2.6012660067	5.883827969	2.4138478242
H	3.4018394888	9.4665170361	0.2783380577
H	10.6833910945	6.0622490589	4.8305522368
H	8.571969533	9.8488934391	3.3165175962
H	8.0408019456	11.305116445	2.4313699594
H	7.9996096677	-1.1251745236	7.400255209
H	7.1131408752	1.513512645	3.2405123758
H	13.5914094833	5.685990293	0.7742287338
H	7.283549969	-0.9752457338	3.1284499214
H	13.1412542975	6.4631981628	5.0141401355
C	7.6535599161	-1.2077529911	5.2563021433
H	7.7229224534	-2.299529605	5.2067978244
C	13.5221539054	6.0988441847	2.9067984996
H	14.5991465327	6.2799911284	2.9874905478
C	8.8371606004	-0.0836189875	0.3488521234
H	8.9747671459	0.6500632078	1.162716043
H	7.8555076247	-0.5721606634	0.4881165074
H	9.6220502563	-0.8544342635	0.4560616703
C	10.3213808939	1.2471978955	-1.2138394083
H	10.4993449091	2.0198973755	-0.4455829344
H	11.119154243	0.4882133776	-1.1183455418
H	10.4192161923	1.7241890301	-2.2053579743
C	8.7922189331	-0.5263770311	-2.1216219528
H	9.6011700552	-1.2668979773	-1.992399193
H	7.8321487515	-1.067124501	-2.0378078517
H	8.8756437575	-0.1220581848	-3.1464171608
C	3.3185161172	7.1392023889	-1.3526297801
H	2.7073964571	8.0438197318	-1.305679347
C	2.5980802912	4.8223909568	2.7202601858
H	2.1036042735	4.2332444002	1.9257169827
C	0.3757509406	5.0594707846	3.864025788
H	-0.0821180273	4.4464602671	3.0676471055
C	1.8693877095	3.1303290748	4.4600550931
H	1.3776200306	2.5253379767	3.6764326447
H	2.8991409048	2.7512677523	4.5822013697
H	1.3318711944	2.9617902934	5.4101885304
C	3.9127047427	5.1931448026	5.4752812296
H	4.4445733388	4.4122145779	4.920595681
C	9.5093530716	5.1867940775	8.3390575717
H	9.6480146928	4.4028466027	7.5854596676
C	12.8687744049	5.0319187132	10.2981542993
H	13.181421888	6.0869775278	10.196818502
H	12.4596274731	4.8861855704	11.3140278648
H	13.7766385333	4.4086543916	10.2157259803
C	11.5175253128	3.1172085172	9.3948603567
H	12.4397501628	2.5099581634	9.3461866307
H	11.0420393843	2.9400114117	10.3760417239
H	10.8310795149	2.7485520194	8.6126628442
C	12.53048788	4.8226611867	7.8196255848
H	13.4617224114	4.2303395776	7.7591241404
H	11.874434466	4.5009467712	6.9915609347
H	12.7892138228	5.8854676253	7.6608412256
C	6.4530430253	8.2849705281	2.39346102
H	7.3149370173	7.9588475926	2.9860761032
C	5.7311230927	11.8016421811	3.888740825
H	4.6713864848	11.6516906396	4.1641013963
H	6.1980938887	12.4075017768	4.685307091
H	5.7681814958	12.3957836049	2.9580349483
C	7.9663853265	10.7688076968	3.3941353717
H	8.418294718	11.4055190108	4.1766257123
C	6.4254656185	9.7220172332	5.1119205826
H	6.8610115238	10.3580325613	5.9048163608

$Au(PPh_3)CCPh$

E = -1480.0142995 H

Au	1.3758865151	-1.1236064355	0.0953378282
C	2.8195419621	-2.4708625717	-0.0266473772
C	3.7244740517	-3.3139330094	-0.1167481437
C	6.8405769559	-6.2060688662	-0.4353696994
C	5.7174686013	-6.4620978863	0.3703261452
C	4.6916502425	-5.5151307728	0.4788209019
C	4.7680777699	-4.2821247163	-0.2219246288
C	5.9085612293	-4.0367314074	-1.0321901428
C	6.9293595645	-4.989754725	-1.1345473049
H	7.6413448316	-6.9496828286	-0.5179867546
H	5.6403075142	-7.4082078435	0.918874456
H	3.8154524564	-5.7118703832	1.1053924703
H	5.9745863786	-3.0885061771	-1.5758509559
H	7.8017343548	-4.7821664412	-1.7653058399
P	-0.3277218515	0.4632346033	0.2154215915
C	-3.8102449404	-0.8381066554	3.0259583724
C	-4.0990595678	-0.0564889495	1.8955539378
C	-3.0679453335	0.338069522	1.0275611568
C	-1.7367765906	-0.0483023168	1.2904729404
C	-1.4532882962	-0.8436331983	2.4224678746
C	-2.4870925022	-1.2317630682	3.287547698
H	-4.6177941956	-1.1485738871	3.69828008
H	-5.1312778554	0.243489307	1.6828349992
H	-3.3000433587	0.9357946993	0.1391233853
H	-0.4227169123	-1.1657405648	2.6145090496
H	-2.2588052717	-1.8519055154	4.1613165368
C	-2.2575926079	1.2910528851	-3.9455082964
C	-1.7893660543	0.0099376317	-3.6086447698
C	-1.1983604074	-0.2170734792	-2.3570122701
C	-1.0814239253	0.8382708104	-1.4254912881
C	-1.5472430389	2.1242962763	-1.7706700349
C	-2.1329859715	2.3465755674	-3.0277563873
H	-2.7109747039	1.4687411308	-4.9270334854
H	-1.8726495867	-0.8139523727	-4.3258668363
H	-0.813565408	-1.2117028052	-2.1015035839
H	-1.440673747	2.9545329419	-1.0638628215
H	-2.4873350691	3.34958416	-3.2906631094
C	1.1516930623	4.5747748587	1.8370710021
C	-0.1654242516	4.1666694398	2.1036896292
C	-0.6299294437	2.9284513408	1.6317778348
C	0.2253872285	2.0899434166	0.8863083353
C	1.5523764156	2.5002348558	0.6303978
C	2.0093917444	3.7403415264	1.100933773

H	1.5130142527	5.5391840163	2.2110957488
H	-0.8337694467	4.8101845741	2.6867040521
H	-1.6532592244	2.607869996	1.8554277352
H	2.2262585495	1.8380968467	0.0734872524
H	3.0414584351	4.0488190339	0.9013777699

E (M^1 = Au(PPh_3), L = PPh_3)

E = -2652.0814371 H

Au	1.1579817615	-1.4286987779	-0.528477178
Au	2.0854901231	-3.0372487001	-2.9579230253
C	2.4661894466	-2.9866506629	-0.9217855973
C	3.2259643294	-3.6649742443	-0.1825444378
C	5.7813060175	-5.9462820106	2.3035594424
C	4.4670768685	-6.386202816	2.0596864944
C	3.6171956281	-5.6376925642	1.2399732608
C	4.081361557	-4.4286221544	0.6496628372
C	5.4126951219	-3.993742763	0.9030076063
C	6.2508423807	-4.7522522724	1.7256093194
H	6.4425605772	-6.5366278074	2.9469008807
H	4.1072892236	-7.3163418992	2.5116798864
H	2.5928047218	-5.9680571163	1.0412471242
H	5.7644016266	-3.0628264223	0.4472591554
H	7.2742562455	-4.4145753377	1.9192643183
P	1.792380231	-3.2601126277	-5.2586355468
C	-0.7041483346	-7.0392953484	-6.3140245884
C	-0.9689978682	-6.3164312649	-5.1383906802
C	-0.2013125681	-5.186565784	-4.8205215209
C	0.8340426533	-4.7687403377	-5.6856787405
C	1.1007476619	-5.4999369266	-6.8629653013
C	0.3300030759	-6.631980296	-7.1726983621
H	-1.2992973618	-7.9260662287	-6.5569054952
H	-1.7681585828	-6.6384912097	-4.4622220404
H	-0.3970777539	-4.6302994836	-3.8956957492
H	1.9140868829	-5.1923694788	-7.5289437608
H	0.5434959979	-7.1992715843	-8.0849056511
C	5.8649133322	-3.7193542503	-7.4571373965
C	5.6667137968	-4.2996305442	-6.1924482343
C	4.4409523633	-4.140191557	-5.5303469837
C	3.4001731919	-3.402974337	-6.1378387032
C	3.6025916352	-2.820197925	-7.406651284
C	4.834849585	-2.9804420965	-8.0610744899
H	6.8254599222	-3.8389367172	-7.9695540081
H	6.4705533593	-4.8712112735	-5.7164240594
H	4.2902248528	-4.5846373063	-4.5389510991
H	2.8041618853	-2.2380210368	-7.8788656505
H	4.988932067	-2.523067679	-9.0442543688
C	-0.3293217179	0.3886138671	-7.2129102378
C	-0.6443131998	-0.9071710752	-7.6524427606
C	-0.0257793907	-2.0228809499	-7.0645991655
C	0.9134893867	-1.8399853712	-6.0281211022
C	1.2206826832	-0.5355122457	-5.5817573119
C	0.6037185352	0.5736005121	-6.1779289095
H	-0.8134192272	1.2559013921	-7.6746559245
H	-1.3735519833	-1.0539916885	-8.4564285405
H	-0.2742536704	-3.0320805261	-7.4098273206
H	1.940730259	-0.3928277931	-4.7671300761
H	0.8469815494	1.5831506437	-5.8298002671
P	-0.2494926718	0.3119189095	0.1180724346
C	-2.6157576015	-0.7559040385	3.9768856837
C	-3.2451654551	-0.0120849478	2.9657772966
C	-2.5506781396	0.3089533364	1.7880552682
C	-1.216633027	-0.1185841785	1.6206434985
C	-0.5887150196	-0.8723377336	2.6371716743
C	-1.2874069321	-1.1846155322	3.8121624295
H	-3.162205853	-1.0069346758	4.8922536664
H	-4.2819071693	0.3185863586	3.0898690109
H	-3.0475766815	0.8841790397	0.9996322308
H	0.4445340875	-1.2158039427	2.5047258262
H	-0.7961581729	-1.7701696851	4.5965489822
C	-3.4332660562	1.4035028177	-3.0922171044
C	-3.0727174312	0.0632840903	-2.8690701224
C	-2.0958329431	-0.2516732421	-1.913721057
C	-1.4805293164	0.7769256564	-1.1662957453
C	-1.8418119116	2.1212713941	-1.3947166945
C	-2.8166491895	2.4292193806	-2.3579465635
H	-4.1935482432	1.6480524527	-3.84182622
H	-3.5485083617	-0.7380536084	-3.444433
H	-1.8062435238	-1.295986795	-1.7464067012
H	-1.3627774582	2.9240234645	-0.8241729952
H	-3.093488874	3.4745145559	-2.5324628588
C	2.1380638962	4.1875974744	1.0706515344
C	0.9838689493	3.8868470978	1.8123151761
C	0.2579096285	2.7150353231	1.545187933
C	0.6891451558	1.8377924284	0.5272260292
C	1.8551014723	2.1396302441	-0.210667258
C	2.5730287961	3.3136895222	0.0597636833
H	2.7042216844	5.1000757147	1.2860701037
H	0.6483503549	4.5624204539	2.6063858628
H	-0.634931726	2.477953631	2.1336328784
H	2.2019327775	1.4491725347	-0.9891486382
H	3.4786410221	3.541187072	-0.5126833847

H (M^1 = Au(PPh_3))

E = -3095.804906 H

Au	6.7146485688	6.2097262429	6.9721244028
Au	6.4496547245	5.2281305467	0.9465322907
Au	7.8880202425	4.4643591041	4.1049941462
C	6.9933534314	4.4218836544	6.1060675803
C	9.3023619705	5.0954183143	2.5448284174
C	11.4601549197	5.8162822933	1.6077192243
C	6.4313216452	1.1351908	6.8691706576
C	10.7338241544	5.2224344724	2.6723613102
C	7.127650895	3.2065933027	5.7391449004
C	7.0715591316	1.765313009	5.7706606324
C	11.4282612089	4.767095283	3.8184102344
C	6.3677838101	-0.2614075391	6.9327538759
C	7.639087993	0.9694306598	4.747290008
C	12.8508809359	5.9447000571	1.6978157571
C	7.5689367752	-0.4272329279	4.8226067776
C	8.1347216155	5.1287481441	2.0302880466
C	12.8200923727	4.9016473949	3.8965351084
H	10.9232839831	6.1692838119	0.7214307152
H	5.9918062708	1.750571568	7.6607067897
H	10.8662945755	4.3066369934	4.6386854097
H	5.8736069403	-0.7406311726	7.7846462241
H	8.1339298746	1.4574713453	3.9001903053
H	13.4048316156	6.4021489509	0.8710847202
H	8.0124878325	-1.0346773203	4.0266184457
H	13.3488181618	4.5440225788	4.7864479744
C	6.9345965858	-1.0461461748	5.9130080346
H	6.8822520413	-2.1385751684	5.9693458378
C	13.5346679987	5.4895298748	2.8390003321
H	14.6231896067	5.5918308327	2.9024385841
P	6.3856294577	8.2662764063	8.0343521534
P	4.5138566653	5.3554024934	-0.3563257945
C	4.5767662864	9.0352085401	-3.2009770205
C	5.1695957118	9.1059769317	-1.9289184057
C	5.1562931576	7.9867283212	-1.0838631607
C	4.5396488112	6.7880056563	-1.5069018295
C	3.9479037684	6.7197033311	-2.7861262218
C	3.9685387832	7.8434062348	-3.6277830759
H	4.5956308098	9.907451927	-3.8631386244
H	5.6526888433	10.0311776105	-1.5968615458
H	5.6313536048	8.0385217996	-0.0965935867
H	3.4820947179	5.7892566887	-3.1279719161
H	3.5124007736	7.7835266034	-4.6217365165
C	0.6682855756	5.6882255624	2.2435293272
C	0.7697095377	6.4447483332	1.0649345542
C	1.9275775718	6.3680918356	0.2734170288
C	2.9927671826	5.5301716458	0.6644055085
C	2.8910989702	4.7781018244	1.8562014683
C	1.7293992182	4.8549325242	2.6379636438
H	-0.2372592729	5.7488611194	2.8569365367
H	-0.0544217781	7.0970302639	0.7564136552
H	2.0031338589	6.9613974212	-0.644041067
H	3.7213093957	4.1344587611	2.1708211139
H	1.655083211	4.2657204691	3.5583876105
C	3.9439903333	1.6028145866	-3.0442674437
C	2.8190001888	2.2174475087	-2.4709444911
C	2.9728922215	3.3441746559	-1.647220167
C	4.2615736265	3.8592794165	-1.3942535235
C	5.3918468929	3.2335312513	-1.9659335604

C	5.229437181	2.1118090114	-2.7918978428
H	3.820203344	0.7222331885	-3.6836869911
H	1.8168486772	1.818609598	-2.6613599036
H	2.0935809928	3.8159304027	-1.1958109094
H	6.3962230866	3.6225701309	-1.7591080474
H	6.1090259351	1.6299254049	-3.2319319
C	3.6480723712	11.0897851038	5.5480384697
C	4.7213844045	11.633951874	6.2718872136
C	5.5656152245	10.7974245869	7.0200998646
C	5.3349419862	9.4058698214	7.0443729763
C	4.2599987952	8.861302397	6.3071633931
C	3.418071649	9.7034845503	5.5666023062
H	2.9931496206	11.7459225449	4.9645979964
H	4.906441062	12.7133796571	6.2543357164
H	6.4063598764	11.2255660169	7.5764036748
H	4.0880663552	7.7781662242	6.3110503486
H	2.5862977872	9.2750477729	4.9971200804
C	10.3873304958	10.5292785337	8.7419882255
C	10.1939547265	9.7658083397	7.5780583283
C	8.9889154033	9.0758844529	7.3821479091
C	7.9631166187	9.1551476485	8.3503016192
C	8.1613908654	9.9207193147	9.5187887574
C	9.3730471914	10.6042820352	9.7102536307
H	11.3323399478	11.0607821654	8.8972508258
H	10.9863825814	9.6988117898	6.8249460629
H	8.844499741	8.4693784333	6.4798745998
H	7.3765056499	9.9751792944	10.2807036635
H	9.5240253326	11.1932161716	10.6212868662
C	4.3779436106	7.7498795682	12.1976116807
C	4.0372613514	8.8557756032	11.4019084037
C	4.6239972816	9.0242846972	10.1371801166
C	5.5582739883	8.0787012539	9.6645897078
C	5.8931605829	6.9636510534	10.4649270497
C	5.3063550867	6.8048510717	11.7286614354
H	3.9153260066	7.6208244981	13.1819529253
H	3.3095374859	9.5903078607	11.7632191315
H	4.3493398001	9.8842336757	9.5169148041
H	6.6103123696	6.2207851116	10.0949474302
H	5.5691507529	5.9379799889	12.3442709784

Au(NHC-Me)CCPh
E = -748.551562 H

Au	-0.2871874122	-3.9162114802	2.5959938841
C	1.4061992461	-3.7187250147	1.5959908861
C	2.4694340733	-3.5945480883	0.9680658218
C	6.1236224096	-3.1677948927	-1.1899731746
C	6.1178886849	-3.0975344887	0.214109575
C	4.9205786106	-3.2367729593	0.9266732006
C	3.6920463538	-3.4517707386	0.2460298915
C	3.7137681533	-3.5207581066	-1.1729707229
C	4.9157218002	-3.3797925459	-1.8773270634
H	7.0625647395	-3.0581382866	-1.744483052
H	7.0551902092	-2.9325570105	0.7586046075
H	4.9137121046	-3.1824782459	2.0203837425
H	2.7716762635	-3.6858803613	-1.7062583168
H	4.9106115758	-3.4359032374	-2.9723393873
C	-2.0351268611	-4.1199466052	3.6281458351
C	-4.1595619762	-4.7123471566	4.2189379472
C	-3.6433188448	-3.9625436413	5.2412598577
H	-4.078203663	-3.6535449149	6.1891647155
H	-5.1320369267	-5.1853695141	4.1020123014
N	-3.1684965916	-4.7976237039	3.2466508133
N	-2.3510143274	-3.6111673781	4.86534216
C	-3.308811281	-5.5190090473	1.9808833891
H	-4.1498323237	-5.1055229478	1.3995083574
H	-2.3729628725	-5.3914335751	1.4161262195
H	-3.4807764472	-6.5917848833	2.1709624179
C	-1.44284788	-2.8002878403	5.6777239626
H	-1.871645901	-1.7974939037	5.8422986223
H	-1.2619558483	-3.2906361763	6.6488683466
H	-0.493231922	-2.7082396028	5.1292756588

E (M^1 = Au(NHC-Me), L = PPh_3)
E = -1920.6186929 H

Au	1.873206982	-1.244642624	-0.3221679362
Au	2.1901784494	-3.0677698461	-2.7242870424
C	2.8003409571	-3.0320736066	-0.723292715
C	3.4971191027	-3.9087227011	-0.1496267183
C	5.8301895427	-6.8545244121	1.8003684465
C	4.4278360823	-6.9690794975	1.7853063066
C	3.6515248999	-6.0004937357	1.1421325894
C	4.2790502767	-4.8965756229	0.4997883734
C	5.6980199084	-4.7910161136	0.5219977148
C	6.4617271955	-5.7667761559	1.1695565753
H	6.4334548182	-7.6157482024	2.306549118
H	3.9414591907	-7.8169880161	2.2786442109
H	2.5597879622	-6.0762909354	1.1242313441
H	6.1762815652	-3.9390886038	0.0284626434
H	7.5532773577	-5.6819699519	1.1852342346
P	1.5842015827	-3.2476649556	-4.9621820061
C	-0.1045146598	-7.4686060663	-5.9417713687
C	-0.3180630344	-6.8912510793	-4.6785758847
C	0.2069576772	-5.6236816223	-4.3875821451
C	0.9441264423	-4.9216550722	-5.3669276419
C	1.1594945224	-5.5058182169	-6.6335110651
C	0.63410943	-6.77690048	-6.9157612127
H	-0.507878999	-8.4621824236	-6.1645139524
H	-0.8862537441	-7.4324974549	-3.9145489486
H	0.0541234178	-5.1791266571	-3.396460895
H	1.7439954502	-4.9750699058	-7.392683448
H	0.8083180583	-7.2286575898	-7.8981252056
C	5.2109734579	-2.5753784101	-7.7930995952
C	5.3837769792	-3.2054460263	-6.5487506649
C	4.2867619704	-3.3863511957	-5.6941771839
C	3.0047030661	-2.9428021397	-6.0870951122
C	2.8345448333	-2.3077794843	-7.3357402611
C	3.9389282003	-2.1265688253	-8.1839943326
H	6.0702889536	-2.4292820861	-8.4562567374
H	6.3760866355	-3.5505567971	-6.2393637683
H	4.4223570587	-3.868617214	-4.7184659313
H	1.8453568236	-1.9498365035	-7.6408962358
H	3.8032055276	-1.6306043371	-9.1510309384
C	-1.6617719964	-0.1526090417	-6.2048650641
C	-1.761632092	-1.4763839433	-6.6611098575
C	-0.7970121294	-2.4274658216	-6.2890526673
C	0.2744085593	-2.0525230666	-5.4519200538
C	0.3663699886	-0.7215626681	-4.9863845047
C	-0.5961150311	0.2237832183	-5.3686169833
H	-2.4154803893	0.5860118016	-6.498163046
H	-2.5925069138	-1.774201054	-7.3096078887
H	-0.8809487786	-3.4590932551	-6.6464568277
H	1.1909105012	-0.4287128351	-4.3253561164
H	-0.5160656663	1.2559032552	-5.0102319401
C	1.0133123743	0.510885575	0.2489686458
C	0.7246276341	2.6761969924	0.8807471875
C	-0.491048417	2.0534656249	0.975820732
H	-1.4634382694	2.4311077853	1.2838975425
H	1.0180455912	3.7027166826	1.0886691346
N	1.6312165349	1.720299924	0.4368544955
N	-0.2966770738	0.7329748966	0.586702525
C	-1.3542448587	-0.2818810484	0.5600986598
H	-1.7380357628	-0.4545058604	1.5789594459
H	-2.1759624214	0.0489544931	-0.0956009527
H	-0.9243209874	-1.2151214116	0.1679216652
C	3.055973481	1.9804469204	0.2090761934
H	3.5310241478	2.3171945417	1.1448742377
H	3.5270654647	1.0438471407	-0.1238857078
H	3.1794440151	2.7518002679	-0.5686294016

H (M^1 = Au(NHC-Me))
E = -1632.8829234 H

Au	6.6531131373	5.8320231292	7.1643641823
Au	6.4641353361	5.3248591015	0.9755250815
Au	7.927020867	4.4991625275	4.1229791482
C	7.0512730331	4.1773617242	6.1186404329
C	9.2604824133	5.4324557474	2.6563112897
C	11.2914446085	6.6223586207	1.9342424572
C	6.943717818	0.801874596	6.6058599535
C	10.6643712814	5.719270557	2.8312021413
C	7.2850676441	3.0277448103	5.6131997967
C	7.3626857459	1.5906112712	5.5030836897
C	11.4305533483	5.1159696428	3.8571892212

C	7.0096295929	-0.5940848643	6.5323172213
C	7.8447610327	0.9506656894	4.3365174349
C	12.6558880517	6.904720967	2.066135978
C	7.9068490262	-0.4472111401	4.275282139
C	8.1057946223	5.3825193202	2.1128516855
C	12.794982622	5.4074002295	3.9795058806
H	10.6984254391	7.0920763352	1.1429259601
H	6.5740134169	1.2958997387	7.5101000937
H	10.9470142048	4.414947582	4.5466124198
H	6.6861596081	-1.1952020067	7.3888676454
H	8.1705590643	1.5599865982	3.4860078043
H	13.1329582314	7.6004956664	1.3675858596
H	8.2840092061	-0.9325899883	3.3688636485
H	13.3800564145	4.9326949424	4.7743372219
C	7.4903053693	-1.2230319491	5.3702754497
H	7.5411760461	-2.3158100269	5.3197258483
C	13.4112801936	6.300403026	3.0865668982
H	14.4788095358	6.5244292628	3.1841658665
C	4.8230797388	5.2526812874	-0.2345549886
N	3.5820417649	4.7492075925	0.0590356607
C	2.7287473911	4.8629998847	-1.0323376629
C	3.4492399209	5.4526727044	-2.0363919909
H	1.6973386903	4.5190612291	-1.0021145942
H	3.1680070363	5.7238194056	-3.0514660558
C	6.2657526914	7.4950670011	8.2801431488
N	6.7304949729	8.7689731708	8.0776715265
C	6.2650191412	9.630379268	9.064182681
C	5.4887793607	8.8813859912	9.9076475398
H	6.52164054	10.6872055436	9.0813158694
H	4.9374664698	9.1580364821	10.8034880403
N	4.7238515412	5.6828534633	-1.5325021535
N	5.4999009884	7.5822357481	9.4139587592
C	5.8106945043	6.3038125873	-2.2958339678
H	5.5270998574	7.3267782733	-2.592663889
H	6.7023441403	6.3417681379	-1.6529534529
H	6.0308176188	5.7035130689	-3.1935770005
C	4.7950036458	6.4586092489	10.0384017044
H	3.7191261711	6.6854990542	10.113640157
H	4.9395970849	5.5695773832	9.4070785544
H	5.2056259603	6.2658295114	11.0430708297
C	7.6060687839	9.1778009331	6.9752372839
H	7.1138819671	9.9593842621	6.3737747833
H	8.5600645368	9.5605445196	7.3732884416
H	7.7999108796	8.2977703737	6.3446512119
C	3.1996639627	4.1586144245	1.3448678398
H	2.3506119556	4.7136481816	1.7761115625
H	2.9208877356	3.1010887455	1.2069261481
H	4.0629484143	4.2237881608	2.0231386641

Au(IPr)CCPh

E = -1603.7381715 H

Au	-0.2211373854	-3.7781005212	2.8872339889
C	1.1357915139	-3.3849704649	1.502040298
C	1.9737814086	-3.144220062	0.6185432353
C	4.8454118027	-2.3256498172	-2.4283800935
C	4.5525161463	-3.6528408665	-2.0687112828
C	3.610959886	-3.9259487836	-1.0689078876
C	2.9357506276	-2.869983295	-0.3991805785
C	3.2433548068	-1.5340118261	-0.7731795368
C	4.1854208589	-1.2701525047	-1.7750128333
H	5.5823385419	-2.1155602226	-3.2119750845
H	5.0622659051	-4.4825906381	-2.5727672122
H	3.3804776772	-4.9589461622	-0.7876982404
H	2.7282573349	-0.7134281008	-0.2626788227
H	4.4073172116	-0.2318159135	-2.0488650495
C	-1.6359697397	-4.1824073707	4.2900935485
C	-3.2528404851	-5.2387979126	5.5204974819
C	-3.1178622409	-3.973854129	6.0237529542
H	-3.622993963	-3.4655973223	6.8412684558
H	-3.8995788007	-6.0640653029	5.8076947904
N	-2.3443249289	-5.3502508437	4.4670391313
N	-2.1307016083	-3.3433874999	5.264820923
C	-1.8627317302	-8.8800588554	2.1777758688
C	-1.1076499314	-8.6933093277	3.342121732
C	-1.2417615169	-7.5264892908	4.1192365637
C	-2.1709637523	-6.5535294062	3.6749395179
C	-2.9470837205	-6.7099610032	2.4999660371
C	-2.769832751	-7.8971630612	1.7633739396
H	-1.7395698044	-9.7946279984	1.5868404697
H	-0.3930298539	-9.4633447655	3.653345113
H	-3.348565041	-8.0468834332	0.8450438934
C	-0.8787539385	0.6371973034	5.9874380405
C	-1.9269586877	0.3859373799	5.0939798048
C	-2.3563599204	-0.9279058741	4.8231882248
C	-1.6874383048	-1.9811368477	5.494548058
C	-0.6196254643	-1.7611522094	6.3995181906
C	-0.2328631873	-0.426509159	6.6290450089
H	-0.5592896693	1.6675472046	6.1801496165
H	-2.4206191558	1.223915562	4.5893104265
H	0.5944069783	-0.2208032914	7.3173089646
C	-3.9265089365	-5.6461653705	2.0059295618
H	-3.9484054542	-4.827700112	2.7478407293
C	-5.3635986284	-6.2027247411	1.8891375993
H	-5.720961514	-6.6105750162	2.8517226302
H	-6.0590108964	-5.4034869978	1.5750064797
H	-5.4260482701	-7.011378612	1.1385237246
C	-3.4458025057	-5.0372932022	0.6683182945
H	-3.4059779038	-5.801392724	-0.1295581515
H	-4.1384141658	-4.2412980269	0.3389512344
H	-2.4368661733	-4.6002651779	0.774216131
C	-0.37716473	-7.3374757169	5.36571528
H	-0.6862927049	-6.3977889684	5.8581093847
C	-0.580196778	-8.4802328389	6.3859974796
H	-0.2616250827	-9.4549415755	5.9741492834
H	0.0201436741	-8.2922694217	7.294533541
H	-1.6390616001	-8.5732316052	6.6872107538
C	1.1120136598	-7.1852933109	4.9781879579
H	1.4914690867	-8.0979103554	4.4833152488
H	1.2553846392	-6.3374811349	4.2852893951
H	1.727357245	-7.0085390408	5.8792049197
C	-3.4899389301	-1.1674927961	3.8267075956
H	-3.6668898299	-2.2562293356	3.763265262
C	-4.8074354058	-0.5094026004	4.2964292905
H	-5.1153385179	-0.879604996	5.2908242423
H	-4.7082654369	0.5892838868	4.3639500324
H	-5.6212361698	-0.7276816064	3.5814028023
C	-3.0935531215	-0.6856383833	2.4121733026
H	-2.9200909437	0.4058332084	2.3922842087
H	-2.170645625	-1.1846213182	2.0686888874
H	-3.9005642724	-0.9106000308	1.6912270511
C	0.1242463823	-2.8981914733	7.0990683567
H	-0.3450833762	-3.8522360359	6.7987529443
C	1.6015496792	-2.9511937234	6.6457849592
H	1.6759441093	-3.067519973	5.5504611713
H	2.1421293969	-2.0295966801	6.9291043156
H	2.1174850893	-3.8041481527	7.1231666745
C	0.0126244268	-2.7916784729	8.6371898577
H	0.4838778142	-1.8658512089	9.0143724106
H	-1.040922191	-2.7911767301	8.9698860341
H	0.5243281901	-3.6450463431	9.1178837351

E (M^1 = Au(IPr), L = PPh_3)

E = -2775.807017 H

Au	1.661716253	-0.6077348009	-0.2333337738
Au	2.4095079511	-2.8544248324	-2.8588811328
C	3.020132319	-1.8685438001	-1.0026221752
C	4.0736618766	-2.555396554	-1.1346671135
C	7.8069027293	-4.5853930617	-1.1505762598
C	6.6429451665	-5.2655698054	-0.7497162488
C	5.4078132001	-4.607091325	-0.7504934612
C	5.3272349843	-3.2505277649	-1.1604069062
C	6.5057805136	-2.5724815502	-1.5675290408
C	7.7358262891	-3.2407836901	-1.5563232547
H	8.7719099634	-5.1034733664	-1.1438197353
H	6.7006898713	-6.3112623729	-0.4294550727
H	4.496716477	-5.1237422768	-0.4315496738
H	6.4380315198	-1.5260657122	-1.8815462923
H	8.6435283358	-2.7115571697	-1.8649964046
P	1.5357936126	-3.7744932304	-4.7963326175
C	-1.0585637402	-7.5343170813	-3.9246807713
C	-1.0260918806	-6.4643586112	-3.0141560901
C	-0.230917341	-5.3395483913	-3.2780081914

C	0.5326644552	-5.2774749717	-4.4647102809
C	0.5002814664	-6.3547942699	-5.3760566637
C	-0.2953907772	-7.4788165492	-5.1023630641
H	-1.6734510693	-8.4155252586	-3.7124771944
H	-1.6130588462	-6.5093093046	-2.0906032998
H	-0.1949289314	-4.5110815372	-2.5601462777
H	1.1017494878	-6.3202581263	-6.2907784091
H	-0.3133654905	-8.3145654806	-5.8100011197
C	4.8772632965	-5.1376903281	-7.7316145234
C	5.0407258096	-5.2915244822	-6.3441574272
C	4.035910144	-4.8618195129	-5.4656048033
C	2.8530000313	-4.2815331622	-5.9749639552
C	2.692369302	-4.1265463697	-7.3680357142
C	3.7057572663	-4.5549773865	-8.2409556801
H	5.6668066483	-5.466945537	-8.4155525875
H	5.9565664245	-5.7388853451	-5.9434942455
H	4.1705462446	-4.9710544168	-4.3828207428
H	1.7832842878	-3.6667877324	-7.7695905325
H	3.5783062711	-4.4287310665	-9.3214089548
C	-1.0983699037	-0.7788047705	-7.1865601169
C	-1.4911300611	-2.1241466312	-7.0999895808
C	-0.7182407287	-3.040241425	-6.3677425576
C	0.4544607151	-2.6061022658	-5.7150070412
C	0.8413501368	-1.2498226634	-5.7954442321
C	0.0681644911	-0.3428187107	-6.5345215007
H	-1.7028894801	-0.0679833115	-7.760164418
H	-2.4015063082	-2.4655988713	-7.6043188945
H	-1.0278948351	-4.0887058162	-6.3026854871
H	1.7461924063	-0.9078601883	-5.278652275
H	0.3750930676	0.7066302437	-6.5976116184
C	0.4073550324	0.6920905454	0.7014893357
C	-0.3444753718	2.501977447	1.8659822585
C	-1.3932892335	1.63110837	1.7373479907
H	-2.4233002793	1.6873686382	2.0805089577
H	-0.27027701	3.4753432572	2.3443121568
N	0.7465391952	1.9137825256	1.2292725553
N	-0.9175304405	0.531357357	1.0243749099
C	4.5669009796	3.7272959838	1.0180957031
C	4.2604168439	2.8672132366	2.0797857192
C	3.0010797877	2.2430452843	2.1744477809
C	2.0645427464	2.5215489804	1.1479789441
C	2.340068339	3.3878520351	0.0604564331
C	3.6158684693	3.9834650424	0.0224230141
H	5.0105446803	2.6764879291	2.8550722182
H	3.8656457335	4.6621382598	-0.8004651644
C	-3.3458067253	-2.7889090904	0.0250432005
C	-3.3139890291	-1.6678355221	-0.8139412056
C	-2.5071442147	-0.553401075	-0.5121152976
C	-1.7332118591	-0.6179014313	0.6736204966
C	-1.7444347714	-1.7338651196	1.5472634972
C	-2.5681940849	-2.8195674994	1.1892869524
H	-3.9876043445	-3.6407645588	-0.2261016377
H	-3.9311655138	-1.6521025298	-1.7189914663
H	-2.6053883588	-3.6990998088	1.8413537221
H	5.5516629516	4.2047501213	0.9685607382
C	-0.9183150176	-1.7979240681	2.8318942889
H	-0.3664714252	-0.8462572227	2.9363787819
C	-2.5004280905	0.6573513121	-1.4455694525
H	-1.7887688767	1.4006682024	-1.0428625942
C	0.1314984298	-2.9311865776	2.7617917458
H	-0.35104104	-3.9211936666	2.6709771628
H	0.8040808502	-2.7967323427	1.895353135
H	0.7465925822	-2.9407753519	3.6794696125
C	-1.8209020066	-1.9475548586	4.0784231848
H	-2.3869546162	-2.8959705364	4.0576910351
H	-1.2067146884	-1.9462120727	4.9965102464
H	-2.5512671061	-1.1226441625	4.1525822217
C	-3.8916313357	1.3305843642	-1.5021014059
H	-4.652928549	0.6476892347	-1.9203585451
H	-4.2354319912	1.6400152838	-0.4992344357
H	-3.8582414661	2.2287590213	-2.144447553
C	-2.0084295207	0.2748651662	-2.8593620639
H	-2.6876978629	-0.4499658319	-3.3430206672
H	-1.9651752583	1.1714888219	-3.503331698
H	-1.0008267704	-0.175079595	-2.8230450394
C	1.3222073962	3.6955860104	-1.0380506929
H	0.4062850335	3.1111025856	-0.8349644456
C	0.926803308	5.1906267345	-1.0337005536
H	0.519203493	5.4998510852	-0.0549829394
H	1.7943304581	5.8385258394	-1.2537771359
H	0.1583220644	5.3875908737	-1.8025948058
C	1.8417164964	3.2601358099	-2.427219554
H	2.7491924727	3.8209891002	-2.7149229191
H	2.0881958778	2.1836234914	-2.4408900997
H	1.0731909726	3.4513571427	-3.1978849758
C	2.6974290816	1.318644958	3.3533891905
H	1.6701774478	0.9294269428	3.231734347
C	2.7469105372	2.084565735	4.6959722005
H	3.7569765119	2.4861342494	4.8939426581
H	2.0411000295	2.9339398604	4.7066464905
H	2.4854899266	1.4105634198	5.5312145102
C	3.6491756001	0.1007141186	3.3702348108
H	4.6999484804	0.4108124826	3.5136903474
H	3.3849397604	-0.5789876056	4.2002649389
H	3.5867872538	-0.4649749997	2.4236616454

H (M^1 = Au(IPr))

E = -3343.2624705 H

Au	7.8336288767	5.0230401401	7.2087935956
Au	5.9372772538	6.5406900927	1.1627122283
Au	8.4053833151	5.8357733937	3.7217311441
C	8.5328779286	4.4412030905	5.4305226802
C	8.5066051687	7.7810308692	2.7342123973
C	9.2202872349	10.1269508824	2.5038299469
C	10.1378016895	1.6661947021	4.2774603769
C	9.502741066	8.8066429328	2.9392210638
C	9.1452653656	3.9131533758	4.4409751098
C	9.9077109352	2.9395516605	3.6950015768
C	10.7551816109	8.5283286408	3.5363475577
C	10.8936228398	0.7082632914	3.5917444387
C	10.4443913774	3.2224766967	2.4166590121
C	10.1777119136	11.1363308037	2.6592569377
C	11.1998069773	2.2558612655	1.7404176995
C	7.4688718839	7.2043291241	2.2623646077
C	11.7052091994	9.5467666434	3.6871842919
H	8.2493240492	10.3440793321	2.0472585697
H	9.718883917	1.4449109839	5.2643868245
H	10.9740360526	7.5083787315	3.8712704858
H	11.0684828635	-0.2707320352	4.0511324844
H	10.2650287819	4.204669706	1.9655282055
H	9.9520268176	12.1517253053	2.3155172387
H	11.6146092918	2.4880617204	0.7535997804
H	12.6734058773	9.3188255895	4.1460056886
C	11.428361424	0.9983752295	2.3240824709
H	12.0224782776	0.2461444981	1.7941248081
C	11.4215718598	10.8515458728	3.2496626151
H	12.1680706989	11.6445404153	3.3661728264
C	4.435848654	5.9320608408	-0.0698291561
N	3.206533678	6.5153119208	-0.2579808661
C	2.4805001477	5.8437510115	-1.240316968
C	3.2698231585	4.8149416471	-1.6796845912
H	1.4818373264	6.1610323952	-1.5298277139
H	3.1022625346	4.0474422217	-2.4310866786
C	7.2268759462	5.5610253169	9.0746752399
N	7.1748144179	6.8227828286	9.6146420077
C	6.7540187508	6.7796861743	10.9427778155
C	6.5370521061	5.462298388	11.2458398787
H	6.65182201	7.6828363563	11.539128599
H	6.2059283362	4.9783138062	12.1611936225
N	4.4588029418	4.8830590713	-0.9559617091
N	6.8298769704	4.7319122071	10.0953630875
C	6.5821317163	0.5090056025	9.8946596672
C	7.7885850654	1.1219505047	10.2548233258
C	7.9037595425	2.5241968442	10.325268113
C	6.7486983543	3.2834667992	10.0114336666
C	5.5112835781	2.6959948443	9.6484592784
C	5.4582088643	1.2894100686	9.5969400858
H	6.5159576185	-0.5836850185	9.8506601049
H	8.6600008648	0.5016996756	10.4917634694
H	4.5181450697	0.7994823893	9.3204440072
C	8.205027402	10.4133135508	7.621909412
C	9.1935884979	9.6703787217	8.2790964896

C	8.8830480275	8.4699139954	8.9471535596
C	7.5311018954	8.0459095262	8.9164144498
C	6.5050412782	8.77472649	8.2652982387
C	6.8767661289	9.9696346293	7.6189148377
H	8.4711395049	11.3452798463	7.1114682872
H	10.2286377859	10.0288098802	8.2780996797
H	6.1102624263	10.5607189303	7.1057247091
C	1.7520421667	9.9026120161	1.8231040623
C	2.4878658019	10.07100775	0.643647863
C	2.9860233325	8.9638593268	-0.0707452606
C	2.7149789579	7.678415192	0.460179356
C	1.9649174729	7.4708436645	1.6443783662
C	1.4932816227	8.6166961272	2.3141064829
H	1.3720288951	10.7790425787	2.3596050506
H	2.6784056417	11.0810036195	0.2645597877
H	0.9115676198	8.4964218535	3.2346371847
C	7.6334898622	2.1400327227	-1.5174067131
C	7.6068792587	3.3351577436	-2.2466934002
C	6.5708595803	4.273905101	-2.0738577278
C	5.5629509534	3.9546884648	-1.1302517597
C	5.5595580526	2.7561441538	-0.3737880559
C	6.6215935948	1.8568484161	-0.5916005089
H	8.4469737007	1.4229391141	-1.6728795069
H	8.4040202906	3.5457594652	-2.9681831744
H	6.653441752	0.9190369538	-0.0264880949
C	9.9862386954	7.6917895508	9.6644825112
H	9.5308183936	6.8026288342	10.1372158133
C	5.0451042261	8.3228183863	8.2519264663
H	4.9804028852	7.3488089846	8.7700950603
C	4.1445725517	9.3179404286	9.0207014997
H	4.4786881991	9.4459173263	10.0655822597
H	4.1499558332	10.3147876819	8.5440983617
H	3.0997843656	8.958820742	9.0368146468
C	4.5330314426	8.1088901063	6.8095543303
H	4.5334879393	9.0526870058	6.2348493395
H	5.1609332442	7.3820240483	6.2657046559
H	3.4955258538	7.7287667005	6.8266562291
C	10.6297706463	8.5338600585	10.7906749674
H	11.1333131768	9.430981236	10.3878399899
H	9.8778920197	8.8729155663	11.5251219293
H	11.3895883202	7.9379353786	11.3272294731
C	11.0520810452	7.1846998637	8.6663630392
H	11.5599556909	8.0245407313	8.1585663307
H	11.8233784073	6.5968114867	9.195906782
H	10.5965702594	6.5421807915	7.8916861184
C	9.2337144943	3.1560963323	10.7367938162
H	9.1165620271	4.2548908676	10.7168287942
C	9.6209279159	2.7576747479	12.1800523839
H	9.7781419718	1.6677479394	12.2686034327
H	10.5609472365	3.2563672433	12.4766921651
H	8.8377487192	3.0428475347	12.9046079942
C	10.3578258919	2.7981408979	9.7380524377
H	10.5500964301	1.7101393572	9.7188740638
H	10.0952346531	3.1169700838	8.7137090449
H	11.2994252373	3.2987477671	10.0267484652
C	4.2635711449	3.5171353048	9.3232807444
H	4.5225665999	4.5879836114	9.4111991036
C	3.1247352835	3.2312751173	10.3294466158
H	3.4395581357	3.4337526952	11.3684339368
H	2.2474790665	3.8650420298	10.1072260843
H	2.7972487316	2.1772358017	10.2790114312
C	3.7962631171	3.2768527237	7.8695605522
H	3.5007038259	2.2240995039	7.7092345869
H	2.9193427026	3.9093822809	7.6416736423
H	4.5965567357	3.5190759811	7.1484580453
C	3.7770012449	9.182258846	-1.3607445598
H	4.039768334	8.1920059339	-1.7758096025
C	1.6663716399	6.0807256661	2.2059411599
H	2.0676256931	5.3299964926	1.5010330264
C	6.5717794176	5.5666334815	-2.8896077936
H	5.6835875893	6.1577553034	-2.6010805723
C	4.4616061193	2.4111204924	0.6324132097
H	3.7595128392	3.2634063061	0.6822071931
C	7.8164953776	6.4262274889	-2.5706053682
H	8.7497637419	5.9036795408	-2.8484270135
H	7.7821923866	7.374095574	-3.1372977843
H	7.8677924664	6.6667156642	-1.4936473562
C	6.4634298319	5.2785530816	-4.404783612
H	7.3354410773	4.7078108868	-4.7714849632
H	5.5568031738	4.6949161039	-4.6439333875
H	6.4216457754	6.2253299417	-4.9724110008
C	3.6561498494	1.1716974551	0.1769371772
H	3.2092842272	1.320831817	-0.822079293
H	4.2968841943	0.2729632321	0.1260657026
H	2.839160507	0.9609080418	0.8901837417
C	5.0356677398	2.2085877572	2.0533446862
H	5.7320472475	1.3516046559	2.0913933687
H	5.5817777333	3.1041813518	2.397677458
H	4.2179199618	2.0052513407	2.7681607677
C	5.1015349395	9.9299641365	-1.0832330833
H	4.9151809814	10.9365621006	-0.6665858424
H	5.7289765209	9.3725214193	-0.3646433342
H	5.6745132482	10.0546731718	-2.0197189274
C	2.9323373046	9.9196538159	-2.4252581396
H	2.6620581436	10.9384489547	-2.0941975937
H	3.5031048826	10.0159712108	-3.366076837
H	1.9949806174	9.3793106403	-2.6463359284
C	0.1460649353	5.8291130154	2.3287430926
H	-0.3221322786	6.5169492997	3.0555298228
H	-0.367712651	5.964004991	1.3606497192
H	-0.0432677911	4.7980995777	2.6773949861
C	2.380566591	5.8658075732	3.5599783838
H	2.0246974537	6.586541242	4.3184184229
H	2.1820429931	4.8477913156	3.9411862463
H	3.4728447041	5.9919759859	3.4578238087

S5.4. B3LYP (Gaussian)

C_6H_6

E = -232.2438192 Hartree

C	-1.15283100	0.78900900	0.00000000
C	-1.25977500	-0.60385200	0.00000000
C	-0.10691000	-1.39279900	0.00000000
C	1.15283200	-0.78900700	0.00000000
C	1.25977700	0.60384800	0.00000000
C	0.10690600	1.39279900	0.00000000
H	-2.04974900	1.40302800	0.00000000
H	-2.23993400	-1.07370200	0.00000000
H	-0.19005100	-2.47657900	0.00000000
H	2.04974900	-1.40302700	0.00000000
H	2.23993000	1.07371000	0.00000000
H	0.19005700	2.47657800	0.00000000

CH_2Cl_2

E = -959.6888593 Hartree

Cl	1.49524000	-0.21685800	0.00000000
H	0.00011500	1.38056000	-0.89861000
H	0.00010200	1.38054900	0.89861700
C	0.00033200	0.76841900	0.00000000
Cl	-1.49537000	-0.21676700	0.00000000

PPh_3

E = -1036.281692 Hartree

P	0.00195100	-0.00054900	-1.20639700
C	-1.43552200	4.03067800	0.65313800
C	-2.01408900	3.51037200	-0.50688500
C	-1.55590000	2.30287600	-1.03414100
C	-0.52572400	1.58444900	-0.40317500
C	0.04898400	2.11945600	0.76030000
C	-0.40161800	3.33446800	1.28215100
H	-1.78392900	4.97628600	1.06030000
H	-2.81450000	4.04964800	-1.00698500
H	-1.99852700	1.91342200	-1.94824200
H	0.85346100	1.58704600	1.25878300
H	0.05624500	3.73601400	2.18278000
C	4.21197200	-0.77646500	0.65149500
C	4.04993500	-0.00357500	-0.50074600
C	2.77519900	0.20550600	-1.02748800
C	1.63843600	-0.33640800	-0.40313600
C	1.81530700	-1.11352900	0.75213900

C	3.09275300	-1.33309400	1.27320900
H	5.20504800	-0.94921900	1.05807300
H	4.91659900	0.42728100	-0.99555300
H	2.65909200	0.79219100	-1.93609600
H	0.95303600	-1.55263900	1.24485900
H	3.21199100	-1.93988200	2.16742400
C	-2.78214000	-3.25270500	0.65152500
C	-2.69280600	-2.00913200	1.27962300
C	-1.86101100	-1.01498500	0.75871100
C	-1.10805500	-1.24889600	-0.40261500
C	-1.21816900	-2.50057100	-1.03262000
C	-2.04015300	-3.49739100	-0.50646100
H	-3.43077600	-4.02447500	1.05771200
H	-3.27145000	-1.81004400	2.17825900
H	-1.80190000	-0.05142800	1.25601500
H	-0.65850800	-2.69198800	-1.94547300
H	-2.10952600	-4.46029700	-1.00604100

[**4**] ([Au(ᵗBuC^N^CᵗBu)(C≡CPh})])

E = -1467.259726 Hartree

Au	-0.00001800	-0.56128500	-0.00001700
C	1.20474300	-3.22782700	0.00014900
C	1.21609200	-4.62773400	0.00016200
C	-0.00007800	-5.31162000	-0.00000300
C	-1.21622900	-4.62770000	-0.00018100
C	-1.20484100	-3.22779300	-0.00019200
N	-0.00004000	-2.60495600	-0.00003700
H	2.15472100	-5.16916100	0.00031800
H	-0.00009200	-6.39820800	0.00000700
H	-2.15487300	-5.16910100	-0.00031300
C	4.47814900	-0.43494900	0.00082600
C	3.13184200	-0.01291800	0.00069200
C	2.06974900	-0.90900900	0.00041200
C	2.35349700	-2.30652000	0.00033500
C	3.68403800	-2.73994000	0.00045800
C	4.72783500	-1.81524800	0.00068100
H	2.90387100	1.04857500	0.00082400
H	3.92244500	-3.80111000	0.00037000
H	5.74571100	-2.18814200	0.00074400
C	-4.47817500	-0.43483200	-0.00076100
C	-3.13185700	-0.01283500	-0.00063600
C	-2.06978700	-0.90895300	-0.00038700
C	-2.35357100	-2.30645800	-0.00037000
C	-3.68412300	-2.73984200	-0.00053200
C	-4.72789700	-1.81512400	-0.00070000
H	-2.90385900	1.04865200	-0.00076100
H	-3.92255600	-3.80100700	-0.00052200
H	-5.74578300	-2.18799000	-0.00080200
C	-5.60404200	0.61413300	-0.00101600
C	-7.00617100	-0.02446500	-0.00079600
H	-7.17300500	-0.64486900	-0.88891500
H	-7.17293500	-0.64441100	0.88765600
H	-7.76886100	0.76250700	-0.00097700
C	-5.47778700	1.49958600	-1.26442100
H	-5.57471700	0.89828000	-2.17577100
H	-6.26748500	2.26091500	-1.27380900
H	-4.51340100	2.01570600	-1.30633700
C	-5.47776500	1.50027700	1.26190300
H	-6.26746000	2.26161200	1.27088400
H	-5.57464700	0.89949100	2.17360200
H	-4.51337200	2.01642300	1.30349800
C	5.60404500	0.61398400	0.00110900
C	7.00615900	-0.02465000	0.00084900
H	7.17303600	-0.64499100	0.88900300
H	7.17284800	-0.64466700	-0.88756800
H	7.76886600	0.76230400	0.00092000
C	5.47782800	1.49938900	1.26455300
H	5.57476900	0.89804500	2.17587700
H	6.26753700	2.26070600	1.27395500
H	4.51345100	2.01552100	1.30650900
C	5.47777100	1.50018300	-1.26177100
H	6.26748900	2.26149400	-1.27073900
H	5.57461600	0.89943000	-2.17349600
H	4.51339100	2.01635800	-1.30332500
C	-0.00000800	1.40883500	-0.00000300
C	0.00000500	2.63095700	-0.00001000
C	0.00019300	6.87812800	-0.00004000
C	-1.20745700	6.17537300	0.01377400
C	-1.21064400	4.78257200	0.01380600
C	0.00006500	4.06026500	-0.00001900
C	1.21084000	4.78246300	-0.01386800
C	1.20778000	6.17526400	-0.01384800
H	0.00024100	7.96485500	-0.00005100
H	-2.15097200	6.71504100	0.02460200
H	-2.14873300	4.23568700	0.02466800
H	2.14887900	4.23549300	-0.02471700
H	2.15134400	6.71484600	-0.02468200

[**5**]$^{+}$

E = -2639.217215 Hartree

Au	-2.06039100	0.86923000	0.23485600
Au	1.06485800	-0.63825900	0.30762100
C	-3.12867300	3.20568200	-1.15283600
C	-4.02019700	3.90971700	-1.96810100
C	-5.10075100	3.23109000	-2.53318700
C	-5.30253000	1.87101500	-2.29843600
C	-4.40067800	1.18266900	-1.47996600
N	-3.36272800	1.88274300	-0.95278000
H	-3.87424500	4.96702500	-2.15373200
H	-5.79836300	3.77233400	-3.16567300
H	-6.14554800	1.35314800	-2.73964800
C	0.34370000	4.59284900	0.97881000
C	-0.08065700	3.24578900	1.02552400
C	-1.19509500	2.79021100	0.33092300
C	-1.93904600	3.71664300	-0.45471300
C	-1.52644300	5.05164700	-0.51758000
C	-0.40112200	5.47850500	0.18764600
H	0.47749600	2.54027600	1.63399500
H	-2.07964000	5.77605800	-1.10996600
H	-0.11604100	6.52151200	0.11747300
C	-4.37496700	-2.94287000	-0.26025700
C	-3.38109600	-2.02879400	0.15511400
C	-3.38245300	-0.69775900	-0.24120300
C	-4.42385300	-0.23595200	-1.09634500
C	-5.41296800	-1.13032500	-1.51842600
C	-5.38466500	-2.46215400	-1.10534300
H	-2.58952700	-2.37419000	0.81307400
H	-6.21859000	-0.80008700	-2.16916000
H	-6.16967400	-3.12394900	-1.45133100
C	-4.31829400	-4.40317000	0.22062900
C	-5.48368800	-5.24889500	-0.32770800
H	-6.45661300	-4.86216900	-0.00445700
H	-5.47729600	-5.29401000	-1.42269700
H	-5.39931800	-6.27581600	0.04388200
C	-4.38244500	-4.43679400	1.76713600
H	-5.31548800	-3.99308700	2.13190800
H	-4.33696400	-5.47256100	2.12368900
H	-3.55154700	-3.88868100	2.22436100
C	-2.99142300	-5.04623500	-0.25218700
H	-2.93363300	-6.08697600	0.08787400
H	-2.92151300	-5.04283400	-1.34610900
H	-2.11735200	-4.51682600	0.14308500
C	1.57303200	5.03672700	1.79083700
C	1.90335500	6.52834900	1.58996100
H	2.12944200	6.76018600	0.54282800
H	1.08301000	7.17702700	1.91668800
H	2.78549700	6.79253800	2.18300800
C	2.80684300	4.20717000	1.35843700
H	3.02632100	4.35287800	0.29424600
H	3.68942400	4.51724800	1.93008100
H	2.66027100	3.13515400	1.53068300
C	1.29828700	4.79909600	3.29589700
H	2.16570400	5.10567400	3.89227100
H	0.43221300	5.37906300	3.63370200
H	1.09865600	3.74391600	3.51217500
C	-0.78816900	-0.13613600	1.40635800
C	-0.29165300	-0.70336100	2.39702100
C	1.11710900	-2.52919500	5.94097400
C	0.45644400	-3.29837000	4.97800000
C	-0.00030400	-2.70567700	3.80460200
C	0.20516600	-1.32790300	3.58377200
C	0.87519500	-0.56036500	4.55912700

C	1.32408300	-1.16228200	5.73094400
H	1.46825300	-2.99490100	6.85723600
H	0.29403500	-4.35884000	5.14557200
H	-0.51988200	-3.29359700	3.05430100
H	1.02661000	0.50100700	4.38874800
H	1.83303000	-0.56658700	6.48274300
P	2.85533700	-0.94147900	-1.15434700
C	2.91200200	-5.16863200	-3.04175000
C	1.70004300	-4.51691500	-2.79819300
C	1.69253500	-3.25142800	-2.21338900
C	2.90305200	-2.62340800	-1.87540500
C	4.11747500	-3.28229700	-2.12075200
C	4.11739400	-4.55176300	-2.70239000
H	2.91590500	-6.15752700	-3.49093600
H	0.76049000	-4.99637700	-3.05684000
H	0.74645300	-2.75283600	-2.01749400
H	5.05907300	-2.81150800	-1.85571800
H	5.06050800	-5.05787000	-2.88671600
C	6.93326700	-0.35306600	0.95951500
C	5.89179500	-1.02973400	1.60049500
C	4.66309100	-1.18675200	0.96117400
C	4.46985100	-0.67396700	-0.33276100
C	5.51785100	0.00549400	-0.97151100
C	6.74453100	0.16435400	-0.32295300
H	7.88808500	-0.22608500	1.46140200
H	6.03403900	-1.42967900	2.60022400
H	3.85402400	-1.70680800	1.46828200
H	5.37936300	0.41304200	-1.96801400
H	7.55062300	0.69424200	-0.82197700
C	2.65559200	2.09033600	-4.64847300
C	3.16298800	0.80957800	-4.87587500
C	3.21704100	-0.11918500	-3.83502900
C	2.76152400	0.23333700	-2.55505700
C	2.24408700	1.52088400	-2.33359700
C	2.19687200	2.44490400	-3.37726600
H	2.61261600	2.80912800	-5.46168500
H	3.51475100	0.52924700	-5.86444800
H	3.60701300	-1.11489600	-4.02239800
H	1.87118300	1.80049400	-1.35156700
H	1.79516900	3.43779700	-3.19724000

[**6**]$^{+}$

E = -3070.176355 Hartree

Au	-3.02832800	-0.54745000	1.01347300
Au	3.02830200	-0.54752700	-1.01351100
Au	0.00003200	1.17907700	0.00004300
C	6.69718800	2.02260800	0.96443000
C	-6.69697400	2.02294000	-0.96458900
C	5.57911900	2.78249100	0.59409500
C	6.40067800	-3.74949700	-0.08890800
C	-6.72924100	0.64075100	-0.78117200
C	-5.57889800	2.78276000	-0.59414800
C	1.22526500	-4.78455100	-2.67232100
C	-4.22329800	-3.20985100	0.96161000
C	-1.22562800	-4.78462700	2.67227500
C	-5.51802500	4.31019300	-0.77043300
C	-1.62876600	0.80931200	1.43527900
C	6.72938700	0.64042500	0.78095600
C	0.91965800	1.65606600	-2.02565500
C	0.97500100	-3.77175500	3.56145900
C	4.47857700	2.09454200	0.03518300
C	4.22310600	-3.20999200	-0.96176200
C	-5.21210300	-4.16146200	0.69121000
C	5.63680900	-0.02538300	0.21617500
C	-0.97530500	-3.77153900	-3.56145500
C	1.21524700	3.68474400	-3.37691600
C	4.48272300	0.71912500	-0.16271800
C	-5.63672700	-0.02512600	-0.21634600
C	-2.08326600	-2.27196700	1.76705100
C	-0.39136400	-3.67412600	2.86082000
C	2.91403900	-3.41636800	-1.59776700
C	5.51831800	4.30991900	0.77046200
C	6.61682100	-2.41186200	0.24359800
C	-2.91428000	-3.41632200	1.59768600
N	4.47319800	-1.92077100	-0.61481900
C	-1.21512100	3.68441500	3.37733000
C	0.39107800	-3.67399100	-2.86084500
C	-4.48262700	0.71931700	0.16264300
C	0.37621400	2.65322500	-2.91102500
C	5.61683700	-1.47410300	-0.03364500
C	2.08308700	-2.27195700	-1.76708500
N	-4.47328300	-1.92060800	0.61468100
C	-2.46853600	-4.66217600	2.05137400
C	-6.40084300	-3.74919700	0.08858900
C	-0.91955600	1.65579200	2.02599100
C	-6.61687600	-2.41154200	-0.24390600
C	-5.61685200	-1.47385300	0.03343400
C	2.46819700	-4.66219000	-2.05144900
C	-0.37608300	2.65294100	2.91133100
C	-0.96145100	2.59555300	-3.34535300
C	-0.72121300	4.63177100	4.27073900
C	0.96162900	2.59532500	3.34552200
C	0.72139500	4.63208500	-4.27037800
C	1.44596000	3.55168600	4.23449300
C	1.62889100	0.80939100	-1.43524800
C	-1.44572200	3.55188900	-4.23438300
H	7.56595500	2.50285600	1.39856200
H	-7.56569300	2.50324200	-1.39875800
H	7.17384800	-4.48269000	0.12180600
H	-7.62066800	0.09348000	-1.07688600
H	0.91723000	-5.76508100	-3.01557800
H	-0.91767300	-5.76518100	3.01553500
H	0.58279600	-5.60603300	4.70931300
H	1.35893900	-5.89513700	3.13745600
H	-2.11183000	-3.89790000	-1.68825100
H	-1.93535700	-2.24368900	-2.29294300
H	7.62081000	0.09310300	1.07659000
H	3.59942500	2.66031500	-0.25886900
H	-5.05625800	-5.20152200	0.95120900
H	2.24660700	3.72734900	-3.04073000
H	7.54578500	-2.10098100	0.70613900
H	-2.24652000	3.72696900	3.04125600
H	-3.08638800	-5.54899300	1.93469900
H	-7.17404300	-4.48233900	-0.12219700
H	-7.54578500	-2.10059400	-0.70651200
H	1.93514600	-2.24384900	2.29306700
H	2.11158800	-3.89803600	1.68830000
H	3.08598700	-5.54905200	-1.93479300
H	-1.60812700	1.80096900	-2.98513100
H	-0.76956700	-1.82730700	-4.58149300
H	-0.19519400	-3.20542000	-5.53223800
H	-1.37426200	5.42025300	4.63284400
H	1.60829900	1.80076600	2.98523400
H	1.37445000	5.42060000	-4.63240100
H	2.47814000	3.50142300	4.56770200
H	-2.47786000	3.50157500	-4.56771400
C	0.60763000	4.56894100	4.69891400
H	0.98868100	5.31102400	5.39440600
C	-0.60739000	4.56918700	-4.69870900
H	-0.98840100	5.31124900	-5.39424600
C	4.35312900	4.66768000	1.72455300
H	3.38746300	4.31994300	1.34245600
H	4.50564000	4.21810500	2.71264900
H	4.28974100	5.75465900	1.85338500
C	5.27778600	4.97639600	-0.60596100
H	4.33741100	4.64693900	-1.06067400
H	5.22971900	6.06598500	-0.49469900
H	6.08956400	4.74188100	-1.30373000
C	6.81922100	4.88636300	1.36205000
H	6.72758100	5.97342100	1.46040100
H	7.03004200	4.48326700	2.35914500
H	7.68446000	4.68654300	0.72000200
C	5.21186600	-4.16167400	-0.69144900
H	5.05593700	-5.20172000	-0.95145700
C	2.08433400	-3.28550700	2.59692100
H	3.06366100	-3.35345200	3.08651700
C	1.31240300	-5.21181900	3.99322400
H	2.29254600	-5.22890100	4.48213300
C	0.96470000	-2.87724900	4.82506000
H	1.93530100	-2.92877600	5.33255200
H	0.76927000	-1.82757900	4.58158900
H	0.19480600	-3.20573000	5.53223300

C	-0.85116900	-2.42409100	2.38986600
H	-0.22403000	-1.54819800	2.52457100
C	-4.47841300	2.09473900	-0.03521100
H	-3.59925200	2.66046300	0.25890700
C	-6.81883900	4.88670800	-1.36214400
H	-7.02956500	4.48366200	-2.35928100
H	-7.68415900	4.68689400	-0.72020300
H	-6.72715100	5.97376700	-1.46044200
C	-5.27763700	4.97659200	0.60605500
H	-5.22951900	6.06618500	0.49485100
H	-6.08950800	4.74207200	1.30371300
H	-4.33732700	4.64708100	1.06086400
C	-4.35271500	4.66796800	-1.72436700
H	-4.28927200	5.75495300	-1.85312500
H	-3.38710400	4.32017200	-1.34218500
H	-4.50512600	4.21846100	-2.71250800
C	0.85096800	-2.42399400	-2.38987300
H	0.22387900	-1.54805700	-2.52454000
C	-1.31272700	-5.21157400	-3.99329300
H	-1.35923600	-5.89494300	-3.13756500
H	-2.29288700	-5.22862200	-4.48217000
H	-0.58314100	-5.60574400	-4.70942700
C	-0.96504000	-2.87696000	-4.82500100
H	-1.93566800	-2.92842900	-5.33244800
C	-2.08459400	-3.28532600	-2.59684100
H	-3.06394000	-3.35321900	-3.08640400

$[Au(PPh_3)]^+$

E = -1171.875864 Hartree

Au	-0.00475300	-0.01032200	2.08528100
P	0.00072800	0.00219500	-0.21930300
C	2.54781200	-3.50695300	-1.77563400
C	1.60211000	-3.72029600	-0.76677100
C	0.84505500	-2.65604500	-0.28455000
C	1.02841600	-1.36767900	-0.81990400
C	1.98022300	-1.15455100	-1.83106200
C	2.73408700	-2.22914300	-2.30571400
H	3.14193900	-4.33793000	-2.14379700
H	1.46080000	-4.71331200	-0.35136400
H	0.11717000	-2.82659700	0.50463100
H	2.13327900	-0.16400200	-2.24625600
H	3.46851900	-2.06357400	-3.08793200
C	1.77159100	3.97119900	-1.74487900
C	2.42780400	3.25201300	-0.73997000
C	1.88327900	2.06162900	-0.26569600
C	0.67610600	1.58103400	-0.80591500
C	0.01667500	2.30588000	-1.81239300
C	0.57135000	3.49885500	-2.27851400
H	2.19565700	4.90292500	-2.10703300
H	3.35852900	3.62290000	-0.32187400
H	2.39322700	1.51030200	0.52020600
H	-0.91672800	1.94455600	-2.23082000
H	0.06158300	4.05814500	-3.05696000
C	-4.30694600	-0.43870300	-1.78952300
C	-3.27926300	-1.18722400	-2.36624600
C	-1.97383600	-1.07564800	-1.88540500
C	-1.69942800	-0.20109300	-0.82060800
C	-2.73731000	0.54960900	-0.23875300
C	-4.03570500	0.43046400	-0.72742800
H	-5.32198500	-0.53503700	-2.16302500
H	-3.49092700	-1.86278300	-3.18933700
H	-1.17978700	-1.66105100	-2.33667500
H	-2.53244500	1.21982300	0.59225700
H	-4.83638200	1.00805200	-0.27586800

$[Au(PPh_3)(C_6H_6)]^+$

E = -1404.165943 Hartree

Au	-1.29638300	-0.09524300	-0.51330700
P	0.95446400	0.00989000	0.05884500
C	2.85646000	3.99984600	-1.30098200
C	1.58126300	3.98402200	-0.72829800
C	1.00718000	2.77592200	-0.33750800
C	1.71210400	1.57230900	-0.50973500
C	2.99187300	1.59231500	-1.08488600
C	3.55821100	2.80650600	-1.47873200
H	3.29964200	4.94143900	-1.61135400
H	1.03241000	4.91112700	-0.59212400
H	0.01280700	2.76850400	0.10236100
H	3.54361300	0.66891800	-1.22892600
H	4.54767800	2.81638600	-1.92599500
C	3.33437900	-3.41700200	-1.93483300
C	2.33116400	-2.74886400	-2.64275400
C	1.60603800	-1.72902600	-2.02937200
C	1.88691500	-1.36467100	-0.70137600
C	2.89490400	-2.03760300	0.00570500
C	3.61380200	-3.06169500	-0.61426100
H	3.89418100	-4.21599800	-2.41187200
H	2.10997000	-3.02574100	-3.66922400
H	0.82448400	-1.21492500	-2.58365800
H	3.11732400	-1.76941800	1.03361100
H	4.39082000	-3.58161500	-0.06187700
C	1.57829600	-0.33812500	4.62746500
C	2.34453400	0.56933900	3.89414600
C	2.15723200	0.69524900	2.51619800
C	1.19372000	-0.09177200	1.86691200
C	0.42144300	-1.00064900	2.61023300
C	0.61801600	-1.12438000	3.98433600
H	1.72574500	-0.43107100	5.69936700
H	3.08932300	1.18287700	4.39219700
H	2.75639500	1.40446800	1.95412700
H	-0.33040100	-1.61116300	2.11606000
H	0.01896000	-1.82901400	4.55350900
C	-4.32147800	1.34656800	0.25228800
C	-4.68816900	0.33675400	1.14515900
C	-4.44872000	-1.00988300	0.84175000
C	-3.85658200	-1.35774000	-0.37205900
C	-3.48746000	-0.34617600	-1.29751300
C	-3.73050300	1.01443800	-0.97251200
H	-4.51758300	2.38674300	0.49289900
H	-5.16914300	0.59799000	2.08324800
H	-4.74434900	-1.78547300	1.54145300
H	-3.70881500	-2.40112300	-0.63405000
H	-3.21883800	-0.61913900	-2.31675100
H	-3.50465400	1.78795000	-1.70062600

$[Au(PPh_3)(CH_2Cl_2)]^+$

E = -2131.59544 Hartree

Au	-1.22431400	0.62304200	-0.07926500
P	0.97365700	-0.07305200	0.00780200
C	3.84342900	3.52859200	-0.35323100
C	2.68808300	3.62535200	0.42809000
C	1.81540500	2.54300300	0.51983100
C	2.09995200	1.35043800	-0.16796800
C	3.26034600	1.25670600	-0.95208700
C	4.12723200	2.34751900	-1.04093600
H	4.51864600	4.37572000	-0.42871900
H	2.46372600	4.54502500	0.95995200
H	0.91637400	2.62588600	1.12564600
H	3.48732500	0.34321300	-1.49226600
H	5.02244200	2.27215300	-1.65079400
C	1.93060700	-3.01051000	-3.42468600
C	1.09692000	-1.91177400	-3.65254100
C	0.79380500	-1.03832600	-2.60986200
C	1.33189600	-1.25816200	-1.33015900
C	2.16842500	-2.36264400	-1.10447500
C	2.46410400	-3.23422900	-2.15414300
H	2.16003000	-3.69385400	-4.23690100
H	0.67777900	-1.73909000	-4.63918900
H	0.14029700	-0.18852800	-2.79131500
H	2.58411500	-2.54517100	-0.11866900
H	3.10933000	-4.08914400	-1.97567100
C	1.86044600	-2.21243400	4.00531100
C	2.76135400	-1.26573500	3.51563500
C	2.50117000	-0.60292300	2.31426500
C	1.32902400	-0.89101700	1.59925200
C	0.42222800	-1.84329000	2.09691700
C	0.69185200	-2.50261600	3.29419700
H	2.06547500	-2.72285200	4.94164200
H	3.66860000	-1.03872800	4.06734800
H	3.20592500	0.13272300	1.94064900
H	-0.48915300	-2.07148100	1.54950000
H	-0.01071600	-3.23788800	3.67490000

Cl	-3.59598500	1.49609400	-0.21800900
H	-5.71956500	0.54493800	0.18208800
H	-4.59243600	0.26894000	1.57121000
C	-4.72776200	0.22341800	0.49334500
Cl	-4.39479700	-1.39930900	-0.09934600

$[Au(PPh_3)_2]^+$

E = -2208.254444 Hartree

Au	-0.00012800	0.00035900	-0.00032000
P	-2.37380500	-0.00085700	-0.00087900
C	-4.06992400	-4.26405500	-0.62064900
C	-2.92950100	-4.06059600	0.16104400
C	-2.41861500	-2.77428600	0.32844400
C	-3.05305800	-1.67741500	-0.27939500
C	-4.19737400	-1.88733600	-1.06364800
C	-4.70056300	-3.17892600	-1.23190000
H	-4.46335400	-5.26731800	-0.75569500
H	-2.43461300	-4.90323900	0.63498400
H	-1.52816200	-2.62275200	0.93407800
H	-4.69238400	-1.04992100	-1.54537600
H	-5.58520700	-3.33485600	-1.84230300
C	-4.07271700	2.66663300	-3.38259300
C	-2.93545600	1.88393100	-3.59945100
C	-2.42403600	1.09559500	-2.56962600
C	-3.05462000	1.07748400	-1.31373900
C	-4.19561900	1.86584700	-1.10111300
C	-4.69958200	2.65730100	-2.13531400
H	-4.46656100	3.28528300	-4.18367100
H	-2.44320600	1.89211500	-4.56754300
H	-1.53527200	0.49337000	-2.74281700
H	-4.68720200	1.86786200	-0.13332900
H	-5.58158500	3.26721300	-1.96330600
C	-4.07725000	1.59490700	3.99808900
C	-4.69890000	0.51438500	3.36990700
C	-4.19346800	0.01387600	2.16822500
C	-3.05596200	0.59641600	1.58935700
C	-2.43015700	1.67975900	2.22973200
C	-2.94329800	2.17823200	3.42627800
H	-4.47239000	1.97988700	4.93362600
H	-5.57830900	0.05722700	3.81392400
H	-4.68163900	-0.82847300	1.68823900
H	-1.54436100	2.13480600	1.79282000
H	-2.45499400	3.01645400	3.91465900
P	2.37357700	0.00098100	0.00078300
C	4.07097800	4.26463000	0.61411300
C	4.70015400	3.18049900	1.22859600
C	4.19653100	1.88879100	1.06237300
C	3.05322000	1.67776100	0.27694500
C	2.42021100	2.77371600	-0.33411800
C	2.93156400	4.06010300	-0.16875900
H	4.46477400	5.26796300	0.74757100
H	5.58400200	3.33728300	1.83993600
H	4.69044600	1.05209400	1.54645800
H	1.53052300	2.62144200	-0.94065600
H	2.43783300	4.90201900	-0.64519100
C	4.07034600	-2.66281400	3.38662800
C	2.93418400	-1.87824000	3.60259900
C	2.42332200	-1.09107700	2.57161400
C	3.05351100	-1.07585700	1.31549700
C	4.19350900	-1.86586000	1.10384500
C	4.69677200	-2.65634700	2.13913900
H	4.46370600	-3.28056600	4.18863900
H	2.44236100	-1.88410900	4.57092300
H	1.53548500	-0.48732500	2.74421600
H	4.68490900	-1.86974800	0.13597800
H	5.57799800	-3.26758100	1.96784700
C	4.07938900	-1.60057700	-3.99483900
C	4.70133800	-0.51990000	-3.36722800
C	4.19518300	-0.01768300	-2.16656500
C	3.05666400	-0.59869100	-1.58816800
C	2.43058600	-1.68223700	-2.22796200
C	2.94442900	-2.18240800	-3.42349200
H	4.47507000	-1.98685700	-4.92961500
H	5.58145000	-0.06387300	-3.81100600
H	4.68353300	0.82478800	-1.68697800
H	1.54399200	-2.13603900	-1.79139300
H	2.45591800	-3.02072400	-3.91150300

HCCPh

E = -308.386937 H

C	0.5808366451	0.0000265802	-0.0000092606
C	-0.6293387221	-0.0000714014	-0.0000082775
H	-1.6953819521	-0.0000738523	0.0000252836
C	4.8187642975	-0.000034304	0.0000050398
C	4.1181001529	-1.2088955343	0.000002252
C	2.7251709701	-1.2133971905	-0.000002328
C	2.0108226477	0.0000057273	-0.0000030688
C	2.7252049376	1.213388276	-0.0000009418
C	4.1181340326	1.2088468361	0.0000029765
H	5.9053361845	-0.000049411	0.000008256
H	4.658523471	-2.1516100267	0.0000034632
H	2.1766580692	-2.1502502665	-0.000004935
H	2.1767186169	2.1502568916	-0.0000026673
H	4.6585837312	2.1515461625	0.00000465

E (M^1 = H, L = PPh_3)

E = -1480.3238333 H

Au	-0.1290747129	-0.9444717121	-0.1929502302
C	0.7921624518	1.593655885	-0.0478950476
C	-0.2569174854	1.1757023949	-0.5793304548
H	-1.1280748212	1.5065380102	-1.1231655322
P	-0.2655458586	-3.2703187853	0.0668223838
C	-2.1502265687	-4.4435693442	4.1248091921
C	-2.6054215687	-3.3169066721	3.4344855612
C	-2.0197792317	-2.9582369827	2.2213425228
C	-0.976839971	-3.7326697223	1.685758435
C	-0.521842012	-4.8625429409	2.3832909373
C	-1.1102830112	-5.2130562507	3.5998276308
H	-2.6032350033	-4.7182379117	5.0728770269
H	-3.411332405	-2.7145157214	3.8430896134
H	-2.373244348	-2.0769513671	1.6916513095
H	0.288740814	-5.4639379169	1.9837514963
H	-0.7531350038	-6.086869304	4.1367103415
C	3.895259874	-5.2841123835	-0.1491122244
C	3.7125699816	-4.1129101894	0.5920582428
C	2.4596592341	-3.5047142742	0.6384702248
C	1.3743577803	-4.071789426	-0.0514314598
C	1.5621189629	-5.246893639	-0.7940931396
C	2.8220372018	-5.8477464887	-0.840581647
H	4.873778443	-5.7535391352	-0.1892014419
H	4.5467299669	-3.6712652086	1.129306814
H	2.3246501874	-2.5918487824	1.2136880485
H	0.733589117	-5.6916506198	-1.3357762622
H	2.9617387827	-6.7563185603	-1.418757164
C	-2.8874859365	-5.1277533571	-3.2618450052
C	-2.9962009111	-5.6033769958	-1.9540228958
C	-2.218575011	-5.0467690225	-0.9365791205
C	-1.3257728872	-4.0044490118	-1.2287542197
C	-1.2233603724	-3.5259393338	-2.5464648993
C	-1.9990886669	-4.0900978215	-3.5578130515
H	-3.4966088666	-5.5613003362	-4.0495194148
H	-3.6881470109	-6.4073271337	-1.7213058305
H	-2.3120131927	-5.4207711068	0.0779774972
H	-0.538400684	-2.7150127932	-2.7823656872
H	-1.9153450216	-3.7157715983	-4.5737774993
C	4.3409391041	2.9099016091	1.7623932422
C	4.3530586706	2.5245861048	0.4160533035
C	3.1856300315	2.0758099669	-0.1871223152
C	1.9886956598	2.010080051	0.5667456129
C	1.9857610773	2.4029125109	1.9271944507
C	3.1616733205	2.8496296082	2.5152958222
H	5.2569121866	3.2621837371	2.2277574836
H	5.2727528376	2.5795361868	-0.1576293535
H	3.1758508294	1.7785378533	-1.2308694432
H	1.061768806	2.3549236264	2.4944672063
H	3.1647254508	3.1544782249	3.5569299811

H (M^1 = H, L = PPh_3)

E = -752.3895555 H

H	9.047367311812	3.940531778188	6.547179673436
H	7.074635950721	5.021377812157	1.747715903475
Au	8.332155991900	3.704604438966	3.861011002525

C	8.531685111902	3.233404729538	5.912834213525
C	9.077276599346	4.253696647329	1.326766854156
C	11.366356463559	4.857886309118	0.731353362692
C	8.000919115293	-0.314704740643	5.927673231960
C	10.284470941826	3.942089751764	0.683775221909
C	7.948582029683	2.127315016220	6.014964002507
C	7.280261835987	0.896027107373	6.087900664526
C	10.408393770472	2.734511503930	-0.049282839905
C	7.337164443042	-1.527743776924	6.042627787091
C	5.890008876979	0.863147975382	6.366313312804
C	12.543851858526	4.563280344265	0.058897980013
C	5.242143070026	-0.358813313801	6.478476338323
C	8.013323337394	4.519603585853	1.936104088280
C	11.593167586659	2.455634150685	-0.715433967798
H	11.258911915880	5.781974859207	1.290178102088
H	9.065884182020	-0.278250106680	5.721881985021
H	9.571865383913	2.044029015946	-0.084954232728
H	7.882584825803	-2.458383873310	5.923566505154
H	5.349120226480	1.795409844796	6.493184726584
H	13.375076052313	5.260316699726	0.089351861450
H	4.178890191680	-0.391523471423	6.693315972488
H	11.694464152338	1.534572355938	-1.280352421608
C	5.963105272366	-1.549099101678	6.316424221589
H	5.449905716555	-2.502129938946	6.406173922054
C	12.656538099942	3.366525949635	-0.660766621413
H	13.580803986315	3.142478808198	-1.185393941988

Au(PPh_3)CCPh

E = -1479.9226409 H

Au	1.3809888142	-1.1295505092	0.085205757
C	2.8369987263	-2.4824466279	-0.0361742672
C	3.7342329311	-3.3147300385	-0.1201851462
C	6.8398065117	-6.1953958001	-0.4200005515
C	5.7277561946	-6.4416202311	0.3896939022
C	4.707312269	-5.498985703	0.4908763383
C	4.7784713631	-4.2830471007	-0.2201429206
C	5.9062624995	-4.0473931131	-1.0336843576
C	6.9229026984	-4.9946052447	-1.129998185
H	7.6345405758	-6.9327891592	-0.4971387404
H	5.6551212523	-7.3733034128	0.9453517549
H	3.8423956163	-5.6888004348	1.1194006031
H	5.9690014776	-3.1139418383	-1.5849540224
H	7.7844958333	-4.7951092904	-1.7624031391
P	-0.3375391712	0.467883731	0.2106875153
C	-3.7877329854	-0.8334901503	3.0309958047
C	-4.0841630045	-0.0744140753	1.8973589868
C	-3.0636888184	0.319688971	1.0296107307
C	-1.7341061846	-0.0434513878	1.2924042883
C	-1.4450066484	-0.8159332515	2.4291995375
C	-2.4671814344	-1.2038042681	3.2953969657
H	-4.5844490107	-1.1427495112	3.7020320654
H	-5.1112534409	0.2083732728	1.683106603
H	-3.3051608433	0.9012303134	0.1449137669
H	-0.4210327259	-1.1209638557	2.6288615695
H	-2.2320757002	-1.8036864969	4.1701171522
C	-2.2755158191	1.2833951599	-3.9284272695
C	-1.8222576345	0.0071252374	-3.5866927324
C	-1.2307477818	-0.2157998041	-2.3435004053
C	-1.0969051419	0.8367213366	-1.4227419108
C	-1.5494912113	2.117096465	-1.7748056241
C	-2.1358147648	2.3367474821	-3.0231012503
H	-2.7284122532	1.4578844847	-4.9005954028
H	-1.9178206067	-0.8140946424	-4.2914754612
H	-0.861281363	-1.2060645208	-2.0898606325
H	-1.4367741147	2.9453555431	-1.0818241549
H	-2.478741726	3.3333062351	-3.2877865928
C	1.1529976089	4.5638819108	1.8086251148
C	-0.1482081998	4.1504909395	2.1007636351
C	-0.6145041679	2.9191760085	1.6364011352
C	0.2208420205	2.0898099904	0.8728016136
C	1.5320590131	2.5078824933	0.5918201125
C	1.9920829405	3.7410223646	1.0539515748
H	1.515015127	5.5205963302	2.1751187766
H	-0.8014241937	4.7833043012	2.6954381745
H	-1.6240232328	2.6012758655	1.8784616755
H	2.1940827115	1.8617440046	0.02117887
H	3.0092285482	4.052340591	0.8332053688

E (M^1 = Au(PPh_3), L = PPh_3)

E = -2651.890994 H

Au	1.536869155	-1.0809745503	-0.6080612437
Au	2.2950533105	-2.915972482	-3.01039855
C	3.0737194714	-2.3895005673	-1.1447494412
C	4.1085134138	-2.7467616913	-0.5532299067
C	7.6128700658	-3.9657462348	1.4483798183
C	6.4223253801	-4.6760825637	1.635504891
C	5.2632549823	-4.2786386412	0.9779558217
C	5.2865908517	-3.1560513257	0.1197561459
C	6.4948953525	-2.4459864867	-0.0618378444
C	7.6475976984	-2.8532442642	0.600944409
H	8.5157282201	-4.2799453721	1.9641623828
H	6.4012473224	-5.5388164983	2.2944993047
H	4.3331822978	-4.821332332	1.1145785614
H	6.5087710976	-1.5848191153	-0.7224689585
H	8.574633516	-2.305919597	0.4592669513
P	1.518741311	-3.5763646491	-5.121291659
C	-1.7177965408	-6.8794273995	-4.8373451268
C	-1.6572146047	-5.8608633161	-3.8828110348
C	-0.6700674874	-4.8799936998	-3.9695067095
C	0.2612982961	-4.9053636812	-5.0212100515
C	0.1972301827	-5.9321747093	-5.9755069119
C	-0.7903558863	-6.9145887032	-5.8801667494
H	-2.4824413177	-7.6474096264	-4.7645167167
H	-2.3724227016	-5.8348321585	-3.0657876911
H	-0.6191954557	-4.0974443089	-3.216425603
H	0.9183807304	-5.9714523511	-6.7858846136
H	-0.8308219819	-7.7086946	-6.6200457599
C	4.9329131734	-5.2737018174	-7.7520824073
C	4.91498775	-5.5046621135	-6.3742534806
C	3.8909208415	-4.97459295	-5.5904379344
C	2.8689804019	-4.2139914497	-6.1827750416
C	2.892952925	-3.9834799171	-7.5667832478
C	3.9238093657	-4.5130672883	-8.3455726823
H	5.7348412416	-5.6813755526	-8.3606986035
H	5.7017430231	-6.0906220022	-5.9081635998
H	3.886855944	-5.1487129044	-4.5172981786
H	2.1158366158	-3.3885546618	-8.0366657106
H	3.9379033019	-4.3276382333	-9.4156665088
C	-0.3406277542	-0.0511741725	-7.4906177739
C	-0.9461206359	-1.3079877306	-7.5439193488
C	-0.4066795016	-2.3791612391	-6.8281677689
C	0.7451070048	-2.1951766236	-6.04864462
C	1.3438997088	-0.9253162139	-5.9898520165
C	0.8057685716	0.1390428187	-6.7130850768
H	-0.7592802315	0.7779084223	-8.0540879768
H	-1.8382025804	-1.4590119826	-8.1448857814
H	-0.8834948199	-3.3530323249	-6.8771748609
H	2.231133201	-0.7691932199	-5.3811185315
H	1.2808247991	1.1149042507	-6.6684083928
P	-0.1366409586	0.3962512452	0.1091120485
C	-3.9150635448	-1.8682516022	1.5494519245
C	-4.0604388404	-0.6774007463	0.8358926326
C	-2.9338596319	0.0139626529	0.3849626255
C	-1.6501352055	-0.4878746463	0.6464220777
C	-1.5105354332	-1.6912600475	1.3585854773
C	-2.6388262939	-2.3737458673	1.8113310016
H	-4.7935324418	-2.4035117563	1.8982122967
H	-5.050906072	-0.2831407178	0.6276970104
H	-3.0574609982	0.9379804812	-0.1711649744
H	-0.5206694267	-2.0943835695	1.55785495
H	-2.5214964433	-3.3020077999	2.3630487142
C	-1.4951944636	3.2886527491	-3.2465697429
C	-1.1400797996	1.9706367639	-3.5449589759
C	-0.7170524965	1.1146294506	-2.5288814342
C	-0.6549890929	1.5687734602	-1.2010956621
C	-1.0092252616	2.8945569465	-0.907971088
C	-1.4273957246	3.7488594147	-1.9302351945
H	-1.8188494614	3.9575703422	-4.0389159032
H	-1.1808522185	1.6086584442	-4.5682577482
H	-0.4302603158	0.0939670677	-2.7687046083
H	-0.9541898432	3.2626965109	0.1117655287
H	-1.6970686934	4.7745876119	-1.6959633553

C	1.2927320841	3.0094168143	3.6568611516
C	-0.0303492335	2.5651648722	3.6219852085
C	-0.4764381936	1.7685797145	2.5655050643
C	0.4057857132	1.4110343786	1.5344877122
C	1.7379941553	1.8550192137	1.579207059
C	2.1761582361	2.6542352833	2.6343621318
H	1.6369615795	3.6258729105	4.4822201459
H	-0.7176435856	2.8346328093	4.4186624864
H	-1.5052022047	1.422204008	2.5505355701
H	2.4324159313	1.5703722482	0.7925201394
H	3.2081140984	2.9917396869	2.6622391756

H (M^1 = Au(PPh_3), L = PPh_3)
E = -3095.5179576 H

Au	6.8102315573	6.0193135928	6.8632003957
Au	6.5844714064	5.3124674214	1.0364876537
Au	8.1715478939	4.341792008	4.0505515571
C	7.3395235293	4.2203314434	6.1012513145
C	9.555167152	4.9482189161	2.3443209125
C	11.6988378941	6.0357447405	1.8487928269
C	8.0788457672	0.962792584	7.0227472987
C	10.990408447	4.9793778714	2.4547136924
C	7.5517596068	3.0218533528	5.796684926
C	7.712344107	1.5905157881	5.8157852333
C	11.6989510021	3.9683024677	3.1300057749
C	8.2187139388	-0.421929751	7.0728871332
C	7.4970410511	0.8073604589	4.6667151618
C	13.0894435629	6.0693512818	1.9150072616
C	7.6443161655	-0.5764116521	4.7272133734
C	8.3650809038	5.0652458811	1.9658388562
C	13.0894574619	4.0146099255	3.1942016187
H	11.1513329561	6.8172315626	1.3311258449
H	8.2520844432	1.5676646713	7.9073008844
H	11.153435358	3.1518607221	3.5939434557
H	8.4993442572	-0.8989103382	8.0074024862
H	7.2139774682	1.2906355823	3.7361655768
H	13.6295982598	6.8841026324	1.4416432068
H	7.4775989244	-1.1737386709	3.8355748645
H	13.6292824615	3.2303743482	3.7167489706
C	8.0040634141	-1.1939624112	5.9278548873
H	8.1176777484	-2.2732227883	5.9712172716
C	13.7872065465	5.0622262747	2.5874431629
H	14.8716845232	5.0937491184	2.637999113
P	6.1794795414	8.0985464795	7.7619982917
P	4.5206039747	5.6112503545	-0.0469456308
C	4.6747452097	9.0159173846	-3.186603953
C	5.4428875385	9.0877224134	-2.0219800285
C	5.3973858749	8.0513747539	-1.0898661401
C	4.5735895567	6.9352609373	-1.3126656584
C	3.8063907868	6.867614337	-2.4859098457
C	3.8595046084	7.9061353961	-3.417404455
H	4.7173369589	9.819589065	-3.9160601575
H	6.0855806981	9.9449551956	-1.8434106919
H	6.008171674	8.1054876433	-0.1921023477
H	3.1762313986	6.00493681	-2.6791789419
H	3.2667703947	7.8438296595	-4.3254345119
C	1.1661610924	6.6764726022	2.9757647354
C	1.2170766411	7.3395714128	1.7479861258
C	2.2236123964	7.0377167321	0.8269282224
C	3.1902042366	6.0689578068	1.1332998675
C	3.1391107817	5.411601524	2.3744362448
C	2.1281435074	5.7105200345	3.2873554068
H	0.3790984673	6.9092173672	3.6874486466
H	0.470995942	8.0896559642	1.5013449608
H	2.2541343961	7.5575603701	-0.1255127854
H	3.8894161717	4.6666051526	2.6269506509
H	2.0911035855	5.1894108948	4.2399388525
C	3.1316465787	1.7976197745	-2.2812569278
C	2.1844950838	2.5991862471	-1.6413401877
C	2.5848726563	3.7463078185	-0.9533053851
C	3.9425478005	4.0964830459	-0.9014033517
C	4.8918883241	3.2817901188	-1.541123739
C	4.4851702302	2.1405179668	-2.2313888479
H	2.816794003	0.9048573196	-2.8138381647
H	1.1320504656	2.3325879844	-1.6745296795
H	1.8417542239	4.3611783401	-0.454935254
H	5.9474933273	3.5381456787	-1.4978821815
H	5.2254987857	1.516447909	-2.7234394061
C	4.1660348183	10.7989316595	4.5770349836
C	5.0122095575	11.3749098635	5.5262364461
C	5.6359131279	10.5770748603	6.4879644114
C	5.4160717064	9.1916361556	6.5017198978
C	4.5704892369	8.6173955926	5.5379053687
C	3.9441663514	9.4190812084	4.5840480559
H	3.6829196537	11.4235676612	3.8309310156
H	5.1898313652	12.4465193392	5.5207669035
H	6.2940686616	11.0333609388	7.220969345
H	4.4042312212	7.5432333869	5.5307788113
H	3.2876946325	8.9643558961	3.8475403741
C	9.8090405657	10.4382428633	9.4413554489
C	9.9437324881	9.6346714518	8.306433499
C	8.8468712414	8.9250313272	7.818887471
C	7.6006001777	9.0212613166	8.4602590234
C	7.4718637082	9.828174853	9.6010765213
C	8.5749572405	10.5326130146	10.0873316227
H	10.6658798799	10.9846127277	9.8249629594
H	10.9041863479	9.5525941185	7.8059116722
H	8.9596797994	8.2910732565	6.9429494394
H	6.5179611327	9.901600573	10.1141733961
H	8.46881184	11.1514774264	10.9736292831
C	3.1472508301	7.6479803015	11.2370647596
C	3.0246072436	8.7243557433	10.3564550451
C	3.9221862759	8.8707854912	9.2969180387
C	4.9513127403	7.9349270803	9.1131652604
C	5.0648063878	6.8498598936	9.9983370798
C	4.168362715	6.711466177	11.0573705514
H	2.4459043365	7.535710509	12.0588633152
H	2.2289593854	9.4514892478	10.4909718988
H	3.8158794432	9.7078587653	8.6137134169
H	5.8514720632	6.1129758606	9.8568592055
H	4.2630223305	5.8693414145	11.736729022

Au(NHC-Me)CCPh
E = -748.4596578 H

Au	-0.2852149751	-3.9095662229	2.5761380354
C	1.4349305695	-3.7213780687	1.5960481907
C	2.4966809443	-3.6052050265	0.991296867
C	6.1717361696	-3.2029862022	-1.1019937789
C	4.9643239934	-2.890716913	-1.7325636497
C	3.7576161183	-3.0212808325	-1.0492204508
C	3.731382488	-3.4700783406	0.2880100916
C	4.9577984196	-3.7818000921	0.911735305
C	6.1608601185	-3.648610496	0.2224984069
H	7.1119204507	-3.1000806187	-1.6375149291
H	4.9627621739	-2.5434175776	-2.7629286322
H	2.8189699896	-2.7790421232	-1.5386008975
H	4.9485515278	-4.1277938091	1.9410222985
H	7.0952725263	-3.8938166845	0.7215159816
C	-2.0665182021	-4.1043145956	3.5914197941
C	-3.7953377081	-4.9607211996	4.7816736375
C	-4.0788651032	-3.6566931548	4.5343208373
H	-4.9315821851	-3.0541022847	4.8066945587
H	-4.3519373947	-5.7173022732	5.3129092406
N	-2.5642921763	-5.2176829165	4.199252946
N	-3.0137043834	-3.1488200871	3.8075357947
C	-1.8934141379	-6.5135672074	4.2415552686
H	-1.6716702571	-6.7893000735	5.2769187439
H	-2.5287180721	-7.2794470409	3.7869117958
H	-0.962278724	-6.4337143339	3.6800119733
C	-2.929077609	-1.7704297011	3.3342033242
H	-2.9818113938	-1.0795574742	4.18084638
H	-1.9752751517	-1.6442831125	2.8213002912
H	-3.7471048704	-1.5601078849	2.6386630718

E (M^1 = Au(NHC-Me), L = PPh_3)
E = -1920.4273084 H

Au	-0.5675467662	-3.8890625095	2.4539865396
Au	0.35106523	-3.3421155717	-0.9545286633
C	0.9671880146	-3.6664151562	1.1579002507
C	2.1021629425	-3.5535890803	0.6508112559
C	6.1716802246	-3.3768651867	-0.5115187334

C	5.5879051469	-4.6050712437	-0.1880881959
C	4.2466468703	-4.6666864822	0.1811880834
C	3.4757683707	-3.4882829893	0.2364685346
C	4.0723913484	-2.2537565842	-0.087667577
C	5.412743574	-2.2039724936	-0.4609435649
H	7.2178885641	-3.3333348438	-0.8000126401
H	6.1791919854	-5.5153130723	-0.2226407693
H	3.7863996539	-5.6159630475	0.437332779
H	3.4792824791	-1.3457370668	-0.0365345238
H	5.8681963992	-1.2495757297	-0.7080108157
C	-0.5586145749	-3.082301975	-2.7617340965
C	-1.6539666911	-2.1646772588	-4.5088358222
C	-1.3806109058	-3.4554465178	-4.8302515774
H	-1.5993698371	-4.0237198001	-5.7211393501
C	-2.0622386195	-4.129653783	3.8448892842
C	-3.6867608552	-5.0345808099	5.1292847175
C	-3.5065872143	-3.7537611106	5.5418604741
H	-3.9923559932	-3.1869055022	6.3210597596
H	-2.1587038444	-1.3893224812	-5.0642916849
H	-4.3598020827	-5.8021468401	5.479017142
N	-2.795697143	-5.2483909366	4.0908983659
N	-1.14450763	-1.9521804269	-3.2390918646
N	-0.7110958127	-4.0037836929	-3.7496246062
N	-2.5094281782	-3.214598274	4.7462796731
C	-0.2297691532	-5.3842207972	-3.7088690982
H	-1.0685459375	-6.0734959714	-3.8379314408
H	0.5041961839	-5.5463180514	-4.5029103963
H	0.2391333177	-5.5594639403	-2.7406935301
C	-1.2324406691	-0.6748011935	-2.5327719059
H	-0.7256924201	0.1039484134	-3.10915051
H	-2.2809815404	-0.4006494425	-2.3882922528
H	-0.7479087264	-0.7812298663	-1.5622731233
C	-2.6670431474	-6.5195261432	3.3807738418
H	-2.3655627902	-7.3070438366	4.0769773095
H	-3.620947172	-6.7858019521	2.917261514
H	-1.9054177793	-6.4091670392	2.6087742986
C	-2.0127769677	-1.8463083519	4.8837559415
H	-1.6028653448	-1.6979683864	5.8865110894
H	-1.2267265129	-1.6867894119	4.1456372065
H	-2.8254349704	-1.1352288471	4.7113672999

H (M^1 = Au(NHC-Me), L = PPh_3
E = -1632.5947035 H

Au	1.536869155	-1.0809745503	-0.6080612437
Au	2.2950533105	-2.915972482	-3.01039855
C	3.0737194714	-2.3895005673	-1.1447494412
C	4.1085134138	-2.7467616913	-0.5532299067
C	7.6128700658	-3.9657462348	1.4483798183
C	6.4223253801	-4.6760825637	1.635504891
C	5.2632549823	-4.2786386412	0.9779558217
C	5.2865908517	-3.1560513257	0.1197561459
C	6.4948953525	-2.4459864867	-0.0618378444
C	7.6475976984	-2.8532442642	0.600944409
H	8.5157282201	-4.2799453721	1.9641623828
H	6.4012473224	-5.5388164983	2.2944993047
H	4.3331822978	-4.821332332	1.1145785614
H	6.5087710976	-1.5848191153	-0.7224689585
H	8.574633516	-2.305919597	0.4592669513
P	1.518741311	-3.5763646491	-5.121291659
C	-1.7177965408	-6.8794273995	-4.8373451268
C	-1.6572146047	-5.8608633161	-3.8828110348
C	-0.6700674874	-4.8799936998	-3.9695067095
C	0.2612982961	-4.9053636812	-5.0212100515
C	0.1972301827	-5.9321747093	-5.9755069119
C	-0.7903558863	-6.9145887032	-5.8801667494
H	-2.4824413177	-7.6474096264	-4.7645167167
H	-2.3724227016	-5.8348321585	-3.0657876911
H	-0.6191954557	-4.0974443089	-3.216425603
H	0.9183807304	-5.9714523511	-6.7858846136
H	-0.8308219819	-7.7086946	-6.6200457599
C	4.9329131734	-5.2737018174	-7.7520824073
C	4.91498775	-5.5046621135	-6.3742534806
C	3.8909208415	-4.97459295	-5.5904379344
C	2.8689804019	-4.2139914497	-6.1827750416
C	2.892952925	-3.9834799171	-7.5667832478
C	3.9238093657	-4.5130672883	-8.3455726823
H	5.7348412416	-5.6813755526	-8.3606986035
H	5.7017430231	-6.0906220022	-5.9081635998
H	3.886855944	-5.1487129044	-4.5172981786
H	2.1158366158	-3.3885546618	-8.0366657106
H	3.9379033019	-4.3276382333	-9.4156665088
C	-0.3406277542	-0.0511741725	-7.4906177739
C	-0.9461206359	-1.3079877306	-7.5439193488
C	-0.4066795016	-2.3791612391	-6.8281677689
C	0.7451070048	-2.1951766236	-6.04864462
C	1.3438997088	-0.9253162139	-5.9898520165
C	0.8057685716	0.1390428187	-6.7130850768
H	-0.7592802315	0.7779084223	-8.0540879768
H	-1.8382025804	-1.4590119826	-8.1448857814
H	-0.8834948199	-3.3530323249	-6.8771748609
H	2.231133201	-0.7691932199	-5.3811185315
H	1.2808247991	1.1149042507	-6.6684083928
P	-0.1366409586	0.3962512452	0.1091120485
C	-3.9150635448	-1.8682516022	1.5494519245
C	-4.0604388404	-0.6774007463	0.8358926326
C	-2.9338596319	0.0139626529	0.3849626255
C	-1.6501352055	-0.4878746463	0.6464220777
C	-1.5105354332	-1.6912600475	1.3585854773
C	-2.6388262939	-2.3737458673	1.8113310016
H	-4.7935324418	-2.4035117563	1.8982122967
H	-5.050906072	-0.2831407178	0.6276970104
H	-3.0574609982	0.9379804812	-0.1711649744
H	-0.5206694267	-2.0943835695	1.55785495
H	-2.5214964433	-3.3020077999	2.3630487142
C	-1.4951944636	3.2886527491	-3.2465697429
C	-1.1400797996	1.9706367639	-3.5449589759
C	-0.7170524965	1.1146294506	-2.5288814342
C	-0.6549890929	1.5687734602	-1.2010956621
C	-1.0092252616	2.8945569465	-0.907971088
C	-1.4273957246	3.7488594147	-1.9302351945
H	-1.8188494614	3.9575703422	-4.0389159032
H	-1.1808522185	1.6086584442	-4.5682577482
H	-0.4302603158	0.0939670677	-2.7687046083
H	-0.9541898432	3.2626965109	0.1117655287
H	-1.6970686934	4.7745876119	-1.6959633553
C	1.2927320841	3.0094168143	3.6568611516
C	-0.0303492335	2.5651648722	3.6219852085
C	-0.4764381936	1.7685797145	2.5655050643
C	0.4057857132	1.4110343786	1.5344877122
C	1.7379941553	1.8550192137	1.579207059
C	2.1761582361	2.6542352833	2.6343621318
H	1.6369615795	3.6258729105	4.4822201459
H	-0.7176435856	2.8346328093	4.4186624864
H	-1.5052022047	1.422204008	2.5505355701
H	2.4324159313	1.5703722482	0.7925201394
H	3.2081140984	2.9917396869	2.6622391756

Au(IPr)CCPh
E = -1603.6848506 H

Au	-0.2012219387	-3.7710620399	2.8457541278
C	1.1852547711	-3.3760216809	1.4731795925
C	2.0404883968	-3.132343218	0.6267276504
C	5.0005492371	-2.2888985274	-2.3028129052
C	4.6717482481	-3.6117064194	-1.9942325916
C	3.7016704241	-3.891715085	-1.0347456592
C	3.0346821573	-2.8490500116	-0.3572395818
C	3.3774705914	-1.5186593329	-0.6790970884
C	4.3479911254	-1.2457176218	-1.6401715571
H	5.7577370031	-2.0731452119	-3.0521783279
H	5.1740567178	-4.4300306677	-2.5045636911
H	3.4451580186	-4.9192546015	-0.7946088603
H	2.8701920772	-0.7087530181	-0.1633235606
H	4.5970980233	-0.213287143	-1.873494497
C	-1.6311663659	-4.1785743721	4.2617704063
C	-3.2094278045	-5.2366288582	5.5098220625
C	-3.0746402338	-3.9819360421	6.0069671536
H	-3.566674113	-3.4820572062	6.8262391661
H	-3.843274261	-6.0574783287	5.8058370655
N	-2.3220237648	-5.3422997479	4.4449066997
N	-2.1078226448	-3.3476835814	5.2351799586
C	-1.9219586706	-8.8570839861	2.1512592164
C	-1.1198804079	-8.6642908373	3.2725104944

C	-1.2230918824	-7.502319856	4.0469097556
C	-2.1710143096	-6.5397662531	3.6471678202
C	-2.9941913356	-6.7043275466	2.5157271071
C	-2.8471659378	-7.8859179235	1.7790219041
H	-1.822907111	-9.7655647234	1.5632589214
H	-0.3966314618	-9.4253747338	3.5505826412
H	-3.4628117103	-8.0428548911	0.8981529088
C	-0.8889363904	0.6289818165	5.9244112681
C	-1.9368322579	0.365867995	5.0466928269
C	-2.3561471745	-0.9451915325	4.7901363605
C	-1.6772984531	-1.9843368639	5.4566192918
C	-0.6111412703	-1.7502674911	6.3473400538
C	-0.2347998038	-0.4193524451	6.5653747698
H	-0.5784397184	1.6543191088	6.1065325626
H	-2.4363016303	1.1906584005	4.546781271
H	0.5864802429	-0.2036189372	7.2425317907
C	-4.0093610643	-5.6568375611	2.0693517124
H	-3.9622863106	-4.8156440833	2.7677442101
C	-5.4481191458	-6.2084643302	2.1144630356
H	-5.7118284773	-6.562682188	3.1178275059
H	-6.1636877262	-5.4279902767	1.8305033941
H	-5.5789809017	-7.0469558906	1.4206541176
C	-3.6663868521	-5.1043457057	0.6716553418
H	-3.7216778022	-5.8869510881	-0.09408676
H	-4.3753421042	-4.3155877682	0.3929227882
H	-2.6563730202	-4.6820121758	0.6517637155
C	-0.3204098609	-7.3217751669	5.2631684141
H	-0.5481199688	-6.3523781686	5.7169175606
C	-0.5891930624	-8.4012739659	6.3303506424
H	-0.3614805486	-9.4047593638	5.952532942
H	0.0378901841	-8.2284709868	7.2128182956
H	-1.637211808	-8.3968305352	6.6518776983
C	1.1671182126	-7.2933997442	4.8594915863
H	1.4827766512	-8.2473915117	4.4210559301
H	1.3617679194	-6.5029037463	4.1272509824
H	1.7937949857	-7.1088565204	5.7402014488
C	-3.5016806456	-1.195224464	3.8144539879
H	-3.6626408392	-2.2754410154	3.7459233116
C	-4.8171537076	-0.5672269679	4.3160321897
H	-5.0932315625	-0.948855949	5.3059225532
H	-4.7385896634	0.5236037886	4.3901762896
H	-5.6358826297	-0.7948858878	3.6234290271
C	-3.1508344844	-0.6998972509	2.3973922314
H	-3.0029169724	0.3862214436	2.3765355877
H	-2.2347970335	-1.1738814991	2.0297464415
H	-3.9646455121	-0.9379064049	1.7020576121
C	0.1379816716	-2.8734637613	7.0574733032
H	-0.3012713225	-3.8266941422	6.7476676395
C	1.6231000826	-2.9043590835	6.6452856591
H	1.7289288594	-3.0085350583	5.5604656657
H	2.1435716722	-1.9889459076	6.9502714321
H	2.1303527425	-3.7505627018	7.1239086829
C	-0.0150554719	-2.7756240396	8.5882806805
H	0.4229694396	-1.8492426585	8.9775317249
H	-1.0689133047	-2.797437458	8.8893841418
H	0.4952423466	-3.6144801361	9.0758530167

E (M^1 = Au(IPr), L = PPh_3)
E = -2775.6568094 H

H (M^1 = Au(IPr), L = PPh_3)
E = -3343.0530772 H

S5.5. Trigold complex $[6]^+$ optimised with BP86-D3 and M06

BP86-D3
E = -3069.68736839138 hartrees

Au1	6.4379230405	5.7021199530	6.3045621070
Au2	6.5433554639	5.6243184659	1.6568596212
Au3	8.4778971956	4.0211183090	4.0772391989
C4	3.7516951293	3.5140370813	-1.8225898713
C5	8.0054065811	9.0658496755	9.5459466825
C6	5.0089837231	2.9083842570	-1.6217254623
C7	2.6104950823	8.3055373069	1.3898410010
C8	6.8250093513	9.1833047342	8.8025381720
C9	8.8286683358	7.9279064652	9.4280086242
C10	7.3210424538	9.3461053813	4.7736682881
C11	3.9413377327	6.9850078846	5.4741944606
C12	3.0715058911	4.1687155318	3.0653648920
C13	10.1263236439	7.7616488761	10.2372920554
C14	7.7614297047	4.2142803596	6.1633550793
C15	3.3664534930	4.6412921528	-1.0862433657
C16	9.4770402853	4.3637211980	2.0859526011
C17	4.1422414050	1.8325343803	2.7424720351
C18	5.8660058484	3.4663261387	-0.6334612608
C19	4.7890447219	7.8637492206	2.3515987087
C20	2.9527789432	7.9850004952	5.4613021612
C21	4.2264926660	5.1840407213	-0.1127186952
C22	9.8321589771	8.7935760999	5.1096449780
C23	11.3645189899	3.8310411793	0.6012612585
C24	5.5006422718	4.5732187106	0.1352689728
C25	6.4406326573	8.1694639254	7.9067580826
C26	5.0701276643	4.8596132516	4.9316510852
C27	4.0921150804	3.2392325853	3.3555724153
C28	5.9707504499	8.0718945893	3.1906155153
C29	5.4644352476	1.6671715097	-2.4093133048
C30	2.7266410380	7.1685863697	0.5794091112
C31	3.9776692649	5.7487462897	4.6897732271
N32	4.8717318011	6.7783281702	1.5243944068
C33	9.2450430388	1.5976068365	7.8676109216
C34	8.4369616952	8.5184200154	4.5315427367
C35	7.2717858647	7.0125542871	7.7442317376
C36	10.8876527038	4.1805982488	1.8879527317
C37	3.8955125837	6.3880659212	0.6544940598
C38	7.0543738825	7.1571838608	3.0174323945
N39	5.0066811052	7.1475325794	6.3153003698
C40	2.9991697398	5.3940628230	3.7403613046
C41	3.1027039977	9.1041747641	6.2917132700
C42	8.3321534510	3.0815751917	6.1401095847
C43	4.2248898758	9.2410864004	7.1196152259
C44	5.2010324277	8.2270643534	7.1259322008
C45	6.1113162859	9.1411170470	4.0965953892
C46	8.9140073105	1.8228903482	6.5087324041
C47	11.8052017205	4.3779229764	2.9477931094
C48	9.7714543555	0.3609931449	8.2553408391
C49	9.1267431907	0.8029586029	5.5512863113
C50	12.7397667705	3.6950442688	0.3839671492
C51	9.6625894565	-0.4256445053	5.9518050081
C52	8.2386661789	4.6058769373	1.9467335913
C53	13.1769214999	4.2313080499	2.7186176278
X54	8.1697595000#	3.9983050000#	6.1974750000#
X55	8.6241420000#	4.3226030000#	1.8992395000#
H56	3.0574308145	3.1126389050	-2.5648614558
H57	8.2753345954	9.8762249034	10.2271685388
H58	1.7105070582	8.9264146811	1.3228837506
H59	6.2050978796	10.0778505146	8.9312470048
H60	7.3925373394	10.1775858654	5.4789644428
H61	2.3087785773	3.9361634580	2.3179682809
H62	2.1693678932	1.8531286643	1.7423273122
H63	3.5200119117	2.4421774736	0.7196531422
H64	9.8333217367	7.0349192121	6.4209712425
H65	10.6248254475	6.7382606987	4.8473664084
H66	2.3887367162	5.0961769137	-1.2839404326
H67	6.8452117261	3.0078710411	-0.4578194818
H68	2.0823794908	7.8795981126	4.8100885579
H69	10.6504424451	3.6770157246	-0.2137488200
H70	1.9283792282	6.8932539257	-0.1140761199
H71	9.0758712863	2.3931264797	8.6007047822
H72	2.1777057045	6.0809781529	3.5063287394
H73	2.3334328618	9.8840056752	6.2923569416
H74	4.3423756890	10.1181316137	7.7604250056
H75	6.2763300449	1.4097025194	3.2129629787
H76	6.0051955833	2.2061837011	1.6384643479
H77	5.2764482287	9.8265464071	4.2802322713
H78	11.4270977175	4.6468865358	3.9409295405
H79	10.8039360278	8.6117916258	3.1346174907

H80	10.2760665724	10.2714757333	3.5304768110
H81	10.0201000823	0.1856949946	9.3075481415
H82	8.8645519015	0.9903826123	4.5033436850
H83	13.1051667638	3.4303600809	-0.6141680826
H84	9.8268325522	-1.2137965243	5.2091478028
H85	13.8834300835	4.3853570440	3.5412498999
C86	9.9835095883	-0.6498450858	7.3017166997
H87	10.3992399239	-1.6144072790	7.6119399280
C88	13.6471165973	3.8913477448	1.4387223727
H89	14.7222861399	3.7786298729	1.2625205204
C90	5.7628484869	0.5149623887	-1.4136272744
H91	6.5612661218	0.7787199086	-0.6984942091
H92	4.8610387621	0.2574046283	-0.8310560482
H93	6.0868981400	-0.3868570636	-1.9638197229
C94	6.7503916490	2.0167374792	-3.2031340449
H95	7.5725136595	2.3291651573	-2.5358677178
H96	7.0948128106	1.1356794714	-3.7743157731
H97	6.5605506684	2.8375802551	-3.9174716940
C98	4.3921076769	1.1782172486	-3.4068065716
H99	4.7623191828	0.2869313209	-3.9427885656
H100	3.4555992887	0.8912650663	-2.8950846402
H101	4.1554467912	1.9453669619	-4.1662110598
C102	3.6324016760	8.6606245370	2.2810198418
H103	3.5466636906	9.5482980462	2.9112671636
C104	5.5960074591	1.4625727590	2.3418019585
H105	5.6094550968	0.4736964770	1.8489689265
C106	3.2382176368	1.7117015299	1.4955302781
H107	3.3372205100	0.7012616405	1.0613748218
C108	3.6418271966	0.8358086359	3.8260076083
H109	3.6647580958	-0.1971234139	3.4314987878
H110	4.2766627395	0.8738060667	4.7315174860
H111	2.6030466771	1.0672693188	4.1286440335
C112	5.0785527955	3.6167124291	4.3004314683
H113	5.8780196842	2.9102193901	4.5404424354
C114	8.4306055828	6.9124142870	8.5160176014
H115	9.0555873677	6.0196014073	8.4047269982
C116	10.4146267065	8.9788228851	11.1423960701
H117	10.5367637181	9.9071031068	10.5548794416
H118	9.6139189185	9.1381015911	11.8868256781
H119	11.3538105568	8.8140114153	11.6985003241
C120	9.9988834500	6.5009780771	11.1330909895
H121	10.9206359707	6.3621138680	11.7265910868
H122	9.1499052704	6.5994334421	11.8327964001
H123	9.8412130822	5.5863406822	10.5351742730
C124	11.3196558458	7.5897013422	9.2604287533
H125	12.2600338492	7.4724701569	9.8283078646
H126	11.2037629232	6.7018721940	8.6153740015
H127	11.4199044326	8.4715426071	8.6031072175
C128	8.2642544834	7.4180119809	3.6572244385
H129	9.1161251107	6.7635883711	3.4566135613
C130	9.7906093817	9.8297351888	6.2501412620
H131	9.1379468959	9.4972541248	7.0753039423
H132	10.8066705729	9.9745492313	6.6577331339
H133	9.4414010484	10.8159911385	5.8959134326
C134	10.7101544479	9.3478639630	3.9527572754
H135	11.7258096053	9.5811257779	4.3223627669
C136	10.4688103319	7.4868179881	5.6433478590
H137	11.4565982561	7.7066765147	6.0866941734

M06

E = -3067.11080431245 Hartrees

Au1	6.3523593325	5.6158949235	6.3856695513
Au2	6.5233719836	5.7332322851	1.6506712186
Au3	8.3358170408	4.1449841125	4.0927024774
C4	3.9134899612	3.7303870588	-1.9738429301
C5	7.7521708279	8.8356050046	9.7933942403
C6	5.1453385524	3.1179453392	-1.7295515352
C7	2.6183634579	8.3745838339	1.3097665803
C8	6.5794648447	8.9418032481	9.0552338502
C9	8.6302770631	7.7652871873	9.6050397011
C10	7.1785444041	9.4193167768	4.8113923743
C11	3.8470485688	6.8594056286	5.5777222732
C12	3.0477803407	4.1454086081	3.0732725844
C13	9.9116098994	7.6032561801	10.4175796451
C14	7.8609583989	4.3022347683	6.2639261279
C15	3.4919614881	4.8217174822	-1.2229584663
C16	9.1295846590	3.8134147882	1.9172629409
C17	4.1210289662	1.8528789627	2.6639407647
C18	5.9356611810	3.6257151291	-0.6797746727
C19	4.7363284234	7.9234870185	2.3431015181
C20	2.8167149390	7.7960635163	5.6285212148
C21	4.2919616905	5.3236728015	-0.1970028993
C22	9.6585752378	8.9232115220	5.2365429741
C23	10.2985903577	2.0997425272	0.6239985410
C24	5.5364607132	4.7034762097	0.0902875920
C25	6.2569457515	7.9839303348	8.0954275186
C26	5.0195883549	4.7859954526	4.9555008117
C27	4.0741713963	3.2283021857	3.3204220490
C28	5.8954934195	8.1283012084	3.2141070121
C29	5.6532787928	1.9322477833	-2.5450705262
C30	2.7684080366	7.2729813877	0.4754991287
C31	3.9314887256	5.6670361524	4.7349627753
N32	4.8423960146	6.8626680099	1.5109552991
C33	10.6587922759	2.7639282468	7.7208237461
C34	8.3030575515	8.6117784817	4.6113776887
C35	7.1398990890	6.8957950930	7.8716298185
C36	10.2613830216	2.9570022202	1.7318366427
C37	3.9235283918	6.5006150329	0.5877331124
C38	6.9978977547	7.2522607017	3.0505539664
N39	4.8878443162	7.0196453719	6.4253764555
C40	2.9673856592	5.3394495798	3.7805533634
C41	2.9074664344	8.8466253617	6.5352571617
C42	8.7930488288	3.4795816747	6.3173896573
C43	4.0075852537	8.9832269622	7.3735221266
C44	5.0262894304	8.0347388163	7.3066509358
C45	5.9967222011	9.1894700902	4.1158509395
C46	9.8654451651	2.5718135625	6.5814360103
C47	11.3264372080	2.9635828003	2.6427988584
C48	11.6912797663	1.8810529467	7.9992620621
C49	10.1223084827	1.4916389301	5.7269652451
C50	11.3917488442	1.2678882970	0.4316878543
C51	11.1646394364	0.6215023801	6.0080186596
C52	8.1249368308	4.5498919739	1.8990609555
C53	12.4095091046	2.1202973255	2.4476424552
X54	8.1697595000#	3.9983050000#	6.1974750000#
X55	8.6241420000#	4.3226030000#	1.8992395000#
H56	3.2680854771	3.3656969535	-2.7692816777
H57	7.9714090027	9.6015532017	10.5332720019
H58	1.7261950352	8.9925080997	1.2218664396
H59	5.9142932841	9.7850110225	9.2422282012
H60	7.2198394099	10.2553927417	5.5069975083
H61	2.2835130175	3.9272983302	2.3299774162
H62	2.1864701314	1.9375603956	1.6301634371
H63	3.5641521577	2.5215375964	0.6564731835
H64	9.7553422823	7.0566261346	6.3724594587
H65	10.6406167127	6.9917551584	4.8295602911
H66	2.5327729650	5.2849875107	-1.4561210381
H67	6.9001617606	3.1594702272	-0.4686157263
H68	1.9507779046	7.6934286877	4.9792701903
H69	9.4644991210	2.0965035593	-0.0771644188
H70	2.0095117100	7.0247757743	-0.2614446971
H71	10.4521393125	3.6067504600	8.3797495026
H72	2.1304853784	6.0125283004	3.5855994831
H73	2.0990734878	9.5736587364	6.5938887553
H74	4.0685264433	9.8047405712	8.0823676422
H75	6.2219247129	1.3677741056	3.1327283378
H76	5.9868733818	2.2213000367	1.5877914620
H77	5.1554409263	9.8668534107	4.2706785311
H78	11.2904557812	3.6334102027	3.5038170073
H79	10.6475575168	8.9963909076	3.2815312835
H80	10.0299903622	10.5648110311	3.8411718187
H81	12.3031439006	2.0289797609	8.8869654020
H82	9.4985360342	1.3493592865	4.8427847373
H83	11.4207336323	0.6058546255	-0.4314872286
H84	11.3658727998	-0.2127098290	5.3384948849
H85	13.2311241762	2.1241923970	3.1616148354
C86	11.9473976025	0.8131774205	7.1435292184
H87	12.7621972584	0.1258977045	7.3637865884
C88	12.4446798670	1.2743993485	1.3424655819
H89	13.2974782125	0.6154434595	1.1897890370
C90	5.8781737915	0.7367768782	-1.6107671307

H91	6.6194791436	0.9515657434	-0.8284677445
H92	4.9413466013	0.4470105301	-1.1124894236
H93	6.2383161254	-0.1294563872	-2.1834785501
C94	6.9767455969	2.3133771663	-3.2210232470
H95	7.7517661993	2.5881688061	-2.4930847760
H96	7.3576436201	1.4674680781	-3.8105974696
H97	6.8407050653	3.1654195154	-3.9009128611
C98	4.6663636185	1.5100231219	-3.6310357138
H99	5.0733058946	0.6561201034	-4.1889270426
H100	3.7013035864	1.1963130469	-3.2090782305
H101	4.4829143846	2.3164736932	-4.3545741893
C102	3.5902420001	8.7104932829	2.2467912403
H103	3.4700937955	9.5832134381	2.8831290283
C104	5.5532466783	1.4734091368	2.2669840049
H105	5.5467674645	0.5043397232	1.7477532696
C106	3.2512742476	1.7828456977	1.4090345145
H107	3.3392689474	0.7851353184	0.9573409312
C108	3.5927964918	0.8347913923	3.6853359286
H109	3.6109118516	-0.1781734675	3.2579746149
H110	4.2011305785	0.8275392868	4.6002236078
H111	2.5571370345	1.0647883543	3.9726304995
C112	5.0489486462	3.5806489855	4.2726206290
H113	5.8566079663	2.8775889910	4.4815307820
C114	8.2944892669	6.8053825158	8.6299419160
H115	8.9651271599	5.9595949841	8.4651685195
C116	10.1328515180	8.7624676655	11.3874722093
H117	10.2141720535	9.7250441813	10.8632259403
H118	9.3256725085	8.8388419201	12.1291692714
H119	11.0693456987	8.6083821607	11.9398434640
C120	9.8270021237	6.3053845610	11.2307747239
H121	10.7408998287	6.1713365407	11.8268027228
H122	8.9728065118	6.3289909358	11.9213083238
H123	9.7128689348	5.4212178285	10.5892419060
C124	11.1169689948	7.5409900641	9.4713669938
H125	12.0450161868	7.4264136602	10.0492589734
H126	11.0570126419	6.6980831351	8.7689530585
H127	11.1992640861	8.4647718699	8.8801519187
C128	8.1753345693	7.5237378238	3.7283363192
H129	9.0385552248	6.8783158423	3.5596280944
C130	9.5374850177	9.8457222342	6.4492670988
H131	8.8988528623	9.4106403742	7.2315281765
H132	10.5333750927	10.0131457342	6.8826654622
H133	9.1396048001	10.8343577000	6.1828685872
C134	10.5063441079	9.6298903122	4.1680347269
H135	11.4993451481	9.8763099720	4.5710907902
C136	10.3750060925	7.6402686956	5.6760321562
H137	11.3135080942	7.8974217415	6.1875951417