Supporting Information

Au(I)-Catalyzed Hydroarylation of Alkenes with *N,N*-dialkylanilines : a dual gold catalysis affair

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I. General Remarks

All reactions were carried out under argon atmosphere and all glassware was flamed before use. The solvents were purified by an Innovative Technology Pure Solv. Device (activated alumina column containing a copper catalyst and molecular sieves) and degassed.

Benzene and 1,2-Dichloroethane were dried under Na metal or K metal and CaH_2 respectively.

Chromatographic purifications were conducted using Merck silica gel Si 60 (40-63 □m) and TLC were performed on silica gel 60-F254 plates (0.1 mm) with UV or $KMnO_4$ detection.

^{1}H, ^{13}C, ^{31}P NMR spectra were recorded on a BRUKER AVANCE III 400 or 500 spectrometer. ^{1}H and ^{13}C NMR chemical shifts δ are reported in ppm using the residual peak of chloroform-*d* (7.26 for ^{1}H NMR; 77.16 ppm for ^{13}C NMR) or Dichloromethane-*d2* (5.32 for ^{1}H NMR; 55.84 ppm for ^{13}C NMR) as internal standard. Coupling constants *J* are reported in Hertz (Hz). Abbreviations are used as follow: s = singlet, d = doublet, t = triplet, q = quadruplet, sept = septuplet, m = multiplet, br = broad.

High Resolution Mass Spectrometry (**HRMS**) was performed on a QTOF Micro WATERS spectrometer or on a GC-MS Mate JEOL spectrometer.

Gas chromatography: was performed on a Shimadzu-2014

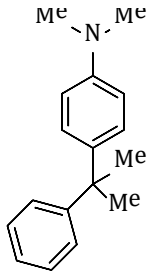
InfraRed spectra (**IR**) were recorded on a Perkin Elmer Spectrum One FTIR spectrometer equipped with an ATR device, and only the strongest or structurally most important peaks are listed.

Melting points (**Mp**) were measured with a Gallenkamp Melting Point Apparatus.

All commercially available compounds were used as received. PPh_3AuCl was prepared according to the literature procedures.[1]

II. Product characterization

Compound 1



Reaction temperature: 135°C, Yellow oil; 95% yield (isolated)

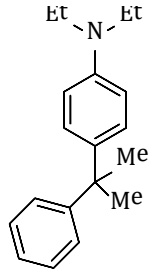
^{1}H NMR (CD_2Cl_2, 400 MHz) δ 7.28 (d, J_{HH} = 4.2 Hz, 4H), 7.21-7.16 (m, 1H), 7.13 (d, J_{HH} = 8.9 Hz, 2H), 6.69 (d, J_{HH} = 8.9 Hz, 2H), 2.92 (s, 6H), 1.68 (s, 6H).

^{13}CNMR (CD_2Cl_2, 100 MHz) δ 151.9 (Cq_{aro}), 149.2 (Cq_{aro}), 139.1 (Cq_{aro}), 128.2 (CH), 127.6 (CH), 127.1 (CH), 125.7 (CH), 112.7 (CH), 42.3 (Cq), 40.9 (CH_3-N), 30.9 (CH_3).

IR (ATR, cm^{-1}) 2965, 2871, 2797, 1682, 1614, 1519, 1493, 1443, 1344, 1202, 1166, 816, 763, 698.

HRMS (ESI) calcd for $C_{17}H_{22}N$ [M+H]: 240.1752, found: 240.1756.

Compound 2



Reaction temperature: 135°C, Yellow oil; 98% yield (isolated)

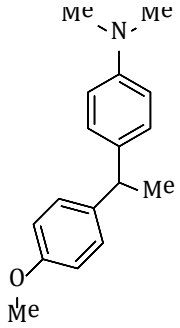
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.27-7.22 (m, 4H), 7.16-7.12 (m, 1H), 7.05 (d, J_{HH} = 8.8 Hz, 2H), 6.58 (d, J_{HH} = 8.8 Hz, 2H), 3.30 (q, J_{HH} = 7.0 Hz, 4H), 1.16 (s, 6H), 1.13 (t, J_{HH} = 7.0 Hz, 6H).

^{13}CNMR ($CDCl_3$, 100 MHz) δ 151.6 (Cq_{aro}), 145.9 (Cq_{aro}), 137.6 (Cq_{aro}), 127.9 (CH), 127.7 (CH), 126.9 (CH), 125.4 (CH), 111.4 (CH), 44.3 (CH_2-N), 42.0 (Cq), 31.0 (CH_3), 12.8 (CH_3).

IR (ATR, cm^{-1}) 2966, 2869, 2797, 1612, 1517, 1493, 1445, 1359, 1264, 1201, 813, 762, 698.

HRMS (ESI) calcd for $C_{19}H_{26}N$ [M+H]: 268.2065, found: 268.2077.

Compound 3



Reaction temperature: 100°C, Yellow oil; 99% yield (isolated)

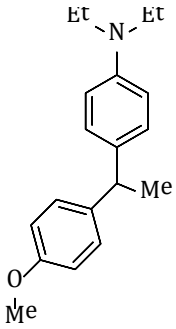
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.13 (d, J_{HH} = 8.6 Hz, 2H), 7.08 (d, J_{HH} = 8.6 Hz, 2H), 6.81 (d, J_{HH} = 8.7 Hz, 2H), 6.68 (d, J_{HH} = 8.7 Hz, 2H), 4.02 (q, J_{HH} = 8.7 Hz, 1H), 3.77 (s, 3H), 2.90 (s, 6H), 1.57 (d, J_{HH} = 7.2 Hz, 3H).

^{13}CNMR ($CDCl_3$, 100 MHz) δ 157.7 (Cq_{aro}), 149.1 (Cq_{aro}), 139.6 (Cq_{aro}), 135.1 (Cq_{aro}), 128.5 (CH), 128.2 (CH), 113.7 (CH), 112.9 (CH), 55.3 (CH_3-O), 43.0 (CH), 40.9 (CH_3), 22.4 (CH_3-N).

IR (ATR, cm^{-1}) 2930, 2833, 2797, 1611, 1508, 1442, 1341, 1242, 1175, 1162, 1032, 946, 831, 813.

HRMS (ESI) calcd for $C_{17}H_{22}NO$ [M+H]: 256.1701, found: 256.1705.

Compound 4



Reaction temperature: 100°C, Yellow oil; 82% yield (isolated)

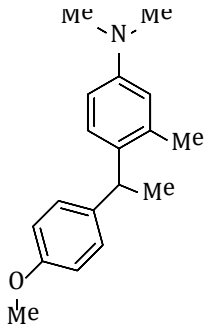
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.15 (d, J_{HH} = 8.6 Hz, 2H), 7.05 (d, J_{HH} = 8.6 Hz, 2H), 6.82 (d, J_{HH} = 8.7 Hz, 2H), 6.61 (d, J_{HH} = 8.7 Hz, 2H), 4.01 (q, J_{HH} = 7.2 Hz, 1H), 3.78 (s, 3H), 3.31 (q, J_{HH} = 7.0 Hz, 4H), 1.58 (d, J_{HH} = 7.2 Hz, 3H), 1.30 (t, J_{HH} = 7.0 Hz, 6H)

^{13}CNMR ($CDCl_3$, 100 MHz) δ 157.7 (Cq_{aro}), 146.2 (Cq_{aro}), 139.7 (Cq_{aro}), 133.7 (Cq_{aro}), 128.5 (CH), 128.3 (CH), 113.7 (CH), 111.9 (CH), 55.3 (CH_3-O), 44.4 (CH_2-N), 43.0 (CH), 22.4 (CH_3), 12.7 (CH_3).

IR (ATR, cm^{-1}) 2965, 2930, 2870, 1610, 1508, 1463, 1372, 1354, 1242, 1176, 1033, 831, 811.

HRMS (ESI) calcd for $C_{19}H_{26}NO$ [M+H]: 284.2014, found: 284.2012.

Compound 5



Reaction temperature: 100°C, white oil; 78% yield (isolated)

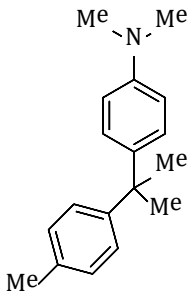
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.13 (d, J_{HH} = 8.5 Hz, 1H), 7.08 (d, J_{HH} = 8.6 Hz, 2H), 6.80 (d, J_{HH} = 8.6 Hz, 2H), 6.61 (dd, J_{HH} = 2.6 Hz, J_{HH} = 8.5 Hz, 1H), 6.56 (d, J_{HH} = 2.6 Hz, 1H), 4.19 (q, J_{HH} = 7.1 Hz, 1H), 3.77 (s, 3H), 2.92 (s, 6H), 2.20 (s, 3H), 1.56 (d, J_{HH} = 7.1 Hz, 3H).

^{13}CNMR ($CDCl_3$, 100 MHz) δ 157.6 (Cq_{aro}), 149.1 (Cq_{aro}), 139.4 (Cq_{aro}), 136.7 (Cq_{aro}), 132.9 (Cq_{aro}), 128.6 (CH), 127.3 (CH), 115.1 (CH), 113.7 (CH), 110.6 (CH), 55.3 (CH_3-O), 40.9 (CH_3-N), 39.5 (CH), 22.6 (CH_3), 20.3 (CH_3).

IR (ATR, cm^{-1}) 2961, 2929, 2833, 1609, 1506, 1442, 1348, 1241, 1175, 1032, 1009, 829, 803.

HRMS (ESI) calcd for $C_{18}H_{24}NO$ [M+H]: 270.1858, found: 270.1861.

Compound 6



Reaction temperature: 100°C, Yellow oil; 96% yield (isolated)

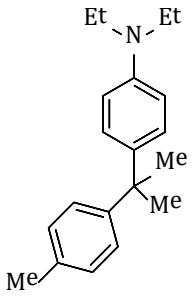
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.14-7.05 (m, 6H), 6.66 (d, J_{HH} = 8.8 Hz, 2H), 2.91 (s, 6H), 2.91 (s, 6H), 2.30 (s, 3H), 1.63 (s, 6H).

^{13}CNMR ($CDCl_3$, 100 MHz) δ 148.6 (Cq_{aro}), 148.5 (Cq_{aro}), 139.1 (Cq_{aro}), 134.8 (Cq_{aro}), 128.7 (CH), 127.5 (CH), 126.8 (CH), 112.4 (CH), 40.8 (CH_3-N), 31.0 (CH), 21.0 (CH_3).

IR (ATR, cm^{-1}) 2964, 2870, 2796, 1613, 1518, 1443, 1344, 1202,1166, 947, 814.

HRMS (ESI) calcd for $C_{18}H_{24}N$ [M+H]: 254.1909, found: 254.1919.

Compound 7



Reaction temperature: 100°C, Yellow oil; 79% yield (isolated)

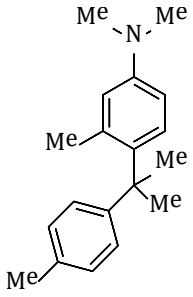
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.15 (d, J_{HH} = 8.2 Hz, 2H), 7.06 (d, J_{HH} = 8.8 Hz, 4H), 6.58 (d, J_{HH} = 8.8 Hz, 2H), 3.31 (q, J_{HH} = 7.0 Hz, 4H), 2.30 (s, 3H), 1.60 (s, 6H), 1.13 (t, J_{HH} = 7.0 Hz, 6H).

^{13}CNMR ($CDCl_3$, 100 MHz) δ 148.6 (Cq_{aro}), 145.5 (Cq_{aro}), 137.7 (Cq_{aro}), 134.8 (Cq_{aro}), 128.7 (CH), 127.7 (CH), 126.8 (CH), 111.4 (CH), 44.4 (CH_2-N), 41.7 (C_q), 31.1 (CH_3), 21.0 (CH_3), 12.8 (CH_3).

IR (ATR, cm^{-1}) 2965, 2927, 2869, 1611, 1515, 1373, 1358, 1264,1201, 1076, 814.

HRMS (ESI) calcd for $C_{20}H_{28}N$ [M+H]: 282.2222, found: 282.2216.

Compound 8



Reaction temperature: 100°C, Yellow oil; 84% yield (isolated)

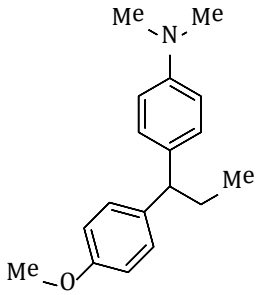
^{1}H NMR (C_6D_6, 400 MHz) δ 7.51 (d, J_{HH} = 8.6 Hz, 1H), 7.19 (d, J_{HH} = 8.0 Hz, 2H), 6.98 (d, J_{HH} = 8.0 Hz, 2H), 6.63 (dd, J_{HH} = 2.8 Hz, J_{HH} = 8.6 Hz, 1H), 6.51 (d, J_{HH} = 2.8 Hz, 1H), 2.59 (s, 6H), 2.13 (s, 3H), 1.92 (s, 3H), 1.67 (s, 6H).

^{13}CNMR (C_6D_6, 100 MHz) δ 149.6 (Cq_{aro}), 149.4 (Cq_{aro}), 137.5 (Cq_{aro}), 136.5 (Cq_{aro}), 134.5 (Cq_{aro}), 129.2 (CH), 127.1 (CH), 126.3 (CH), 117.7 (CH), 110.4 (CH), 42.6 (C_q), 40.5 (CH_3-N), 31.5 (CH_3), 22.6 (CH_3), 20.9 (CH_3).

IR (ATR, cm^{-1}) 2964, 2870, 2795, 1609, 1506, 1349, 1290, 1153,1014, 841, 814, 799.

HRMS (ESI) calcd for $C_{19}H_{26}N$ [M+H]: 268.2065, found: 268.2067.

Compound 9



Reaction temperature: 135°C, Yellow oil; 79% yield (isolated)

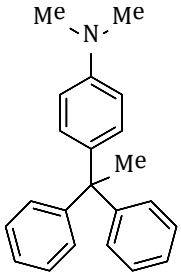
^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.05 (d, J_{HH} = 8.6 Hz, 2H), 7.00 (d, J_{HH} = 8.6 Hz, 2H), 6.72 (d, J_{HH} = 8.7 Hz, 2H), 6.59 (d, J_{HH} = 8.8Hz, 2H), 3.68 (s, 6H), 3.57 (t, J_{HH} = 7.8 Hz, 1H), 2.81 (s, 6H), 1.92 (qd, J_{HH} = 1.9 Hz, J_{HH} = 7.7 Hz, 2H), 0.80 (t, J_{HH} = 7.3 Hz, 3H),

^{13}CNMR ($CDCl_3$, 125 MHz) δ 157.7 (Cq_{aro}), 149.1 (Cq_{aro}), 138.3 (Cq_{aro}), 133.9 (Cq_{aro}), 128.8 (CH), 128.5 (CH), 113.7 (CH), 112.9 (CH), 55.3 (CH_3-O), 51.5(CH), 40.8 (CH_3-N), 29.0 (CH_2), 13.0 (CH_3).

IR (ATR, cm^{-1}) 2957, 2930, 2871, 1610, 1508, 1441, 1343, 1244, 1175,1035, 947, 806.

HRMS (ESI) calcd for $C_{18}H_{24}NO$ [M+H]: 270.1858, found: 270.1871.

Compound 10



Reaction temperature: 145°C, white solid; m.p. 77-79°; 90% yield (isolated)

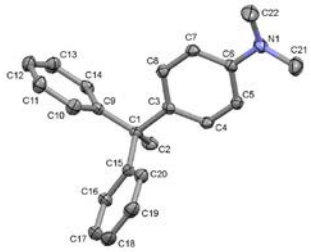
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.29-7.26 (m, 4H), 7.28-7.19 (m, 2H), 7.15-7.13 (m, 4H), 6.98 (d, J_{HH} = 8.9Hz, 2H), 6.68 (d, J_{HH} = 8.7Hz, 2H), 2.95 (s, 6H), 2.18 (s, 3H).

^{13}CNMR ($CDCl_3$, 100 MHz) δ 149.9 (Cq_{aro}), 148.6 (Cq_{aro}), 137.2 (Cq_{aro}), 129.5 (CH), 128.9 (CH), 127.9 (CH), 125.8 (CH), 112.1 (CH), 51.8(C_q), 40.8 (CH_3-N), 30.6 (CH_3).

IR (ATR, cm^{-1}) 3050, 2975, 2795, 1609, 1517, 1442, 1346, 1202, 1125, 1024, 811, 758, 701.

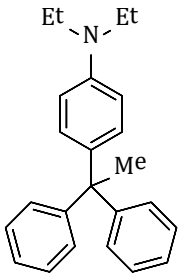
HRMS (ESI) calcd for $C_{22}H_{24}N$ [M+H]: 302.1909, found: 302.1917.

X-Ray Crystal Structure of 10



Single crystals of **10** suitable for X-ray crystallographic analysis were obtained by slow evaporation of CH_2Cl_2 solution. X-ray diffraction experiments for monocrystal of **10** were performed at 150 K with graphite–monochromatized Mo K_α radiation (λ = 0.71073 Å) on a Bruker–Nonius Kappa CCD area detector diffractometer. Formula $C_{22}H_{23}N$, formula weight 301.41, crystal system triclinic, space group *P*-1, *a* = 9.7438(15) Å, *b* = 9.9224(16) Å, *c* = 10.9840(19) Å, α = 64.086(6)°, β = 78.354(7)°, γ = 63.503(6)°, V = 854.8(2) Å^3, Z = 2, calculated density = 1.171 g/cm^3, μ = 0.067 mm^{-1}, R_{int} = 0.0404, R[$F^2>2\sigma(F^2)$] = 0.0778, wR(F^2) = 0.2795. Selected bond lengths (Å), angles (deg) and dihedral angles (deg): C1-C3 1.536(4), C1-C2 1.548(4), C1-C9 1.529(4), C1-C15 1.541(4), C3-C1-C9 110.4(2), C3-C1-C15 110.8(2), C9-C1-C15 108.2(2), C3-C1-C2 107.7(2), C9-C1-C2 110.7(2), C15-C1-C2 109.0(2). Program(s) used to solve structure: SHELXS97. Program(s) used to refine structure: SHELXL–2014. Software used to prepare material for publication: SHELXTL. CCDC 1835022 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Compound 11



Reaction temperature: 145°C, white solid; m.p. 78-80°; 74% yield (isolated)

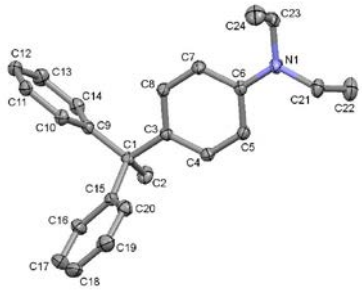
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.27-7.24 (m, 4H), 7.20-7.17 (m, 2H), 7.14-7.12 (m, 4H), 6.91 (d, J_{HH} = 8.9Hz, 2H), 6.58 (d, J_{HH} = 8.7Hz, 2H), 3.33 (q, J_{HH} = 7.0Hz, 4H), 2.16 (s, 3H), 1.16 (t, J_{HH} = 7.0Hz, 6H).

^{13}CNMR ($CDCl_3$, 100 MHz) δ 150.0 (Cq_{aro}), 145.9 (Cq_{aro}), 135.7 (Cq_{aro}), 129.6 (CH), 128.8 (CH), 127.8 (CH), 125.7 (CH), 111.1 (CH), 51.7(C_q), 44.3 (CH_2-N), 30.6 (CH_3), 12.8 (CH_3).

IR (ATR, cm^{-1}) 2968, 2928, 2889, 1607, 1516, 1443, 1373, 1268, 1200, 1153, 1025, 803, 757, 699.

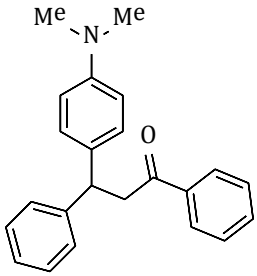
HRMS (ESI) calcd for $C_{24}H_{28}N$ [M+H]: 330.2222, found: 330.2213.

X-Ray Crystal Structure of 11



Single crystals of **11** suitable for X-ray crystallographic analysis were obtained by slow evaporation of CH_2Cl_2 solution. X-ray diffraction experiments for monocrystal of **11** were performed at 150 K with graphite–monochromatized Mo K_α radiation (λ = 0.71073 Å) on a Bruker–Nonius Kappa CCD area detector diffractometer. Formula C24H27N, formula weight 329.46, crystal system triclinic, space group P-1, a = 8.3046(2) Å, b = 10.7954(2) Å, c = 12.0469(2) Å, α = 109.6395(9)°, β = 100.9597(8)°, γ = 104.3515(9)°, V = 940.16(3) Å3, Z = 2, calculated density = 1.164 g/cm3, μ = 0.066 mm–1, Rint = 0.0277, R[F2>2σ(F2)] = 0.0456, wR(F2) = 0.1296. Selected bond lengths (Å), angles (deg) and dihedral angles (deg): C1-C3 1.5403(12), C1-C2 1.5492(13), C1-C9 1.5413(12), C1-C15 1.5438(13), C3-C1-C9 109.99(7), C3-C1-C15 112.51(7), C9-C1-C15 106.69(7), C3-C1-C2 107.70(7), C9-C1-C2 110.90(8), C15-C1-C2 109.09(7). Program(s) used to solve structure: SHELXS97. Program(s) used to refine structure: SHELXL–2014. Software used to prepare material for publication: SHELXTL. CCDC 1835023 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Compound 12



Reaction temperature: 145°C, yellow oil; 34% yield (isolated)

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.93-7.91 (m, 2H), 7.53 (t, J_{HH} = 7.3Hz, 1H), 7.44-7.40(m, 2H), 7.25-7.24 (m, 4H), 7.17-7.11 (m, 3H), 6.65(d, J_{HH} = 8.7Hz, 1H), 4.73 (q, J_{HH} = 7.3Hz, 1H), 2.80 (s, 6H), 3.69 (d, J_{HH} = 7.3Hz, 2H), 2.80 (s, 3H).

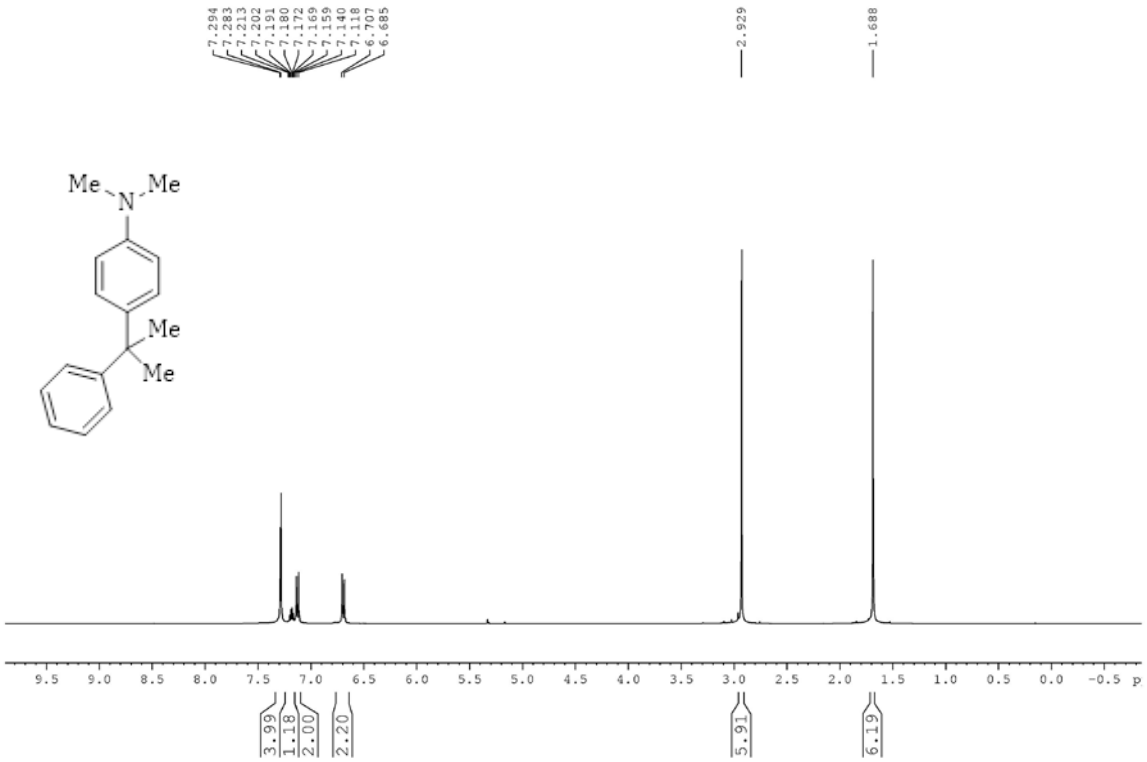
^{13}CNMR ($CDCl_3$, 100 MHz) δ 198.5 (CO), 149.3 (Cq_{aro}), 145.0 (Cq_{aro}), 137.3 (Cq_{aro}), 133.1 (CH), 132.3 (CH), 128.7 (CH), 128.6 (CH), 128.5 (CH), 128.2 (CH), 127.9 (CH), 126.2 (CH), 112.9 (CH), 45.2 (CH), 45.1 (CH_2), 40.7 (CH_3-N).

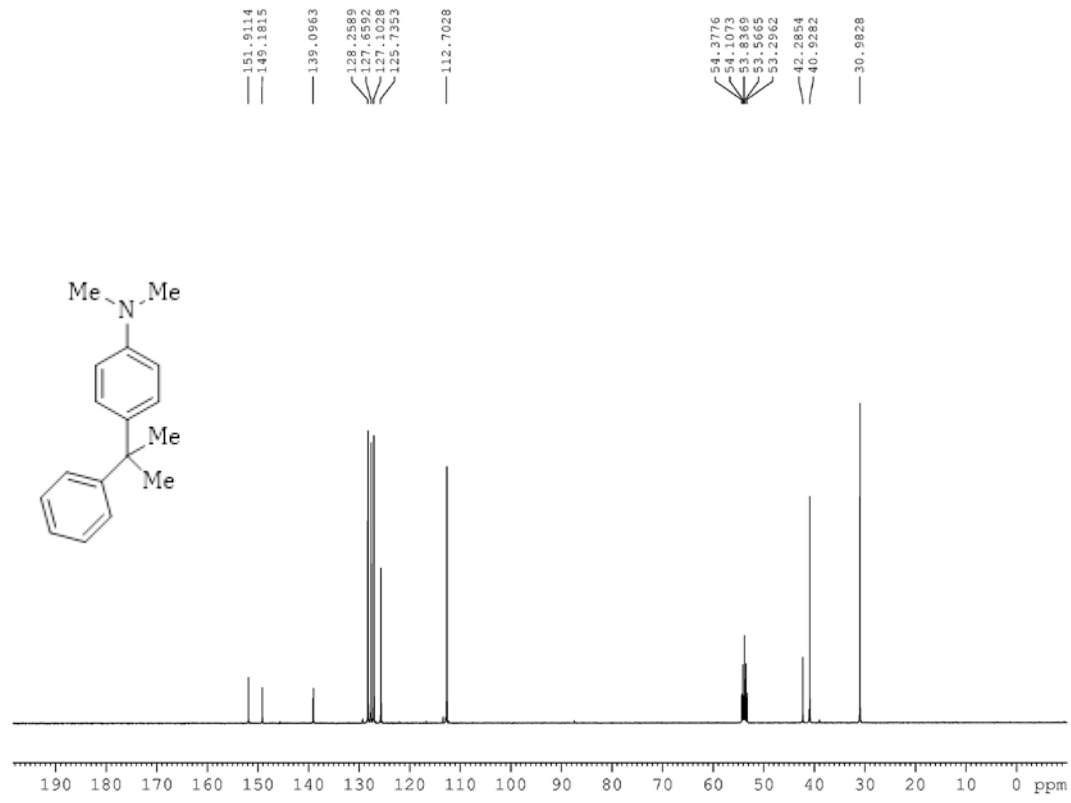
IR (ATR, cm^{-1}) 3059, 3026, 2888, 2798, 1682, 1613, 1518, 1447, 1344, 1202, 1161, 981, 816, 747, 689.

HRMS (ESI) calcd for $C_{23}H_{24}NO$ [M+H]: 330.1858, found: 330.1861.

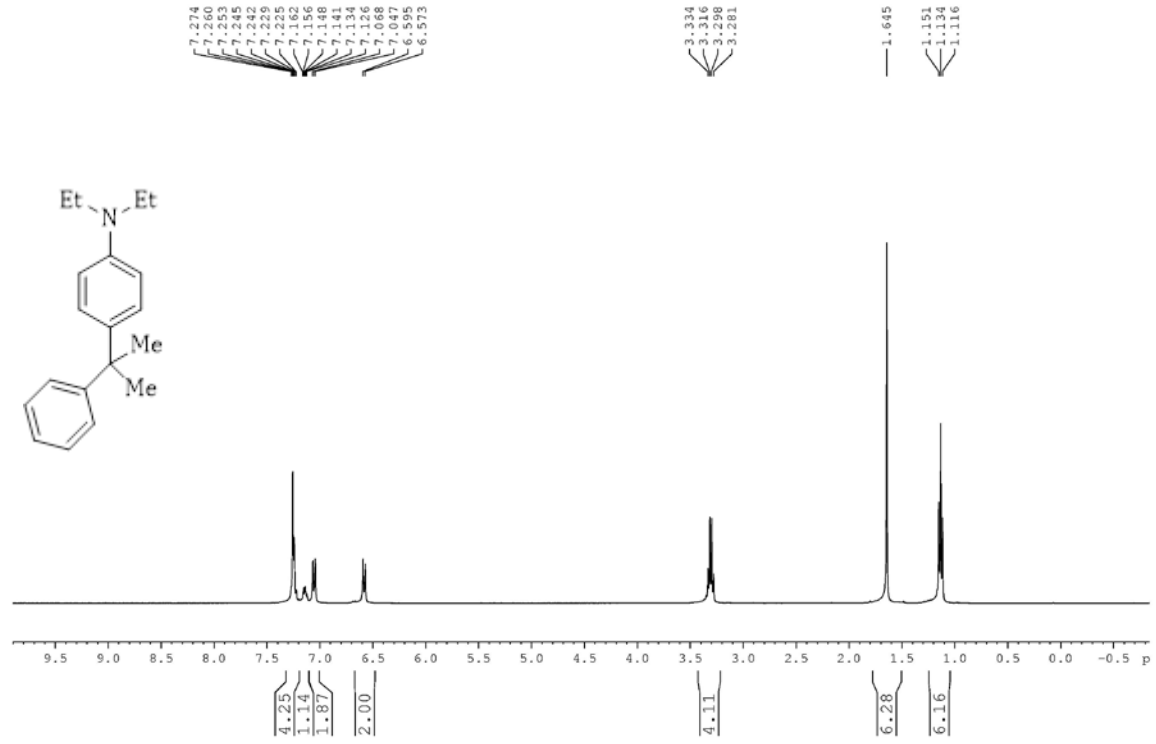
III. NMR Spectra

Compound 1





Compound 2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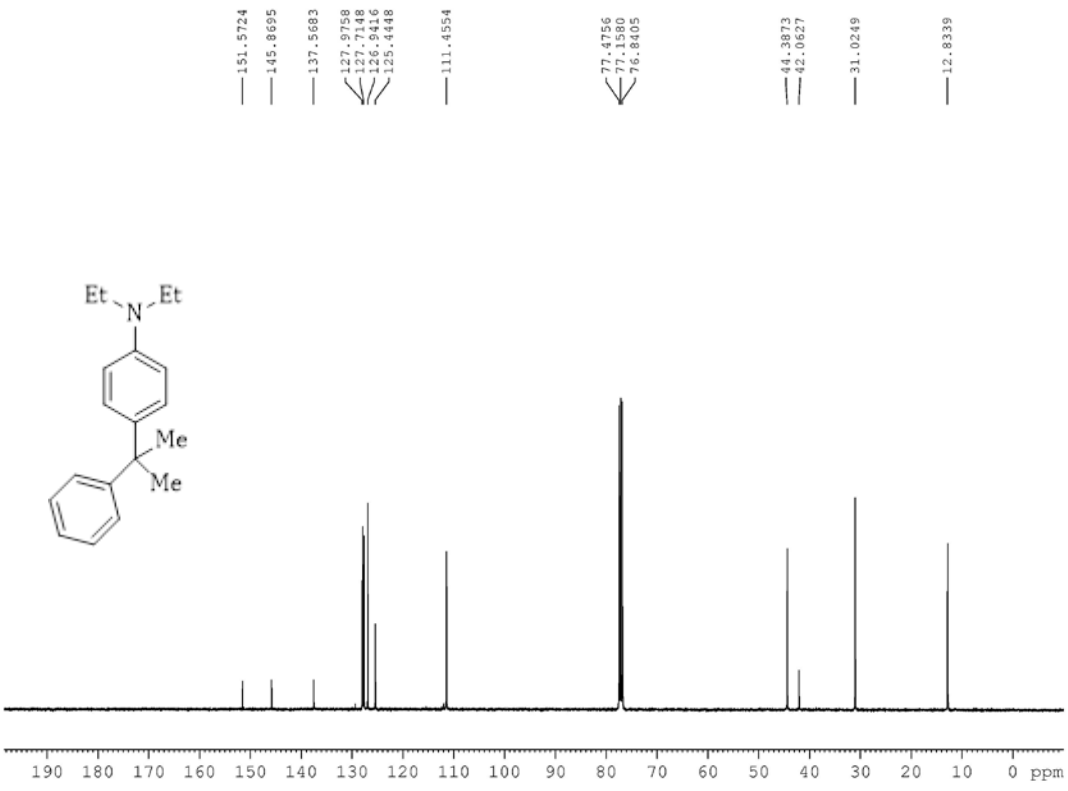
7.260
7.253
7.245
7.242
7.229
7.225
7.162
7.156
7.148
7.141
7.134
7.126
7.068
7.047
6.595
6.573
3.334
3.316
3.298
3.281
1.645
1.151
1.134
1.116
Et
N
Et
Me
Me
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 p
4.25
1.14
1.87
2.00
4.11
6.28
6.16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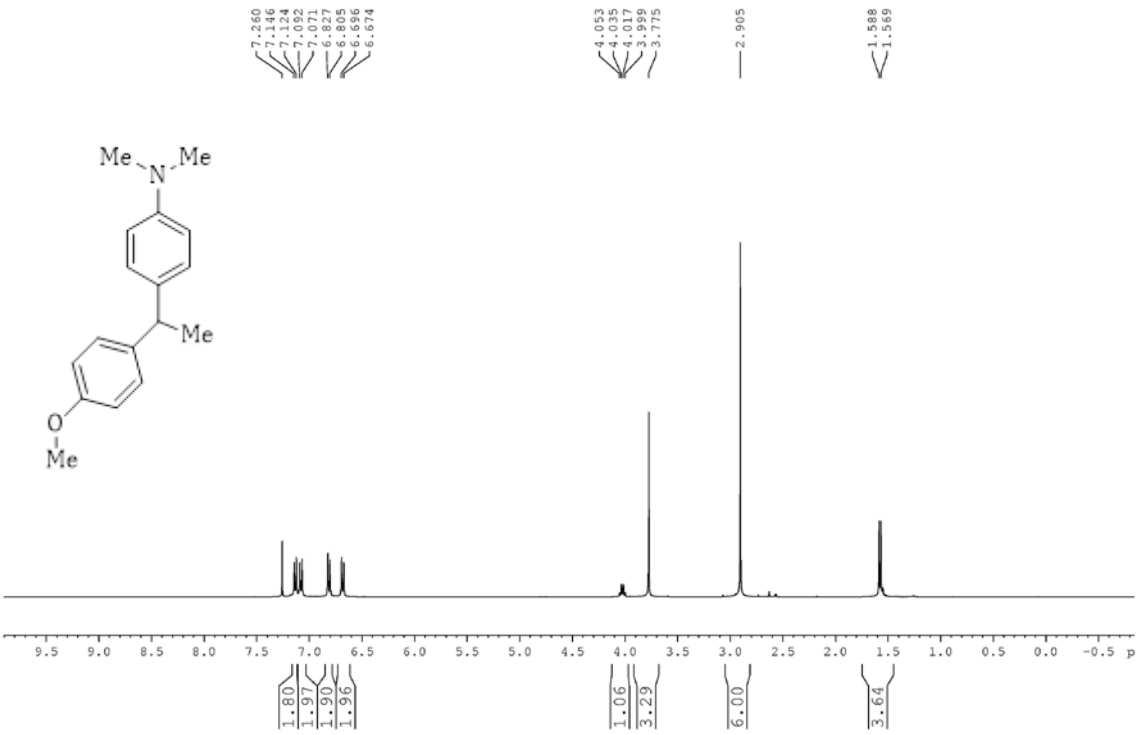
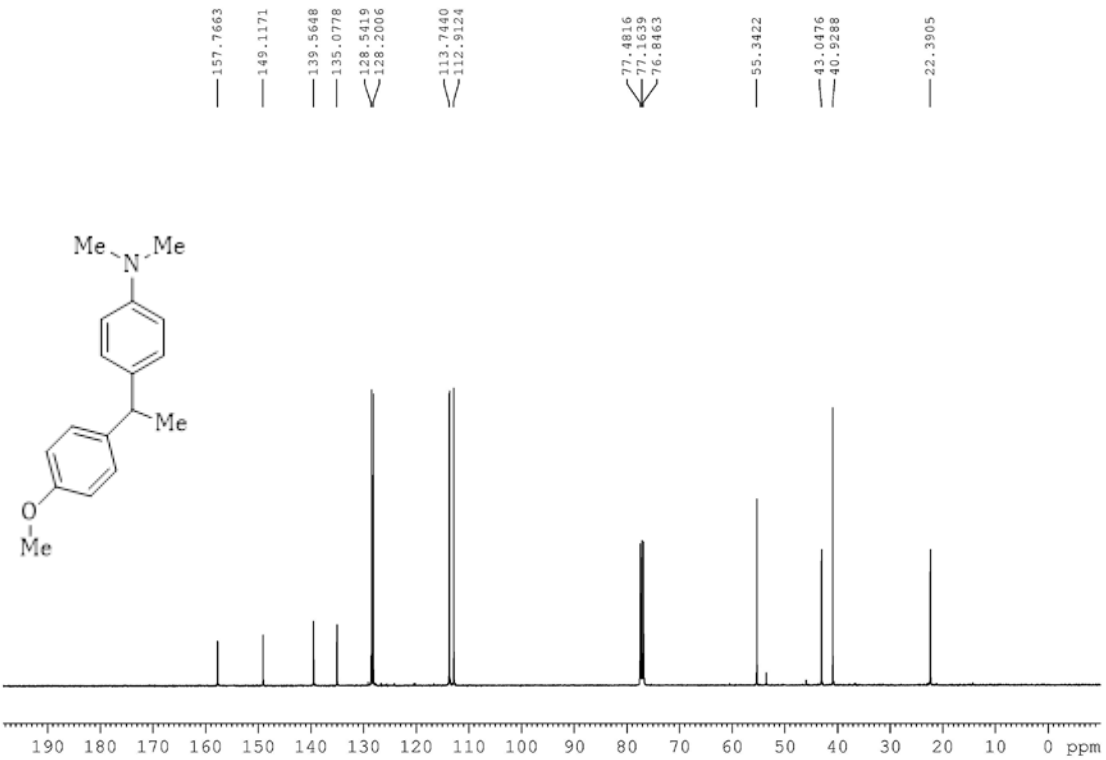
145.8695
137.5683
127.9758
127.7148
126.9416
125.4448
111.4554
77.4756
77.1580
76.8405
44.3873
42.0627
31.0249
12.8339
Et
N
Et
Me
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Compound 3


7.260
7.146
7.124
7.092
7.071
6.827
6.805
6.696
6.674
4.053
4.035
4.017
3.999
3.775
2.905
1.588
1.569
Me
N
Me
Me
O
Me
1.80
1.97
1.90
1.96
1.06
3.29
6.00
3.64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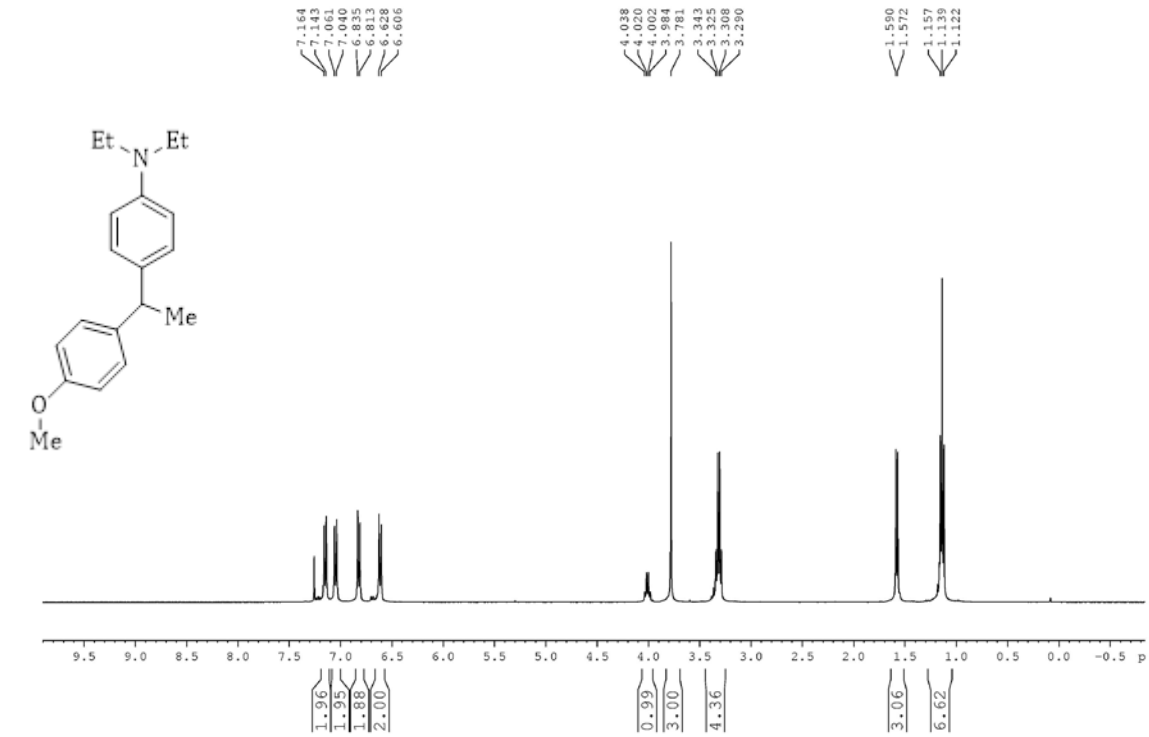
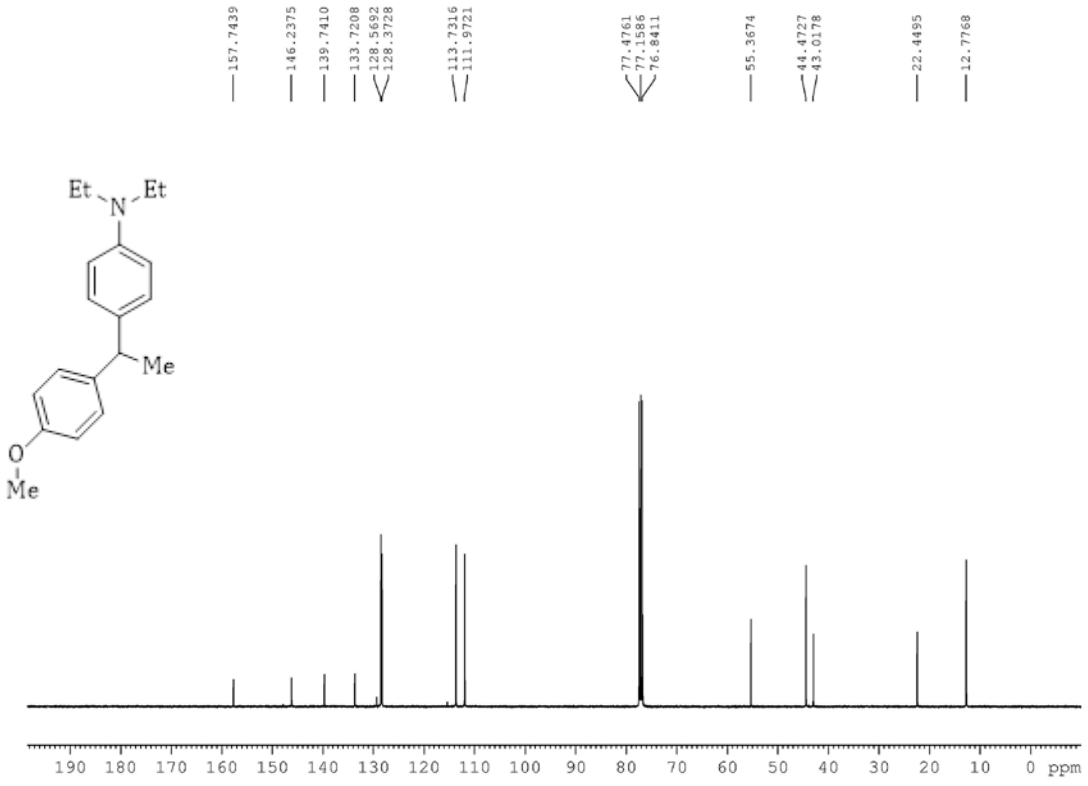
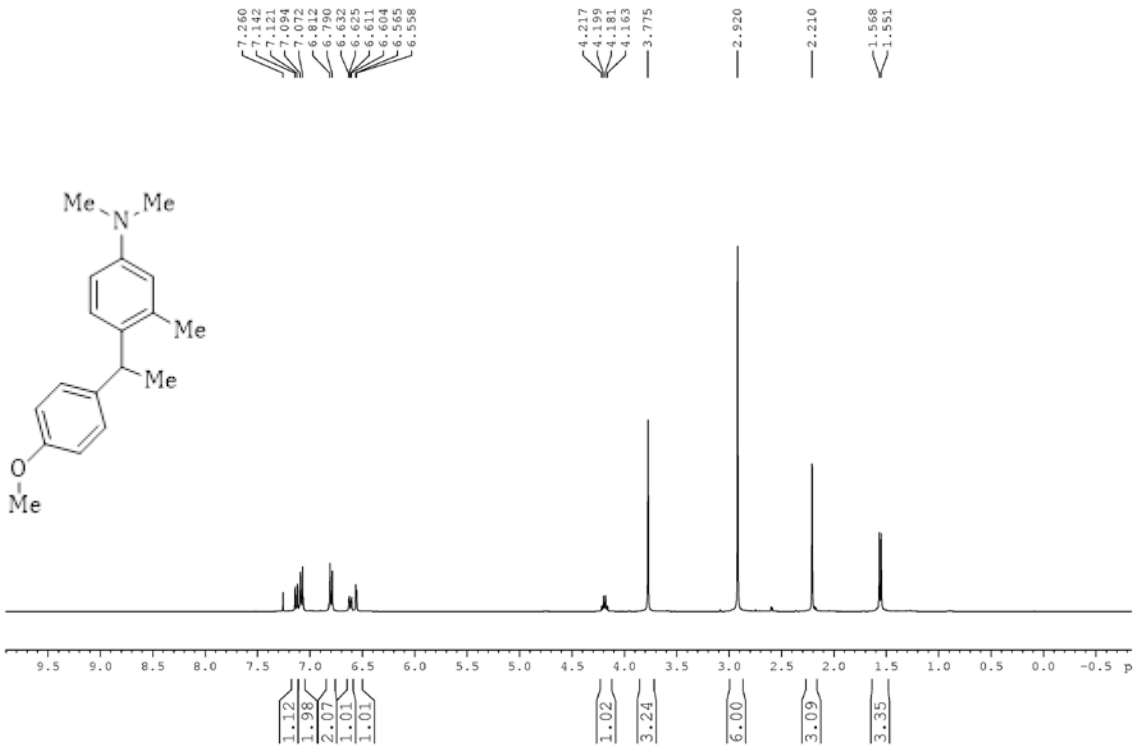
149.1171
139.5648
135.0778
128.5419
128.2006
113.7440
112.9124
77.4816
77.1639
76.8463
55.3422
43.0476
40.9288
22.3905
Me
N
Me
Me
O
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

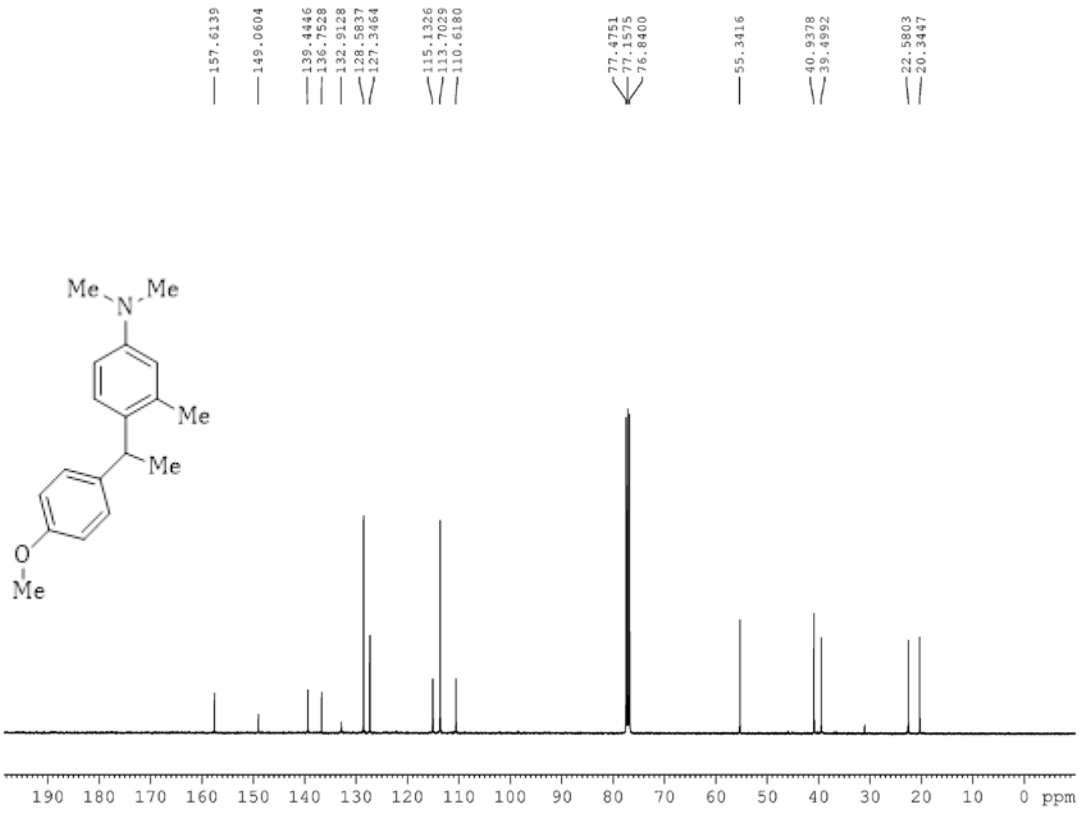
Compound 4


7.164
7.143
7.061
7.040
6.835
6.813
6.628
6.606
4.038
4.020
4.002
3.984
3.781
3.343
3.325
3.308
3.290
1.590
1.572
1.157
1.139
1.122
Et
N
Et
Me
O
Me
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 p
1.96
1.95
1.88
2.00
0.99
3.00
4.36
3.06
6.62

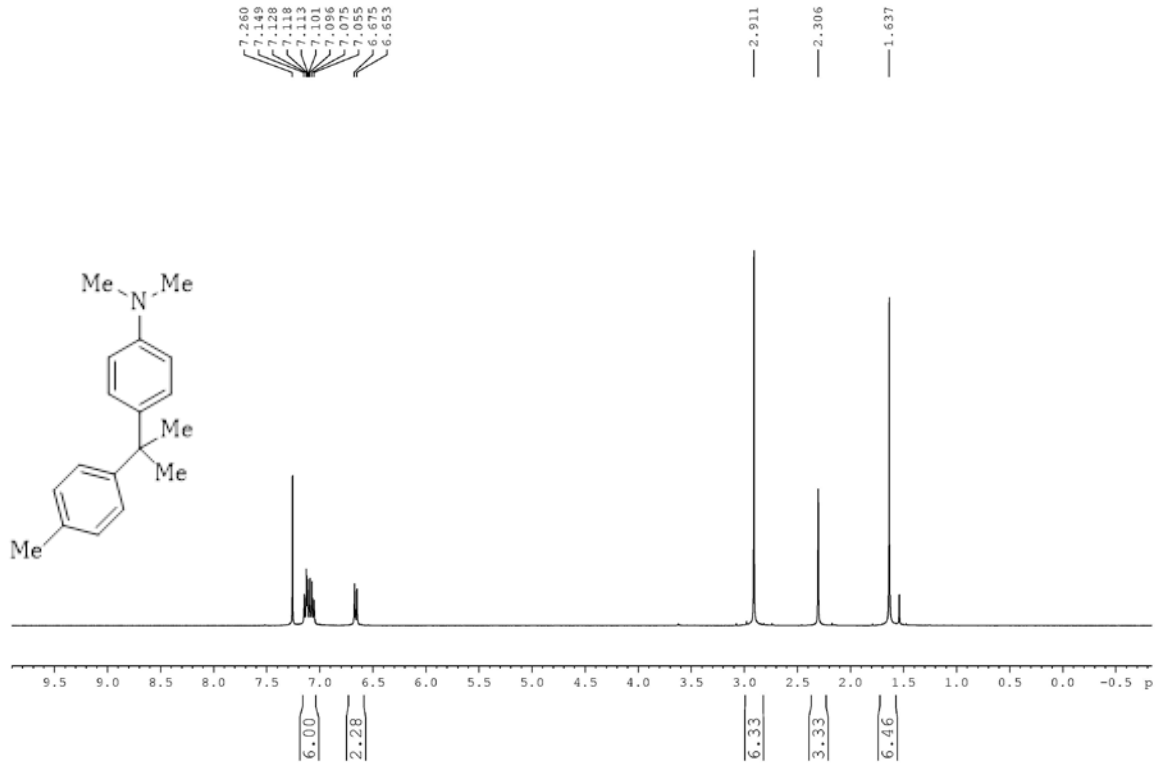

157.7439
146.2375
139.7410
133.7208
128.5692
128.3728
113.7316
111.9721
77.4761
77.1586
76.8411
55.3674
44.4727
43.0178
22.4495
12.7768
Et
N
Et
Me
O
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

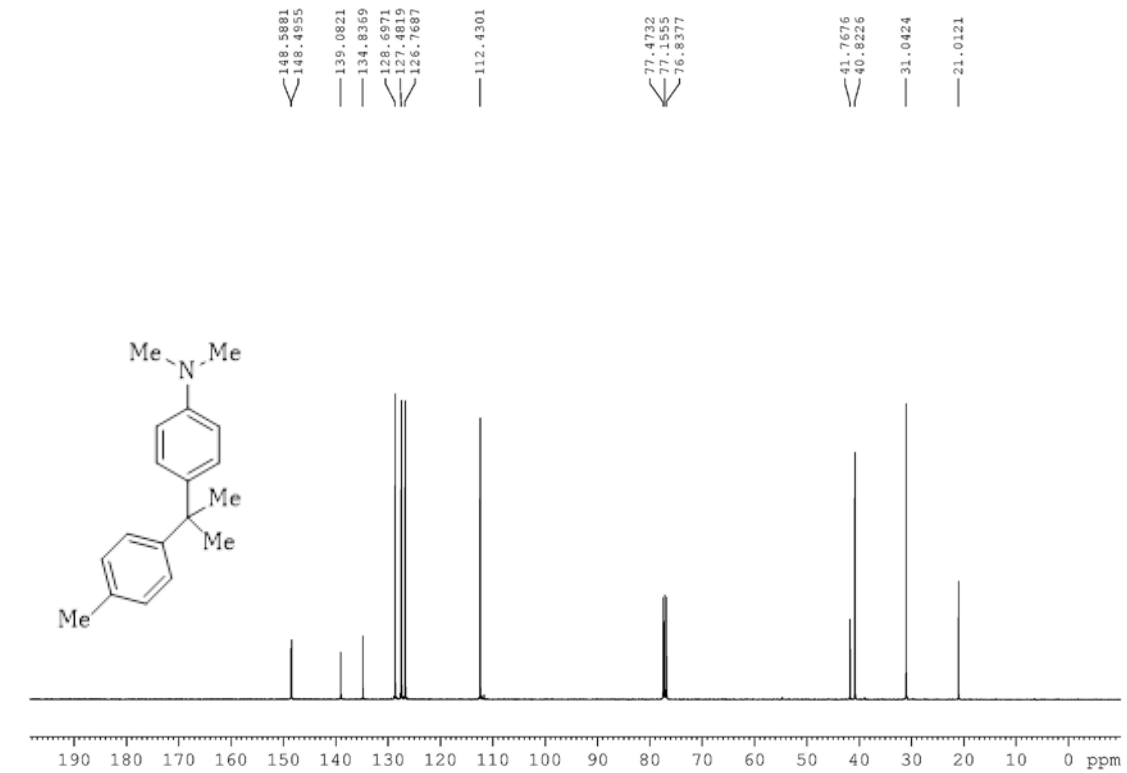
Compound 5


7.260
7.142
7.121
7.094
7.072
6.812
6.790
6.632
6.625
6.611
6.604
6.565
6.558
4.217
4.199
4.181
4.163
3.775
2.920
2.210
1.568
1.551
Me
N
Me
Me
Me
O
Me
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 p
1.12
1.98
2.07
1.01
1.01
1.02
3.24
6.00
3.09
3.35

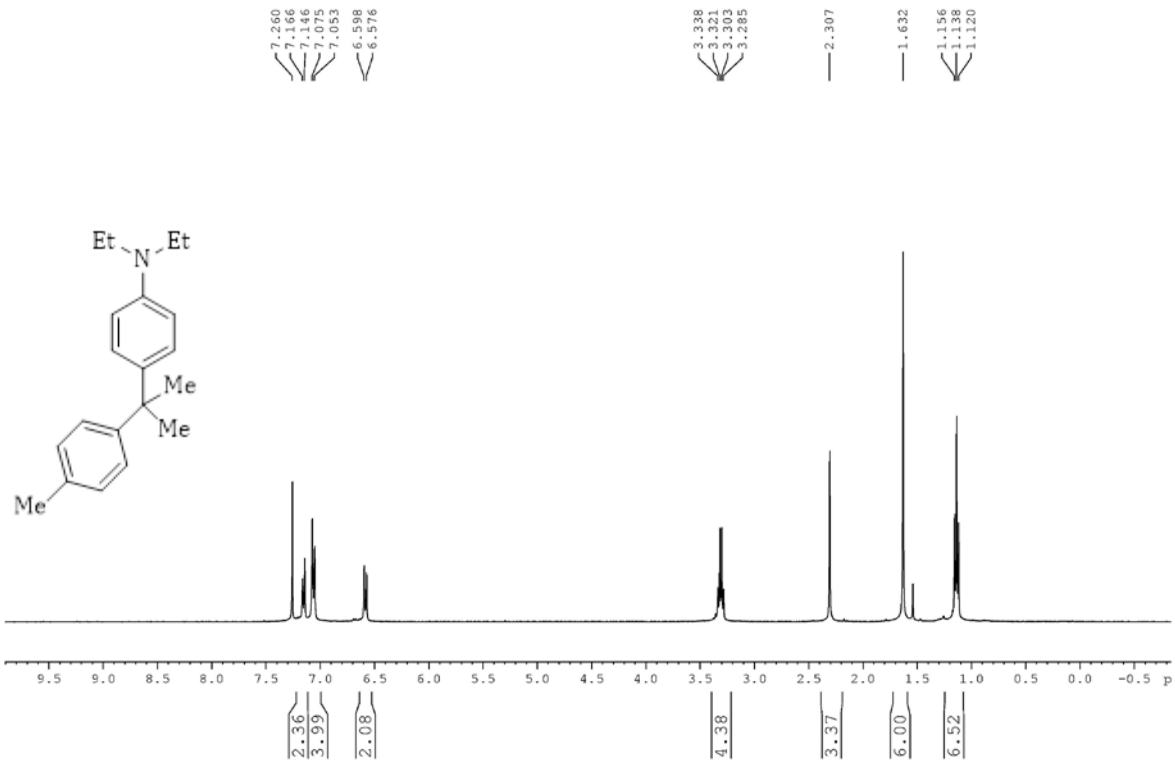

157.6139
149.0604
139.4446
136.7528
132.9128
128.5837
127.3464
115.1326
113.7029
110.6180
77.4751
77.1575
76.8400
55.3416
40.9378
39.4992
22.5803
20.3447
Me
N
Me
Me
Me
O
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

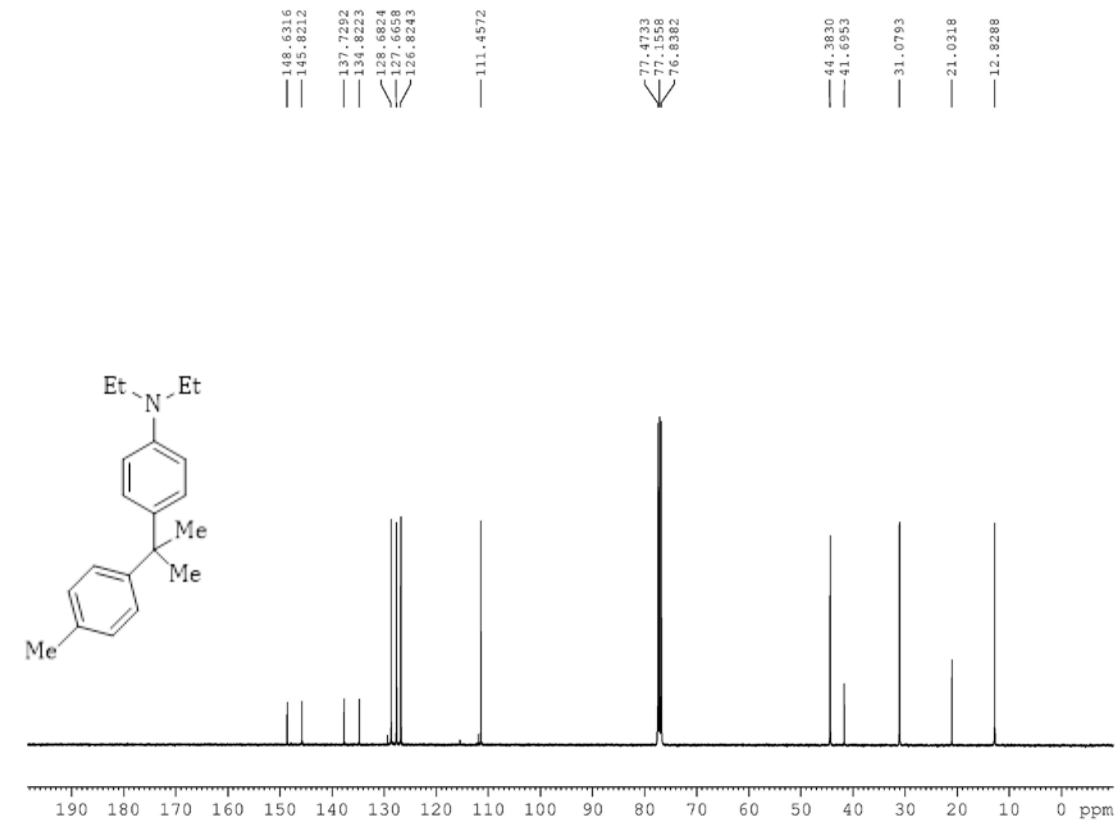
Compound 6


7.260
7.149
7.128
7.118
7.113
7.101
7.096
7.075
7.055
6.675
6.653
2.911
2.306
1.637
Me
N
Me
Me
Me
Me
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 p
6.00
2.28
6.33
3.33
6.46

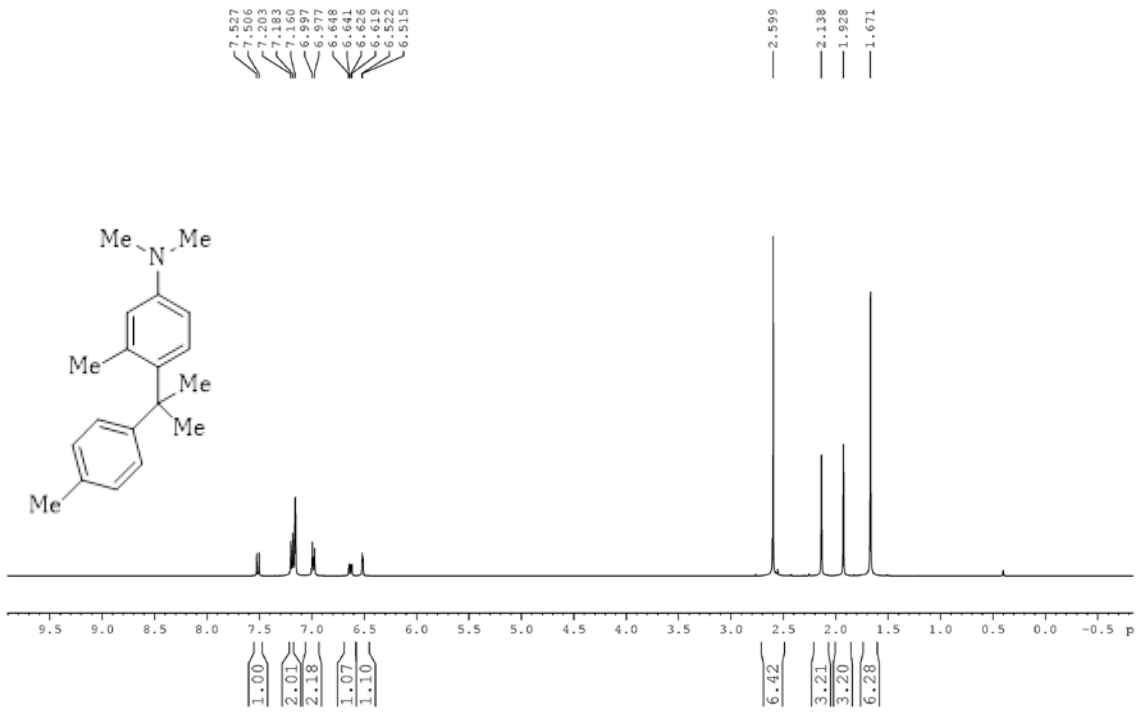

148.5881
148.4955
139.0821
134.8369
128.6971
127.4819
126.7687
112.4301
77.4732
77.1555
76.8377
41.7676
40.8226
31.0424
21.0121
Me
N
Me
Me
Me
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Compound 7


7.260
7.166
7.146
7.075
7.053
6.598
6.576
3.338
3.321
3.303
3.285
2.307
1.632
1.156
1.138
1.120
Et
N
Et
Me
Me
Me
2.36
3.99
2.08
4.38
3.37
6.00
6.52


148.6316
145.8212
137.7292
134.8223
128.6824
127.6658
126.8243
111.4572
77.4733
77.1558
76.8382
44.3830
41.6953
31.0793
21.0318
12.8288
Et
N
Et
Me
Me
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Compound 8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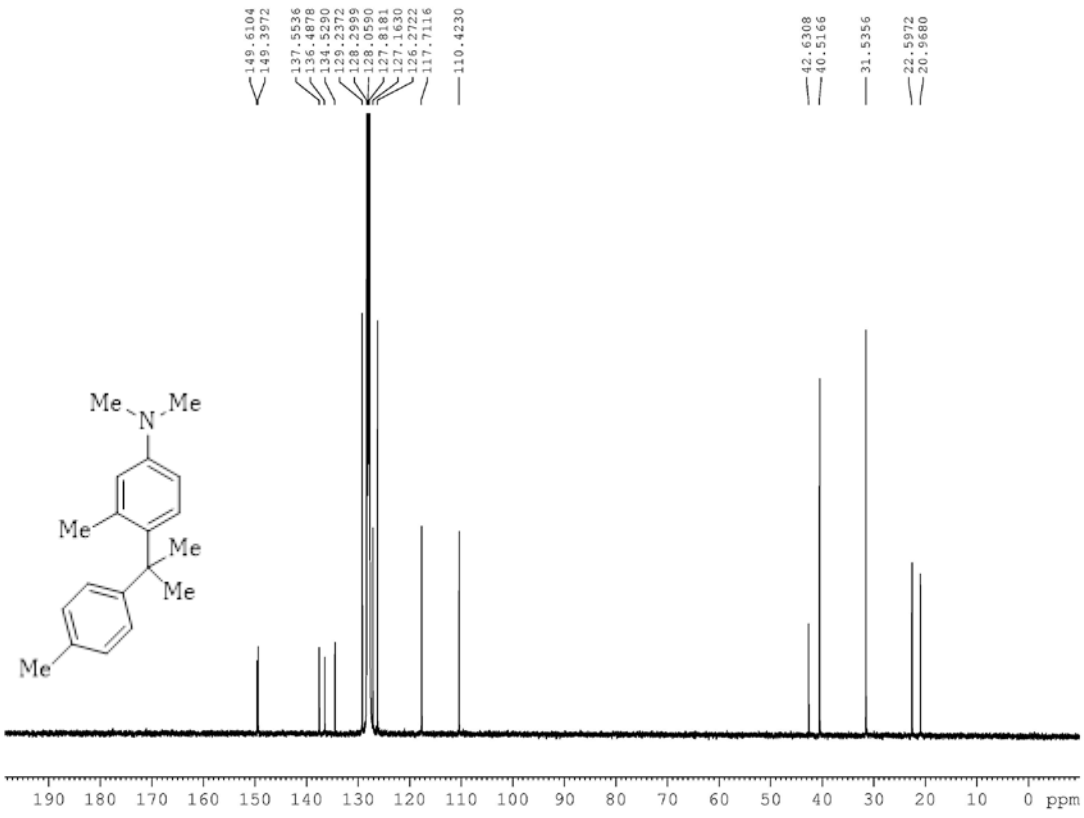
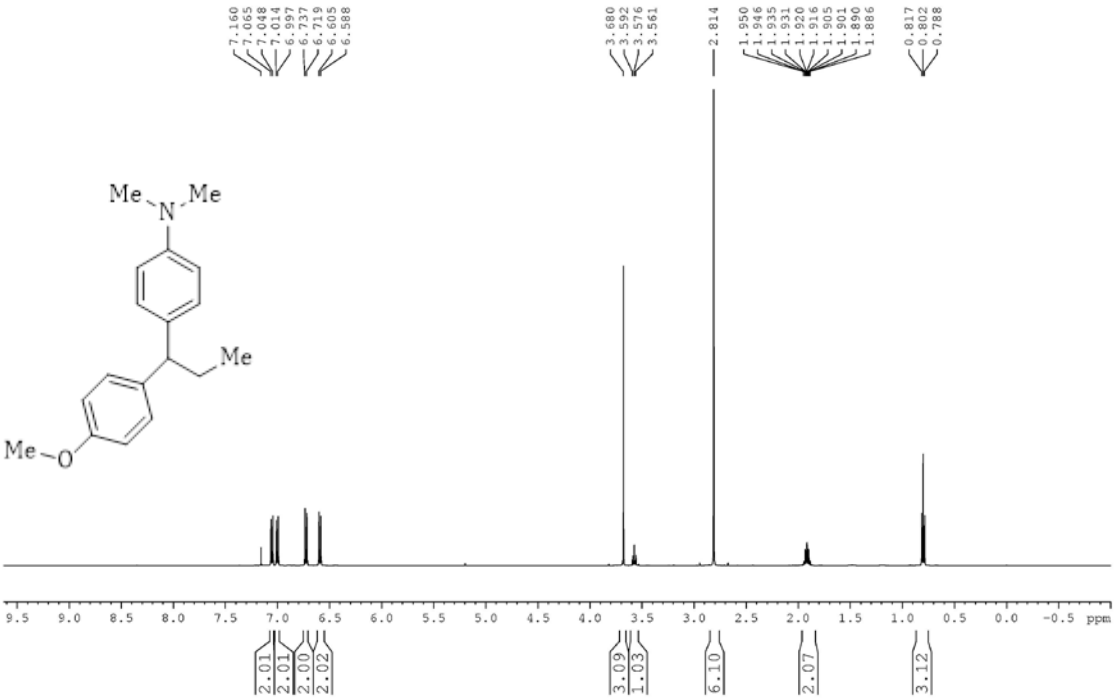
7.506
7.203
7.183
7.160
6.997
6.977
6.648
6.641
6.626
6.619
6.522
6.515
2.599
2.138
1.928
1.671
Me
N
Me
Me
Me
Me
Me
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 p
1.00
2.01
2.18
1.07
1.10
6.42
3.21
3.20
6.28

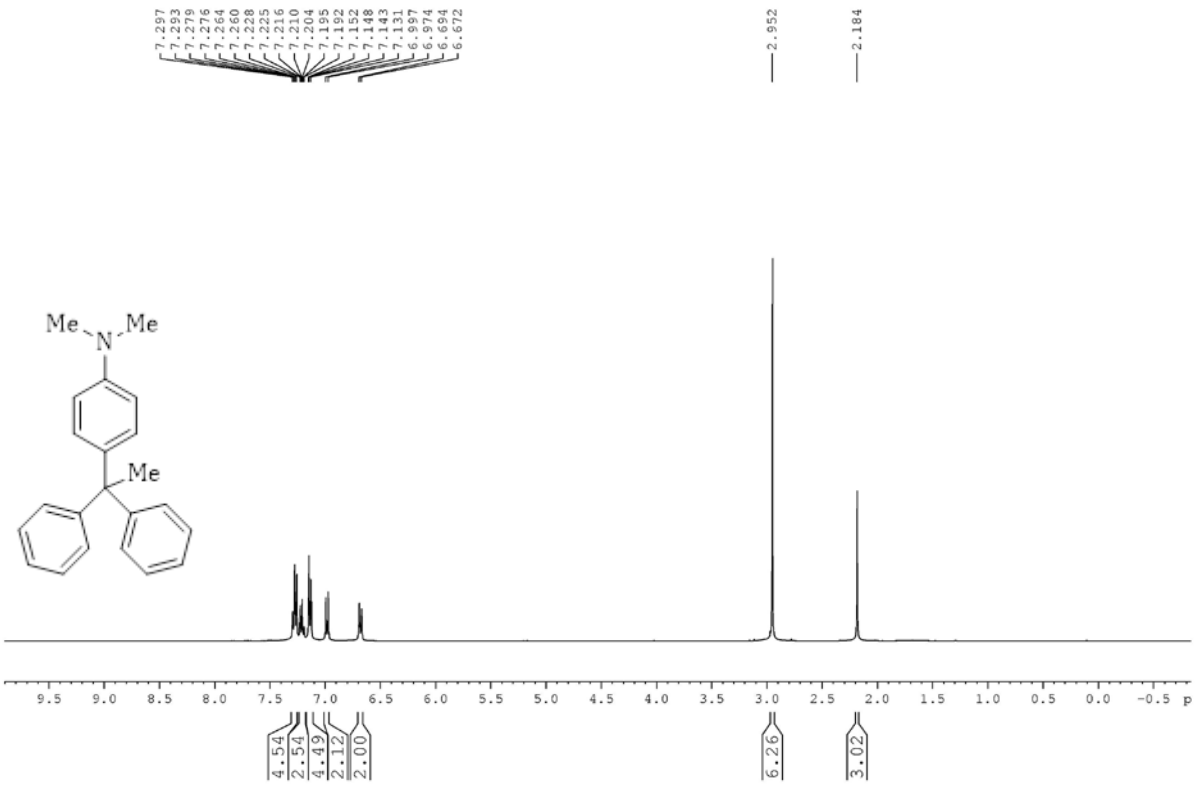

149.6104
149.3972
137.5536
136.4878
134.5290
129.2372
128.2999
128.0590
127.8181
127.1630
126.2722
117.7116
110.4230
42.6308
40.5166
31.5356
22.5972
20.9680
Me
N
Me
Me
Me
Me
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Compound 9


7.160
7.065
7.048
7.014
6.997
6.737
6.719
6.605
6.588
3.680
3.592
3.576
3.561
2.814
1.950
1.946
1.935
1.931
1.920
1.916
1.905
1.901
1.890
1.886
0.817
0.802
0.788
Me
N
Me
Me
Me
O
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm
2.01
2.01
2.00
2.02
3.09
1.03
6.10
2.07
3.12


157.7263
149.0724
138.3566
133.9033
128.8207
128.4819
113.7514
112.9168
77.4151
77.1610
76.9069
55.3251
51.4935
40.9213
29.0537
13.0189
Me
N
Me
Me
Me
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Compound 10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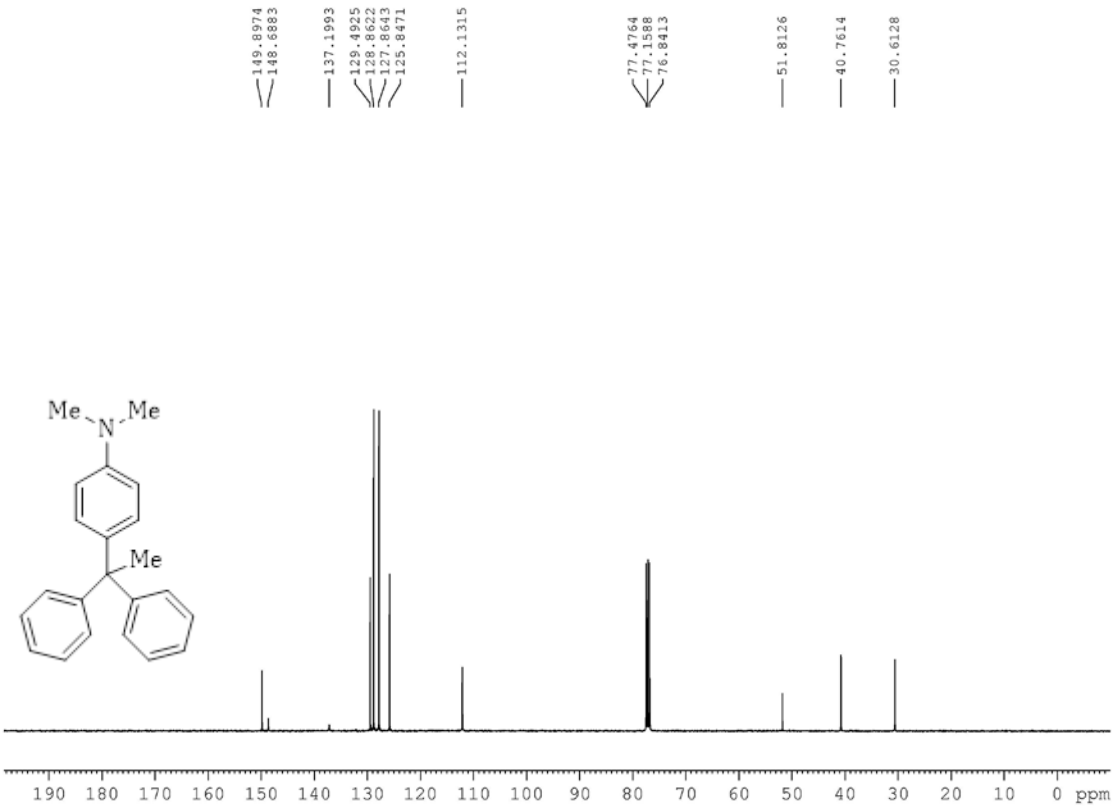
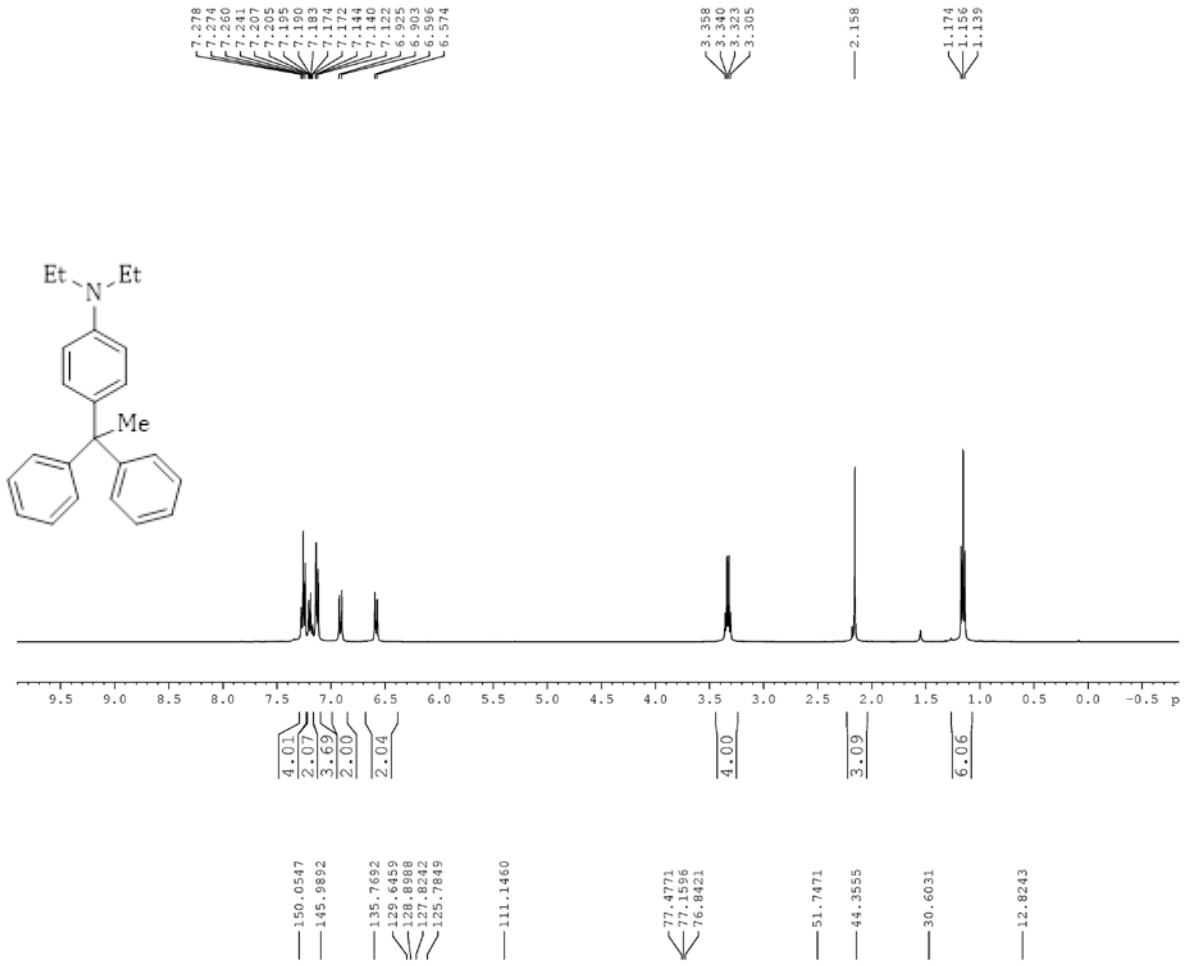
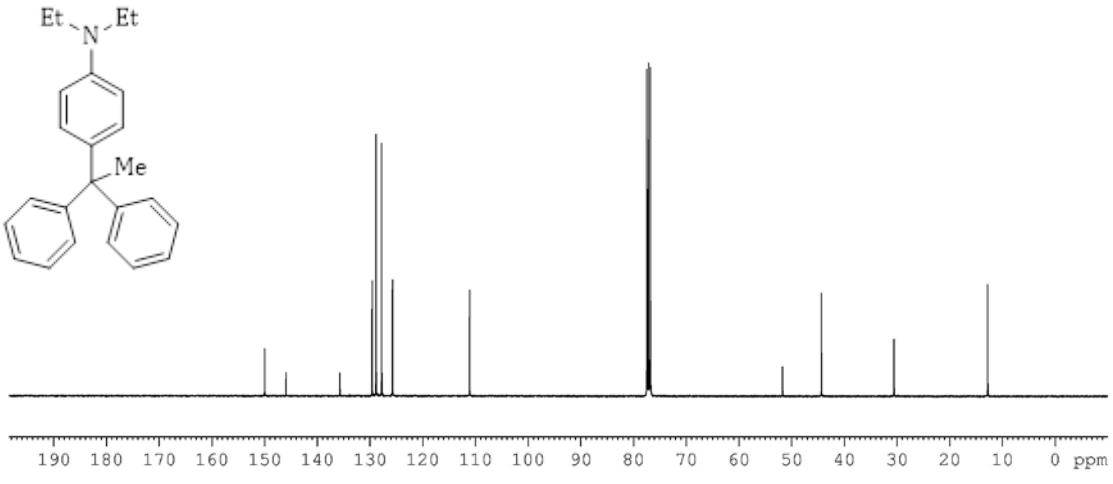
7.293
7.279
7.276
7.264
7.260
7.228
7.225
7.216
7.210
7.204
7.195
7.192
7.152
7.148
7.143
7.131
6.997
6.974
6.694
6.672
2.952
2.184
Me
N
Me
Me
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 p
4.54
2.54
4.49
2.12
2.00
6.26
3.02

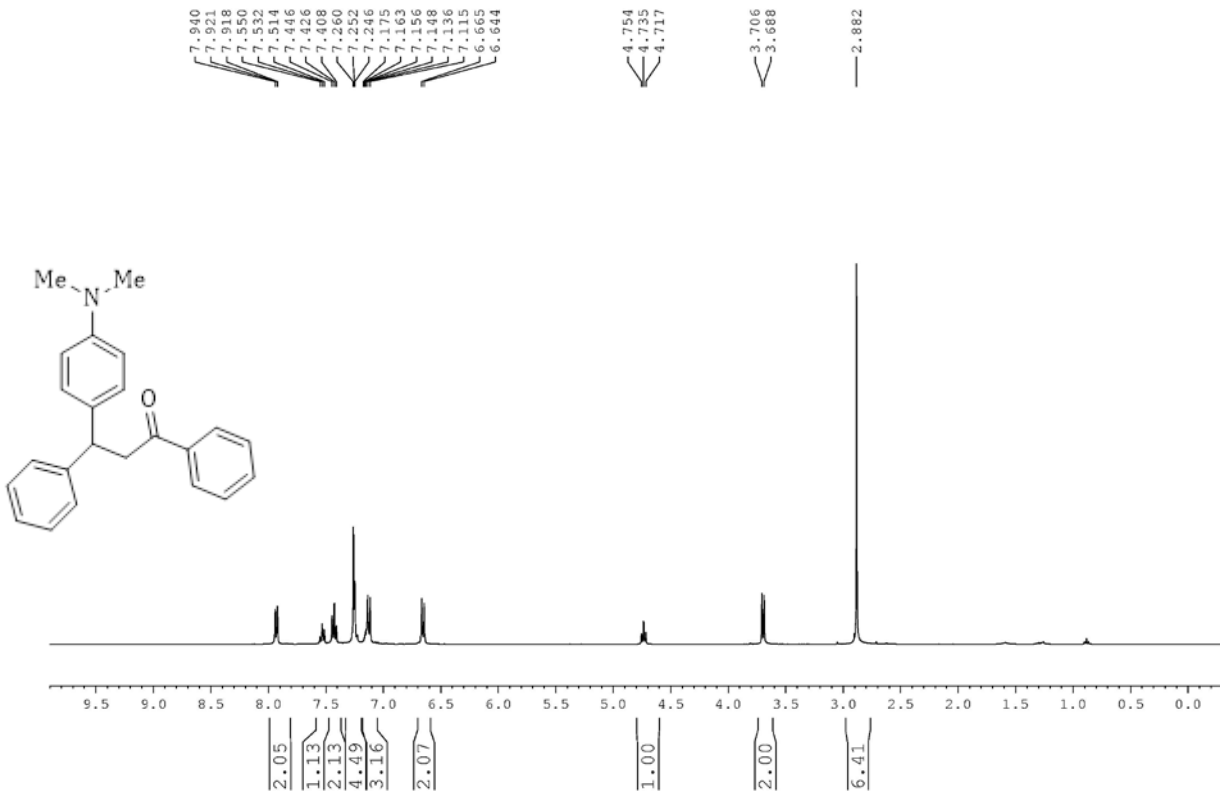

149.8974
148.6883
137.1993
129.4925
128.8622
127.8643
125.8471
112.1315
77.4764
77.1588
76.8413
51.8126
40.7614
30.6128
Me
N
Me
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

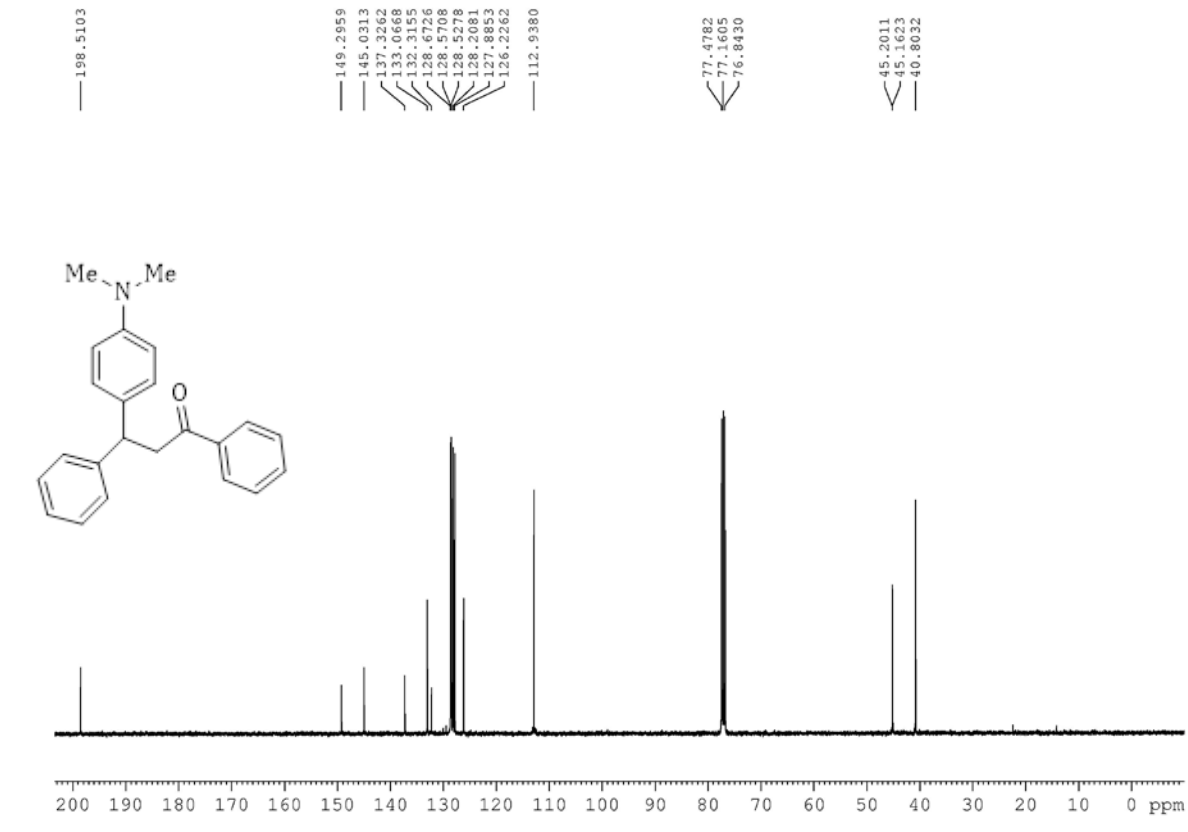
Compound 11


7.278
7.274
7.260
7.241
7.207
7.205
7.195
7.190
7.183
7.174
7.172
7.144
7.140
7.122
6.925
6.903
6.596
6.574
3.358
3.340
3.323
3.305
2.158
1.174
1.156
1.139
Et
N
Et
Me
4.01
2.07
3.69
2.00
2.04
4.00
3.09
6.06


150.0547
145.9892
135.7692
129.6459
128.8988
127.8242
125.7849
111.1460
77.4771
77.1596
76.8421
51.7471
44.3555
30.6031
12.8243
Et
N
Et
Me
ppm

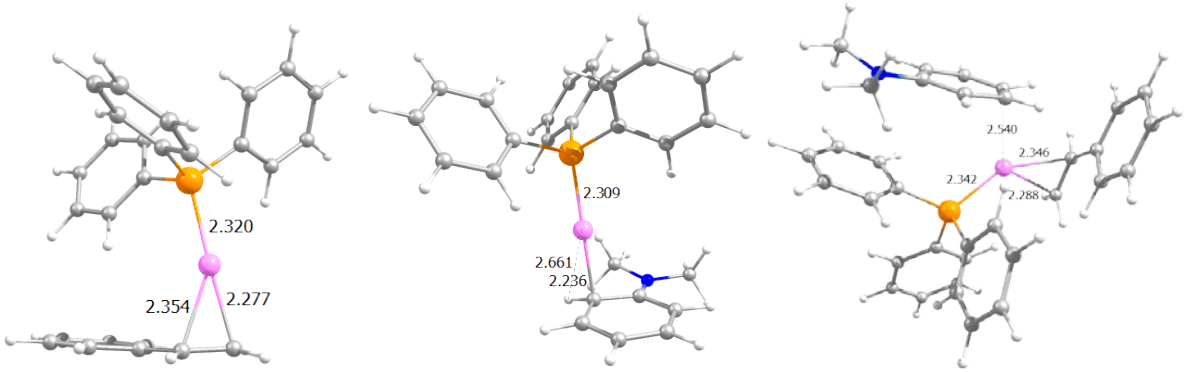
Compound 12


7.940
7.921
7.918
7.550
7.532
7.514
7.446
7.426
7.408
7.260
7.252
7.246
7.175
7.163
7.156
7.148
7.136
7.115
6.665
6.644
4.754
4.735
4.717
3.706
3.688
2.882
Me
N
Me
O
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
2.05
1.13
2.13
4.49
3.16
2.07
1.00
2.00
6.41


198.5103
149.2959
145.0313
137.3262
133.0668
132.3155
128.6726
128.5708
128.5278
128.2081
127.8853
126.2262
112.9380
77.4782
77.1605
76.8430
45.2011
45.1623
40.8032
Me
N
Me
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

IV. Computational data

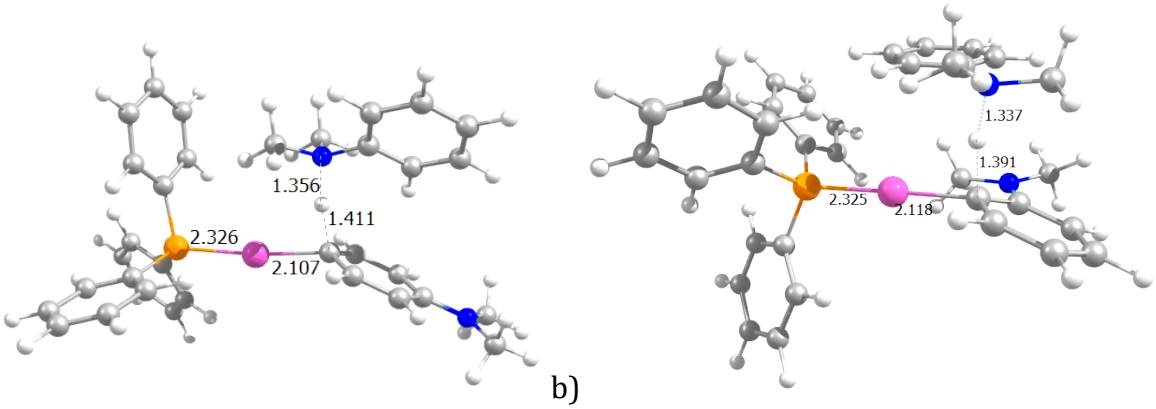
Alternative initial intermediates with arylated styrene and/or *N,N*-dimethylaniline



(a) (b) (c)

Figure S1. Molecular structure of the computed intermediates corresponding to the interaction of $[(PPh_3)Au]^+$ with (a) the arylated styrene, (b) *N,N*-dimethylaniline, and (c) arylated styrene and *N,N*-dimethylaniline (selected distances in Å).

Deprotonation of the aniline



a) b)

Figure S2. Transition states corresponding to the proton transfer from $[(PPh_3)Au(N,N$-dimethylaniline$)]^+$ to a free *N,N*-dimethylaniline molecule (selected distances in Å) in a) para and b) ortho.

An alternative reaction could be the C-H bond cleavage once the aniline is bound to $[(PPh_3)Au]^+$, together with the coordination of a styrene substrate. The energy barrier for such a process is 45.3 kcal/mol, consequently generating a hydride, and, even more importantly, the metal centre necessarily might switch from Au(I) to Au(III). Presumably, due to the positive charge, this step is also highly unfavored from a thermodynamic point of view (by 42.2 kcal/mol).

C-C bond formation

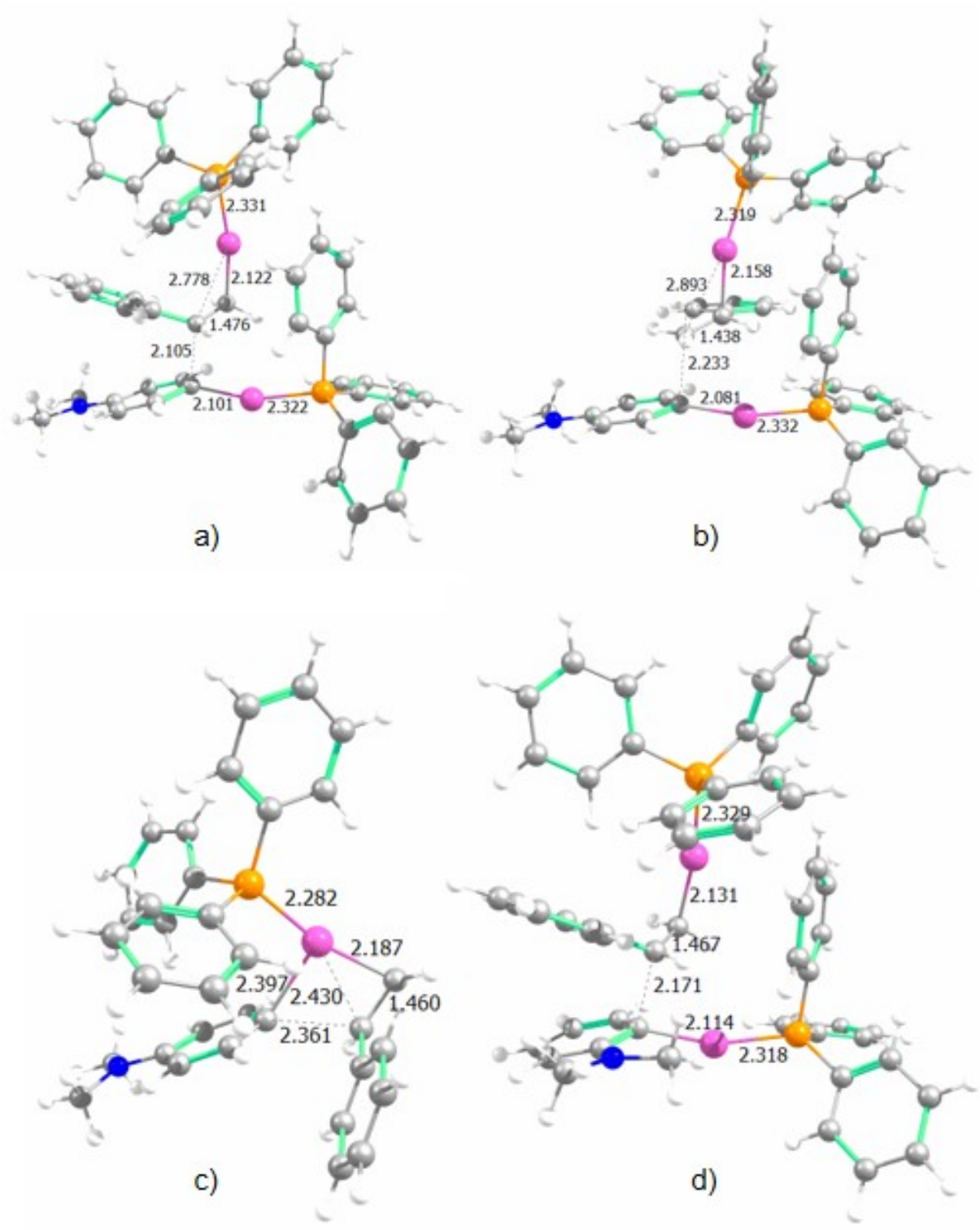


Figure S3. Molecular structures of the computed transition states corresponding to the C-C bond formation following (a) the Markovnikov rules and the (b) anti-Markovnikov rules for the bimetallic mechanism, (c) the Markovnikov rule with only a gold moiety, bearing the *para* substitution of the aniline in all cases, and (d) the Markovnikov rule bearing the bimolecular mechanism and *ortho* substitution of the aniline (selected distances in Å).

Protonation and release of the alkane product

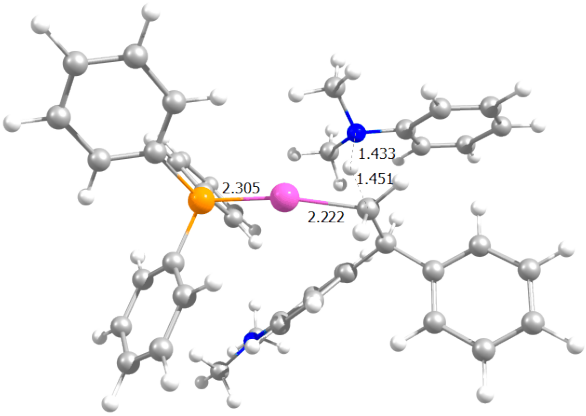
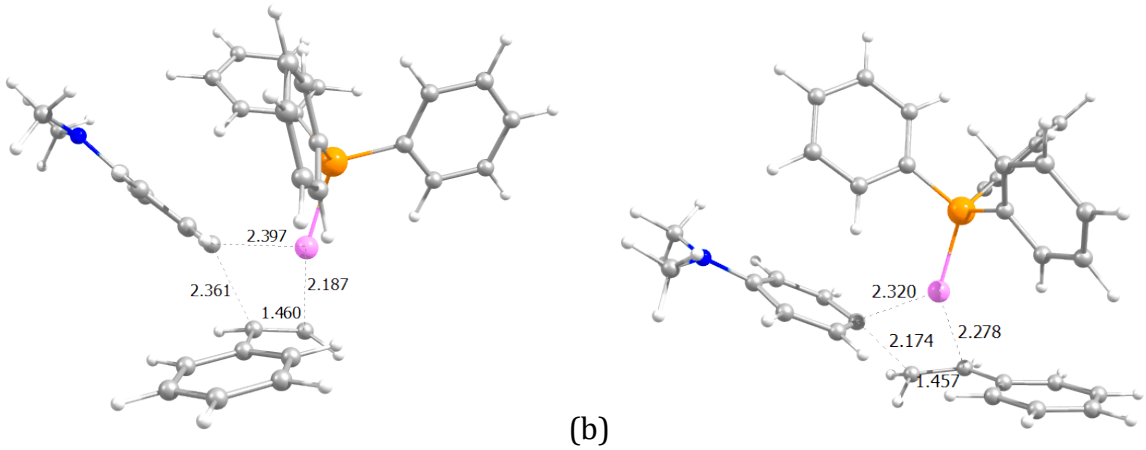


Figure S4. Molecular structure of the computed transition state corresponding to the protonation of the arylated styrene following the Markovnikov rule by a protonated *N,N*-dimethylaniline (selected distances in Å).



(a) (b)

Figure S5. Molecular structures of the computed transition states corresponding to the C-C bond formation following (a) the Markovnikov rules and the (b) anti-Markovnikov rules for the monometallic mechanism (selected distances in Å).

Summary

Overall, Firstly, a dual gold mechanism was determined (Scheme 4), pointing out that the activation of the catalyst led to the catalytically active cationic species, $[(PPh_3)Au]^+$, which is prone to coordinate and activate an incoming alkene derivative. Secondly, the coordination of the dialkylaniline requires its deprotonation and here a free dialkylaniline acts as a base. Thirdly, the C-C bond formation exclusively leads to the Markovnikov product. Here the strong π-π interaction between the six-membered rings that bear the aniline and the styrene moieties help to explain this high selectivity. Finally, the protonated aniline generated in the activation of the precatalyst easily protonates and generates the organic product in an exothermic step. Further, calculations also help to rationalize why the aryl rings on the alkene and aniline help to favor the *para*

Markovnikov products. It is noteworthy that the more hindered the alkene or the aniline are, the more selective the reaction becomes towards the *para* Markovnikov product.

References:

1 N. Mézailles, L. Ricard, F.Gagosz, *Org. Lett*. 2005, **19**, 4133-4136.

Table S1. *xyz* coordinate data sets and absolute energies in a.u. for DFT optimized complexes.

$[(PPh_3)Au]^+$

-1171.45539750 A.U.

P	0.000058	0.001667	-0.190917
C	0.694932	1.571056	-0.782258
C	1.684104	1.576677	-1.791769
C	0.188411	2.785251	-0.260142
C	2.155869	2.806041	-2.281953
H	2.079045	0.631761	-2.195368
C	0.667227	4.003810	-0.760408
H	-0.574586	2.774873	0.535757
C	1.650786	4.014001	-1.769344
H	2.924955	2.817284	-3.069417
H	0.277939	4.951065	-0.356994
H	2.029645	4.973490	-2.154206
C	-1.700061	-0.175125	-0.802153
C	-2.185762	0.684056	-1.813671
C	-2.506549	-1.221141	-0.293687
C	-3.481043	0.483159	-2.319751
H	-1.557939	1.498452	-2.206427
C	-3.795875	-1.410700	-0.809788
H	-2.126385	-1.881215	0.503503
C	-4.282736	-0.558710	-1.821008
H	-3.864655	1.147931	-3.108827
H	-4.428059	-2.221757	-0.417208
H	-5.298807	-0.706611	-2.218515
C	1.010880	-1.375339	-0.804975
C	2.317959	-1.548273	-0.290375
C	0.518024	-2.223090	-1.822754
C	3.133191	-2.564920	-0.806483
H	2.693097	-0.891010	0.511486
C	1.346168	-3.238989	-2.329005
H	-0.499445	-2.088916	-2.220877
C	2.647142	-3.410135	-1.823770
H	4.150232	-2.704565	-0.409350
H	0.968960	-3.901240	-3.123261
H	3.288223	-4.212145	-2.221335
Au	-0.005558	-0.017698	2.092589

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

-1480.95355107 A.U.

P	-1.098126	0.144656	0.001589
H	1.968370	-3.876181	0.083685
C	2.314027	-2.887724	0.428801
C	2.838086	-1.982049	-0.498170
C	3.849865	-0.267552	1.079524
C	3.544429	-0.716435	-0.231853
C	4.452635	0.979346	1.276131
C	3.868694	0.114293	-1.334884
C	4.763846	1.799329	0.171453
H	4.687302	1.318596	2.296577
C	4.472843	1.364474	-1.133959
H	3.633650	-0.224923	-2.356719
H	5.242791	2.777798	0.332435
H	4.720915	1.999349	-1.998193
C	-0.459512	1.775731	0.536012
C	-1.297967	2.676767	1.228920
C	0.867567	2.143561	0.214932
C	-0.807575	3.942707	1.591894
H	-2.328719	2.388288	1.489323
C	1.346504	3.410493	0.581258
H	1.534970	1.441808	-0.312694
C	0.511084	4.310270	1.268641
H	-1.459946	4.644190	2.134495
H	2.382547	3.688244	0.333740
H	0.891642	5.301661	1.559826
C	-2.495978	-0.274677	1.099477
C	-3.829692	-0.048998	0.696704
C	-2.216046	-0.787808	2.386203

C	-4.879140	-0.335565	1.587108
H	-4.048388	0.344001	-0.308596
C	-3.270448	-1.067668	3.268529
H	-1.172925	-0.968123	2.695916
C	-4.601410	-0.841767	2.869139
H	-5.920569	-0.163577	1.274152
H	-3.053957	-1.469078	4.270517
H	-5.427560	-1.067451	3.561141
C	-1.776469	0.345232	-1.683626
C	-2.041294	1.624546	-2.217599
C	-2.074895	-0.816514	-2.431854
C	-2.610748	1.735322	-3.498268
H	-1.803255	2.530225	-1.638028
C	-2.647330	-0.694855	-3.707047
H	-1.861314	-1.814836	-2.014579
C	-2.914567	0.580480	-4.240452
H	-2.817144	2.732258	-3.917413
H	-2.882051	-1.598813	-4.290001
H	-3.358822	0.673431	-5.243642
Au	0.622843	-1.409614	0.054275
H	2.509651	-2.790416	1.510636
H	2.781953	-2.266138	-1.566395
H	3.609112	-0.896278	1.950150

[(PPh_3)Au(alkene)(*para*-aniline)]$^+$

-1846.95077013 A.U.

P	1.114924	0.822060	0.075304
H	-1.874207	2.855602	-2.384520
C	-2.231496	2.385089	-1.453961
C	-3.096206	1.282853	-1.525541
C	-3.598809	1.034642	0.953337
C	-3.863301	0.700707	-0.400790
C	-4.278195	0.386316	1.992628
C	-4.837738	-0.288760	-0.674728
C	-5.239164	-0.603675	1.705857
H	-4.054797	0.654616	3.037021
C	-5.520943	-0.934143	0.368480
H	-5.059917	-0.556235	-1.720721
H	-5.770280	-1.112986	2.524806
H	-6.275983	-1.700659	0.135563
C	2.111542	2.261646	-0.479472
C	3.518303	2.267452	-0.346661
C	1.449483	3.403088	-0.982716
C	4.249724	3.410526	-0.711644
H	4.043902	1.380253	0.039304
C	2.186510	4.542806	-1.341434
H	0.354491	3.394466	-1.096391
C	3.586847	4.547755	-1.206456
H	5.346070	3.410598	-0.609466
H	1.665692	5.429670	-1.734492
H	4.164393	5.440198	-1.493552
C	2.313415	-0.564311	0.090053
C	2.856988	-1.063383	1.290901
C	2.773754	-1.052397	-1.152793
C	3.871809	-2.036135	1.245115
H	2.500468	-0.681283	2.260127
C	3.799487	-2.007647	-1.190182
H	2.336387	-0.672501	-2.090232
C	4.351210	-2.498888	0.008809
H	4.298176	-2.422833	2.183792
H	4.172362	-2.371488	-2.160497
H	5.156873	-3.248775	-0.024099
C	0.708276	1.150129	1.839863
C	1.435844	2.094594	2.596221
C	-0.342531	0.424174	2.447177
C	1.114766	2.304651	3.948817
H	2.249356	2.672017	2.130170
C	-0.654248	0.637432	3.799180
H	-0.920908	-0.303739	1.858764
C	0.073064	1.577972	4.552058
H	1.682373	3.045220	4.533416
H	-1.474349	0.068542	4.264767
H	-0.176299	1.748635	5.610919

Au	-0.914425	0.555423	-1.062655
H	-2.153717	2.999097	-0.541536
H	-3.364414	0.911052	-2.531108
H	-2.832741	1.785626	1.201187
C	-0.702459	-2.776293	0.515104
C	0.344379	-3.372558	-0.256926
C	-1.720261	-2.043517	-0.100867
C	0.319054	-3.169584	-1.675577
C	-1.717859	-1.812434	-1.506736
H	-2.558904	-1.663194	0.504997
C	-0.674617	-2.402921	-2.275906
H	1.095881	-3.617149	-2.308430
H	-2.626131	-1.443791	-2.005917
H	-0.672147	-2.277929	-3.370050
H	-0.748477	-2.929280	1.600803
N	1.328327	-4.130516	0.333153
C	1.345208	-4.302568	1.779672
H	2.299496	-4.774273	2.077774
H	1.291767	-3.318356	2.289499
H	0.508931	-4.940709	2.149798
C	2.147472	-5.025217	-0.479789
H	2.705363	-4.469174	-1.259274
H	2.896193	-5.518426	0.166003
H	1.536693	-5.812931	-0.976898

[(PPh_3)Au(alkene)(*ortho*-aniline)]$^+$

-1846.95646327 A.U.

P	0.145011	1.046551	-0.030150
H	-0.387688	-3.054627	2.764144
C	-0.966626	-2.827637	1.853911
C	-1.831308	-1.713060	1.847352
C	-3.242102	-2.335558	-0.173648
C	-2.902035	-1.432863	0.865850
C	-4.207579	-1.989125	-1.128990
C	-3.569040	-0.183966	0.927660
C	-4.845510	-0.734502	-1.070131
H	-4.469041	-2.703952	-1.924761
C	-4.524632	0.164153	-0.036905
H	-3.314785	0.526805	1.729424
H	-5.598225	-0.462219	-1.825963
H	-5.021574	1.144785	0.018743
C	-0.647172	1.239550	-1.670614
C	-0.540966	2.441432	-2.410291
C	-1.470097	0.197221	-2.147402
C	-1.236704	2.581443	-3.622298
H	0.082444	3.270593	-2.040723
C	-2.170564	0.347895	-3.354507
H	-1.577058	-0.732929	-1.568506
C	-2.050361	1.535613	-4.096656
H	-1.145886	3.516000	-4.197412
H	-2.816173	-0.469652	-3.710232
H	-2.595442	1.650848	-5.046506
C	1.740907	1.963207	-0.086394
C	2.278197	2.511366	1.099880
C	2.465217	2.082811	-1.293972
C	3.519036	3.170178	1.075107
H	1.723286	2.444516	2.047952
C	3.699659	2.754065	-1.314377
H	2.062052	1.657905	-2.223958
C	4.230853	3.297501	-0.131621
H	3.924926	3.598670	2.004573
H	4.247762	2.853805	-2.264310
H	5.197320	3.824459	-0.150338
C	-0.930255	1.988286	1.140962
C	-1.913768	2.892884	0.689952
C	-0.815925	1.718258	2.524687
C	-2.769628	3.517735	1.614111
H	-2.035410	3.092734	-0.384951
C	-1.664145	2.354624	3.444862
H	-0.074798	0.983675	2.882178
C	-2.648168	3.251907	2.989172
H	-3.542209	4.214351	1.253062
H	-1.565717	2.139998	4.520387
H	-3.324254	3.740170	3.707989

Au	0.112322	-1.202442	0.711549
H	-1.118643	-3.673778	1.163049
H	-1.821966	-1.046818	2.728253
H	-2.750507	-3.318700	-0.234009
C	1.755664	-2.701552	-0.323023
C	2.840787	-1.757826	-0.474610
C	0.870243	-2.957698	-1.415760
C	2.925734	-1.057996	-1.720119
C	0.967949	-2.243173	-2.609698
H	0.100425	-3.735554	-1.291983
C	2.009777	-1.296504	-2.744364
H	3.725084	-0.325198	-1.880740
H	0.261820	-2.419769	-3.433328
H	2.108366	-0.731384	-3.684834
H	1.777362	-3.428685	0.501911
N	3.734321	-1.540144	0.543336
C	3.478522	-2.124087	1.850342
H	4.262959	-1.807337	2.560344
H	2.484402	-1.798890	2.252129
H	3.479934	-3.234799	1.817235
C	4.741651	-0.488077	0.425675
H	4.285078	0.525230	0.383369
H	5.415997	-0.531655	1.299901
H	5.365661	-0.631947	-0.480433

[(PPh_3)Au(*para*-aniline)]$^+$

-1537.49129268 A.U.

P	-1.406074	0.143918	0.009103
C	3.896745	-0.651008	-1.236579
C	4.383302	-0.102354	0.000959
C	2.983610	-1.697820	-1.245302
C	3.903687	-0.685566	1.225275
C	2.455119	-2.250291	-0.023783
H	2.664241	-2.126759	-2.208150
C	2.990336	-1.732319	1.209608
H	4.267512	-0.321574	2.194288
H	2.012661	-3.262880	-0.036772
H	2.677020	-2.188393	2.161923
C	-2.711217	-0.688857	-0.967115
C	-3.573845	0.042910	-1.811116
C	-2.871024	-2.086116	-0.825695
C	-4.594463	-0.626831	-2.508475
H	-3.448154	1.130900	-1.926414
C	-3.895855	-2.744842	-1.521935
H	-2.191132	-2.656785	-0.171257
C	-4.756786	-2.015895	-2.364107
H	-5.265843	-0.057562	-3.169860
H	-4.020213	-3.833220	-1.411839
H	-5.556259	-2.535865	-2.914493
C	-1.211499	1.818037	-0.709050
C	-1.868507	2.935640	-0.151376
C	-0.425992	1.965057	-1.874694
C	-1.741075	4.194002	-0.765437
H	-2.476483	2.825642	0.760200
C	-0.310075	3.223591	-2.484616
H	0.093807	1.091467	-2.302453
C	-0.966738	4.338478	-1.929974
H	-2.252027	5.066463	-0.329499
H	0.298016	3.336782	-3.395581
H	-0.871216	5.326163	-2.407363
C	-2.080164	0.372932	1.694870
C	-3.471629	0.336628	1.930689
C	-1.186683	0.643750	2.755444
C	-3.962801	0.577665	3.225387
H	-4.169082	0.117953	1.106876
C	-1.686636	0.886778	4.044172
H	-0.099809	0.660453	2.569166
C	-3.073968	0.853843	4.279396
H	-5.047654	0.546642	3.410709
H	-0.990793	1.096644	4.871224
H	-3.463703	1.038679	5.292506
Au	0.573514	-1.043096	-0.001937
H	4.254798	-0.259554	-2.196986
N	5.278322	0.927988	0.012813

C	5.787542	1.482793	-1.241998
H	6.471838	2.320290	-1.019053
H	6.352646	0.725594	-1.828310
H	4.963747	1.876267	-1.875744
C	5.792627	1.449323	1.279844
H	6.363591	0.678084	1.841740
H	6.472692	2.295291	1.076799
H	4.970999	1.822010	1.928733

[(PPh_3)Au(*ortho*-aniline)]$^+$

-1537.49391303 A.U.

P	-1.256567	0.022705	0.059930
C	3.078597	-0.537818	-1.177614
C	3.737972	0.141792	-0.064872
C	3.010893	-1.980924	-1.184468
C	4.141831	-0.665617	1.048228
C	3.438182	-2.731850	-0.092667
H	2.621280	-2.476656	-2.087670
C	3.995843	-2.051955	1.018950
H	4.603217	-0.201701	1.929281
H	3.357359	-3.828158	-0.096508
H	4.337135	-2.633785	1.889993
C	-2.438385	-0.941472	-0.949819
C	-3.672132	-0.387929	-1.355899
C	-2.117135	-2.278811	-1.274230
C	-4.581862	-1.178500	-2.079211
H	-3.920627	0.656903	-1.111513
C	-3.033686	-3.061275	-1.993279
H	-1.147405	-2.703595	-0.965353
C	-4.265500	-2.511636	-2.395562
H	-5.543506	-0.747822	-2.398563
H	-2.783814	-4.103136	-2.246699
H	-4.980909	-3.125584	-2.964485
C	-1.715062	1.784258	-0.145143
C	-2.425319	2.484778	0.852164
C	-1.365405	2.428949	-1.354259
C	-2.784568	3.827050	0.635142
H	-2.697373	1.985601	1.795183
C	-1.733615	3.766433	-1.564402
H	-0.810768	1.878549	-2.132732
C	-2.441615	4.466577	-0.568775
H	-3.337858	4.374761	1.413706
H	-1.466233	4.266351	-2.508325
H	-2.726257	5.517449	-0.733406
C	-1.581674	-0.406386	1.808190
C	-2.838664	-0.912453	2.205109
C	-0.574649	-0.171470	2.771133
C	-3.084527	-1.173521	3.563921
H	-3.621354	-1.106434	1.454883
C	-0.830640	-0.431807	4.126510
H	0.411090	0.210185	2.456394
C	-2.084879	-0.931979	4.523173
H	-4.063475	-1.571034	3.873497
H	-0.045761	-0.250108	4.876981
H	-2.281660	-1.140996	5.586204
Au	0.942060	-0.334338	-0.549760
H	3.040277	-0.032998	-2.157955
N	3.941743	1.490798	-0.091153
C	3.365214	2.288134	-1.166725
H	3.607811	3.353736	-1.009801
H	3.763466	1.990214	-2.159720
H	2.252214	2.176691	-1.195127
C	4.511047	2.175016	1.070551
H	5.497970	1.747252	1.342644
H	4.665943	3.240563	0.824626
H	3.841186	2.114815	1.957761

[(PPh_3)Au(*para*-aniline)]$^+$ (TS extraction proton by a second aniline)

-1903.46043587 A.U.

P	-2.520076	0.196246	-0.081797
C	4.369496	-1.472836	0.632580
C	3.318132	-2.358837	0.314771
C	5.685427	-1.788036	0.265967
C	3.595262	-3.554666	-0.374260

C	5.967572	-2.982603	-0.420647
H	6.496188	-1.085799	0.514268
C	4.919301	-3.860607	-0.738225
H	2.796007	-4.263711	-0.629518
H	7.001501	-3.227721	-0.708001
H	5.126980	-4.800279	-1.273076
C	-2.732789	-1.486705	0.633547
C	-3.146008	-2.583509	-0.149025
C	-2.318863	-1.691313	1.971512
C	-3.142330	-3.877879	0.404312
H	-3.468538	-2.428159	-1.190551
C	-2.323822	-2.983225	2.518270
H	-1.996047	-0.831686	2.582343
C	-2.730341	-4.079962	1.732780
H	-3.469337	-4.732376	-0.208523
H	-2.011349	-3.137271	3.563087
H	-2.732197	-5.093962	2.162226
C	-3.350443	0.158995	-1.713606
C	-4.744681	0.349947	-1.830296
C	-2.576443	-0.113896	-2.863635
C	-5.357226	0.259511	-3.090971
H	-5.350917	0.579310	-0.939895
C	-3.197335	-0.208912	-4.120224
H	-1.485179	-0.244274	-2.771550
C	-4.586734	-0.022680	-4.234026
H	-6.443625	0.414164	-3.181519
H	-2.592054	-0.419433	-5.015584
H	-5.071497	-0.089808	-5.220482
C	-3.478954	1.325238	0.991541
C	-4.610729	0.880487	1.711452
C	-3.084990	2.680169	1.059488
C	-5.346070	1.793183	2.486132
H	-4.911839	-0.178674	1.674583
C	-3.827873	3.586428	1.833485
H	-2.192856	3.020488	0.508032
C	-4.957538	3.143970	2.545718
H	-6.227120	1.446218	3.048204
H	-3.519619	4.642128	1.885490
H	-5.535919	3.855157	3.155872
Au	-0.222616	0.558225	-0.111303
H	4.159522	-0.522978	1.146538
N	1.957917	-1.972551	0.683035
C	1.727853	-1.879244	2.146467
H	0.746515	-1.388326	2.311563
H	1.723970	-2.887780	2.609564
H	2.520454	-1.265493	2.611458
C	0.871968	-2.724156	0.021406
H	0.825598	-3.774188	0.377489
H	-0.093474	-2.234904	0.260176
H	1.019348	-2.703606	-1.074456
C	3.828395	1.505937	-1.316621
C	4.346663	2.224483	-0.189663
C	2.644598	0.782564	-1.218919
C	3.591488	2.166344	1.029929
C	1.877638	0.696001	-0.008473
H	2.300836	0.227561	-2.107877
C	2.409424	1.435706	1.102944
H	3.935958	2.704065	1.923299
H	1.817280	-0.678780	0.301249
H	1.870943	1.420081	2.065493
H	4.367902	1.507473	-2.272772
N	5.520546	2.928223	-0.268436
C	6.256036	2.995851	-1.528449
H	7.163368	3.610552	-1.389844
H	6.576683	1.987689	-1.872553
H	5.649475	3.461231	-2.336605
C	6.025042	3.654142	0.893715
H	6.200065	2.975497	1.757508
H	6.989189	4.129176	0.638538
H	5.325568	4.455934	1.219621

[(PPh_3)Au(*ortho*-aniline)]$^+$ (TS extraction proton by a second aniline)

-1903.46606053 A.U.

P	-1.944083	-0.180304	-0.031971

C	1.265508	2.271613	1.027263
C	2.614037	1.851680	0.977145
C	0.840059	3.378297	0.274615
C	3.527351	2.568958	0.175471
C	1.745775	4.082002	-0.533257
H	-0.215941	3.681614	0.321845
C	3.090465	3.674466	-0.572731
H	4.583236	2.276799	0.117051
H	1.406372	4.946433	-1.123472
H	3.818272	4.225214	-1.188664
C	-2.809964	-0.212714	1.585653
C	-4.210602	-0.373680	1.664624
C	-2.059189	-0.022644	2.766713
C	-4.849173	-0.332398	2.915619
H	-4.802179	-0.537883	0.750301
C	-2.702881	0.023900	4.013682
H	-0.963298	0.075449	2.703825
C	-4.099075	-0.130187	4.088354
H	-5.940899	-0.462868	2.974398
H	-2.112886	0.171071	4.931639
H	-4.604215	-0.100928	5.066319
C	-2.971155	-1.168937	-1.183787
C	-4.029984	-0.586042	-1.914684
C	-2.709007	-2.552520	-1.298776
C	-4.826145	-1.390127	-2.747869
H	-4.227799	0.494920	-1.837482
C	-3.511340	-3.349083	-2.131401
H	-1.871646	-3.001623	-0.739123
C	-4.569766	-2.769125	-2.854627
H	-5.650352	-0.935513	-3.319280
H	-3.304917	-4.426848	-2.221061
H	-5.194666	-3.394788	-3.510840
C	-2.086867	1.553902	-0.629634
C	-2.794545	2.543117	0.083743
C	-1.448875	1.884629	-1.846733
C	-2.866076	3.854229	-0.424272
H	-3.292313	2.292006	1.033332
C	-1.530077	3.190582	-2.351261
H	-0.890942	1.112910	-2.401071
C	-2.238541	4.178203	-1.640015
H	-3.420545	4.624556	0.133925
H	-1.035620	3.441812	-3.302354
H	-2.300813	5.203982	-2.035434
Au	0.280154	-0.851535	0.047597
H	0.527836	1.746417	1.646857
N	3.009125	0.628348	1.656379
C	2.335478	0.375362	2.953031
H	1.252569	0.221578	2.785057
H	2.742172	-0.558742	3.382165
H	2.491742	1.217817	3.656502
C	4.459358	0.338478	1.714538
H	5.001442	1.097615	2.315018
H	4.589485	-0.664638	2.162151
H	4.874478	0.297875	0.691404
C	2.295995	-1.497564	0.127808
C	3.294835	-1.306812	-0.918430
C	2.483162	-2.615000	1.017803
C	4.402253	-2.209885	-0.977409
C	3.568609	-3.484823	0.936745
H	1.742018	-2.766450	1.820374
C	4.527400	-3.270059	-0.079277
H	5.154719	-2.106126	-1.771605
H	2.532243	-0.363027	0.897307
H	5.385813	-3.953696	-0.178393
H	3.674778	-4.323780	1.640808
N	3.257891	-0.230048	-1.785308
C	2.025645	0.429152	-2.204903
H	2.154409	0.815742	-3.235889
H	1.185699	-0.298625	-2.222386
H	1.735270	1.279726	-1.550112
C	4.464212	0.209593	-2.478927
H	4.647073	-0.338061	-3.432761
H	4.370073	1.288768	-2.713424
H	5.357988	0.089650	-1.833917

[(PPh_3)Au(*para*-aniline)]

-1537.06376633 A.U.

P	-1.729450	-0.005025	0.007833
C	4.825787	-1.220076	-0.042231
C	5.563672	-0.002119	-0.029287
C	3.422475	-1.215339	-0.029421
C	4.812643	1.206858	0.019245
C	2.661913	-0.018876	0.004212
H	2.906243	-2.190114	-0.043169
C	3.409538	1.186183	0.031234
H	5.323093	2.180155	0.047142
H	2.882662	2.154713	0.066660
C	-2.450879	1.657904	-0.322311
C	-3.619666	2.126244	0.315514
C	-1.796441	2.474765	-1.272118
C	-4.132550	3.396113	-0.003486
H	-4.127159	1.501104	1.067241
C	-2.316949	3.739334	-1.590412
H	-0.870828	2.115723	-1.752489
C	-3.485481	4.201608	-0.957125
H	-5.042826	3.758465	0.500162
H	-1.801369	4.371439	-2.330506
H	-3.888584	5.196998	-1.202452
C	-2.514510	-0.540938	1.586084
C	-3.757880	-1.208568	1.627458
C	-1.839379	-0.242483	2.790602
C	-4.323879	-1.562142	2.864602
H	-4.281051	-1.457695	0.690543
C	-2.411971	-0.594764	4.023812
H	-0.856212	0.255940	2.753039
C	-3.654428	-1.253737	4.062461
H	-5.292565	-2.086083	2.891896
H	-1.879392	-0.361774	4.959308
H	-4.098783	-1.536114	5.030109
C	-2.493031	-1.092754	-1.268078
C	-3.675275	-0.746961	-1.957333
C	-1.859419	-2.326026	-1.539693
C	-4.222245	-1.634150	-2.901031
H	-4.165654	0.219723	-1.760533
C	-2.413753	-3.210514	-2.478818
H	-0.921720	-2.581757	-1.018615
C	-3.595607	-2.866056	-3.160334
H	-5.143003	-1.358331	-3.439310
H	-1.913870	-4.169525	-2.687406
H	-4.025271	-3.557165	-3.902788
Au	0.617503	-0.023984	0.012410
H	5.347107	-2.187751	-0.064389
N	6.957815	0.006263	-0.062971
C	7.687010	-1.244812	0.011322
H	8.773451	-1.043301	-0.052543
H	7.497780	-1.803931	0.960694
H	7.425220	-1.925972	-0.830489
C	7.673792	1.259700	0.073017
H	7.482458	1.767649	1.050376
H	8.762087	1.073574	-0.004797
H	7.401556	1.979929	-0.732082

[(PPh_3)Au(*ortho*-aniline)]

-1537.06436098 A.U.

P	1.343272	-0.031416	0.023334
C	-5.321588	-0.046964	0.158199
C	-3.946742	0.270628	0.042607
C	-5.761823	-1.382074	0.122419
C	-2.987216	-0.779596	-0.100735
C	-4.835988	-2.420704	-0.050270
H	-6.837607	-1.603030	0.218916
C	-3.465914	-2.108699	-0.163008
H	-5.171254	-3.470109	-0.084408
H	-2.743344	-2.934912	-0.271500
C	1.983434	0.447101	1.682871
C	3.053588	1.351523	1.854348
C	1.375978	-0.142457	2.814245
C	3.518160	1.651855	3.146710

H	3.520303	1.826755	0.976988
C	1.848242	0.157590	4.102326
H	0.522131	-0.827257	2.679126
C	2.919822	1.053737	4.270136
H	4.351408	2.360745	3.275935
H	1.369139	-0.303557	4.980274
H	3.284390	1.293618	5.281567
C	1.898855	1.324096	-1.094135
C	3.148612	1.302297	-1.750071
C	1.033524	2.427286	-1.270050
C	3.531163	2.381345	-2.566142
H	3.819686	0.437434	-1.626533
C	1.423425	3.503629	-2.083031
H	0.047266	2.430866	-0.777557
C	2.672169	3.482600	-2.731070
H	4.505636	2.358889	-3.079351
H	0.743403	4.359346	-2.218946
H	2.973565	4.324557	-3.374289
C	2.372994	-1.476803	-0.468844
C	3.607169	-1.776557	0.146236
C	1.897421	-2.292022	-1.520675
C	4.361905	-2.877678	-0.295183
H	3.976174	-1.151542	0.974760
C	2.658720	-3.386579	-1.960960
H	0.922338	-2.067837	-1.984664
C	3.891301	-3.680866	-1.349056
H	5.322906	-3.110242	0.190487
H	2.282490	-4.019021	-2.780431
H	4.483640	-4.544506	-1.690659
Au	-0.964026	-0.418546	-0.049926
H	-6.067307	0.755458	0.265269
N	-3.502341	1.631085	0.099324
C	-4.360207	2.585521	0.778553
H	-3.782387	3.511948	0.986285
H	-5.266390	2.891619	0.188338
H	-4.703368	2.170566	1.747454
C	-2.954424	2.174166	-1.140461
H	-2.296966	1.429091	-1.629306
H	-3.756972	2.462923	-1.871439
H	-2.349044	3.082737	-0.927203

[(PPh_3)Au(*para*-aniline)+(PPh_3)Au(alkene)]$^+$ adduct

-3018.07535840 A.U.

P	-3.903705	-0.871514	0.009688
H	0.522041	1.264674	0.747016
C	0.062320	1.735261	-0.139188
C	-0.016010	0.943407	-1.312628
C	-0.362976	3.662892	1.351033
C	-0.428495	3.084277	0.055148
C	-0.814209	4.969065	1.579864
C	-0.938186	3.875979	-1.013521
C	-1.305006	5.738952	0.510160
H	-0.765976	5.395831	2.593486
C	-1.379079	5.181278	-0.784446
H	-0.982118	3.456908	-2.029748
H	-1.645249	6.771560	0.684606
H	-1.773508	5.780996	-1.619440
C	-4.990718	0.350162	0.839706
C	-5.948666	-0.056782	1.795758
C	-4.875802	1.714730	0.492333
C	-6.794042	0.897491	2.385973
H	-6.023613	-1.116151	2.088909
C	-5.725208	2.661789	1.086752
H	-4.110759	2.036530	-0.233818
C	-6.685140	2.254307	2.030887
H	-7.539132	0.579289	3.131711
H	-5.629624	3.724845	0.816735
H	-7.347011	2.999330	2.499431
C	-3.721498	-2.247660	1.209065
C	-4.066912	-3.575147	0.884318
C	-3.136875	-1.955018	2.462671
C	-3.821442	-4.605874	1.810212
H	-4.523826	-3.806761	-0.090461
C	-2.905391	-2.986211	3.385062

H	-2.861191	-0.917315	2.712626
C	-3.241901	-4.314367	3.057372
H	-4.087761	-5.642893	1.553476
H	-2.453784	-2.755200	4.362310
H	-3.052207	-5.124218	3.778810
C	-4.841643	-1.561383	-1.407216
C	-6.236069	-1.769068	-1.320222
C	-4.146556	-1.930621	-2.580392
C	-6.923764	-2.351467	-2.397220
H	-6.787481	-1.468265	-0.415645
C	-4.840707	-2.516136	-3.652401
H	-3.061197	-1.751463	-2.653796
C	-6.227918	-2.727928	-3.560994
H	-8.011444	-2.508376	-2.328699
H	-4.296608	-2.800672	-4.566405
H	-6.771870	-3.181846	-4.403982
Au	-1.859309	0.036017	-0.617804
H	-0.225691	1.432051	-2.281013
H	0.680111	0.087458	-1.372549
H	0.048709	3.067251	2.180103
P	3.365499	-1.805959	0.051000
C	2.197430	4.564545	-1.339173
C	2.126821	5.336509	-0.139843
C	2.583010	3.221403	-1.302137
C	2.550676	4.700922	1.067979
C	2.938720	2.554160	-0.096332
H	2.589107	2.662590	-2.252625
C	2.941560	3.357714	1.074767
H	2.567910	5.260283	2.013005
H	3.247012	2.916372	2.038037
C	3.729756	-2.508724	1.711536
C	4.052773	-3.872975	1.882218
C	3.639848	-1.663607	2.839645
C	4.274222	-4.384843	3.170632
H	4.142174	-4.536012	1.007705
C	3.858661	-2.182797	4.127563
H	3.406024	-0.594634	2.702185
C	4.174452	-3.542445	4.293917
H	4.532076	-5.447815	3.298663
H	3.792148	-1.518613	5.003459
H	4.353610	-3.947241	5.302380
C	4.500706	-2.638169	-1.125340
C	4.242834	-3.922999	-1.655209
C	5.689605	-1.959926	-1.475136
C	5.173993	-4.523234	-2.518988
H	3.308287	-4.449492	-1.403832
C	6.618099	-2.568206	-2.336056
H	5.879861	-0.950301	-1.074586
C	6.361677	-3.848898	-2.857414
H	4.969794	-5.523511	-2.932107
H	7.543076	-2.035519	-2.606259
H	7.088057	-4.322513	-3.536289
C	1.680960	-2.445786	-0.356869
C	0.784960	-2.830975	0.663457
C	1.243995	-2.442761	-1.702340
C	-0.524740	-3.224770	0.341592
H	1.116023	-2.836162	1.713832
C	-0.066760	-2.836192	-2.018904
H	1.935905	-2.140240	-2.504981
C	-0.953437	-3.228284	-0.997820
H	-1.212820	-3.536802	1.140327
H	-0.396407	-2.838274	-3.069901
H	-1.979241	-3.545127	-1.241498
Au	3.299430	0.536163	-0.033067
H	1.932575	5.012310	-2.306366
N	1.650821	6.636529	-0.141931
C	1.362965	7.297764	-1.406082
H	0.927499	8.294587	-1.208506
H	2.274476	7.432355	-2.034041
H	0.622177	6.718070	-1.997241
C	1.727903	7.439996	1.069835
H	2.778838	7.624313	1.393479
H	1.244176	8.418357	0.892838
H	1.191897	6.947569	1.909223

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3018.05949556 A.U.

P	3.764235	-1.198265	-0.039651
H	-0.843726	-0.019007	-1.497191
C	-0.015433	0.702110	-1.348928
C	-0.148638	1.501496	-0.114732
C	1.380307	3.416700	-0.796039
C	0.845002	2.566839	0.199033
C	2.340048	4.388588	-0.467852
C	1.293848	2.725621	1.532252
C	2.784345	4.528206	0.859454
H	2.751517	5.036401	-1.257942
C	2.259874	3.687820	1.860208
H	0.884449	2.066667	2.315150
H	3.541399	5.286288	1.114768
H	2.608384	3.784060	2.900559
C	5.087304	0.078372	-0.201972
C	6.453663	-0.244095	-0.349826
C	4.693660	1.437634	-0.162576
C	7.413201	0.779265	-0.433632
H	6.778310	-1.292596	-0.418867
C	5.659966	2.453416	-0.234637
H	3.628139	1.712126	-0.090467
C	7.020945	2.127843	-0.367925
H	8.475983	0.517645	-0.554964
H	5.334735	3.504403	-0.197686
H	7.777211	2.925709	-0.433159
C	4.406254	-2.785703	-0.683582
C	5.476944	-3.475475	-0.065950
C	3.797957	-3.330627	-1.836421
C	5.936983	-4.687053	-0.606375
H	5.943079	-3.073310	0.847458
C	4.263151	-4.543637	-2.372272
H	2.954948	-2.798004	-2.307117
C	5.332897	-5.220226	-1.760235
H	6.770646	-5.219576	-0.122611
H	3.787022	-4.962027	-3.272667
H	5.696343	-6.170625	-2.181404
C	3.523286	-1.428372	1.779237
C	3.236971	-0.276701	2.548242
C	3.451907	-2.700713	2.385284
C	2.886937	-0.399789	3.901360
H	3.275548	0.721824	2.085293
C	3.101440	-2.817362	3.742920
H	3.657329	-3.610590	1.801602
C	2.815431	-1.670629	4.502979
H	2.668369	0.504454	4.491179
H	3.049165	-3.815297	4.205552
H	2.539222	-1.765947	5.564617
Au	1.751522	-0.374954	-0.879620
H	0.147940	1.290378	-2.273698
H	-0.410179	0.907491	0.777315
H	1.046674	3.307553	-1.837864
P	-3.657570	-1.408071	0.053526
C	-1.623703	4.796271	1.015111
C	-1.484004	5.465390	-0.248336
C	-1.844544	3.430090	1.066786
C	-1.654905	4.678086	-1.439864
C	-1.940759	2.605169	-0.108214
H	-1.899058	2.949831	2.058078
C	-1.873917	3.312920	-1.356172
H	-1.583937	5.146210	-2.430581
H	-1.940439	2.735802	-2.293804
C	-4.444702	-2.087958	-1.454931
C	-5.189180	-3.287013	-1.423650
C	-4.250772	-1.409945	-2.679313
C	-5.729116	-3.804166	-2.613100
H	-5.354561	-3.812457	-0.469862
C	-4.787904	-1.936617	-3.865356
H	-3.682214	-0.464954	-2.697571
C	-5.527213	-3.132968	-3.832868
H	-6.314930	-4.736187	-2.585743
H	-4.636605	-1.405102	-4.817781

H	-5.955026	-3.540604	-4.762145
C	-4.630478	-2.009392	1.481325
C	-4.374757	-3.261121	2.084059
C	-5.684013	-1.197024	1.955355
C	-5.180738	-3.698072	3.149009
H	-3.543014	-3.888603	1.725514
C	-6.487620	-1.643239	3.017047
H	-5.866023	-0.212830	1.492729
C	-6.237033	-2.892943	3.612937
H	-4.981499	-4.673327	3.620145
H	-7.308956	-1.009347	3.385788
H	-6.864952	-3.239091	4.448800
C	-2.012188	-2.237719	0.170225
C	-1.502563	-3.050492	-0.862106
C	-1.204547	-1.940989	1.294312
C	-0.196663	-3.566215	-0.764866
H	-2.121541	-3.277849	-1.744074
C	0.092798	-2.462954	1.389512
H	-1.596500	-1.292380	2.095372
C	0.598433	-3.276634	0.356057
H	0.203126	-4.195554	-1.575064
H	0.723595	-2.223431	2.259278
H	1.620866	-3.678084	0.421895
Au	-3.071582	0.837939	-0.007012
H	-1.534350	5.356872	1.954613
N	-1.179040	6.795402	-0.315494
C	-0.922437	7.557808	0.905746
H	-0.637599	8.590993	0.638320
H	-1.823630	7.609220	1.554783
H	-0.091369	7.111294	1.493490
C	-1.032225	7.457556	-1.610120
H	-1.959140	7.375499	-2.217070
H	-0.827207	8.531142	-1.450793
H	-0.190475	7.028130	-2.197514

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ Intermediate Markovnikov

-3018.09087586 A.U.

P	4.113653	-0.427318	-0.095070
H	-0.691342	0.108288	-1.299581
C	0.049712	0.925837	-1.128374
C	-0.397152	1.816744	0.058348
C	0.709719	4.026213	-0.617925
C	0.598827	2.954319	0.291177
C	1.690785	5.017936	-0.443169
C	1.485365	2.905288	1.389019
C	2.570947	4.958179	0.652709
H	1.766777	5.845321	-1.166458
C	2.462378	3.898717	1.571055
H	1.426695	2.060013	2.095035
H	3.336492	5.737286	0.792943
H	3.145306	3.843543	2.433672
C	5.275494	0.924645	-0.563411
C	6.658059	0.714744	-0.754480
C	4.741049	2.228860	-0.687487
C	7.496644	1.801665	-1.053684
H	7.083920	-0.297560	-0.683085
C	5.588572	3.312333	-0.970008
H	3.658958	2.400131	-0.561923
C	6.966173	3.101045	-1.154372
H	8.573551	1.631322	-1.209029
H	5.159203	4.323000	-1.052339
H	7.629507	3.949300	-1.385654
C	4.835732	-2.011091	-0.673148
C	5.952292	-2.615826	-0.050710
C	4.237168	-2.634513	-1.791019
C	6.465060	-3.824891	-0.549553
H	6.412774	-2.148470	0.834425
C	4.756162	-3.842237	-2.287201
H	3.354530	-2.168576	-2.260005
C	5.869964	-4.437354	-1.668039
H	7.334421	-4.292413	-0.061210
H	4.287493	-4.321770	-3.160850
H	6.275101	-5.385211	-2.055762
C	4.187893	-0.482243	1.748609

C	4.255057	0.730865	2.469362
C	4.020415	-1.695827	2.452341
C	4.150304	0.727679	3.869925
H	4.387009	1.683178	1.932773
C	3.919931	-1.693488	3.854517
H	3.974121	-2.650687	1.905986
C	3.980003	-0.482370	4.566709
H	4.209169	1.679263	4.421709
H	3.798299	-2.646704	4.392866
H	3.903269	-0.482652	5.665218
Au	1.932532	0.113185	-0.739226
H	0.097371	1.525251	-2.065445
H	-0.369859	1.195110	0.980495
H	0.025613	4.083416	-1.480488
P	-3.141860	-1.894008	0.091863
C	-3.607001	3.728268	1.054311
C	-4.182065	4.087823	-0.209754
C	-2.485664	2.905793	1.126185
C	-3.568774	3.546474	-1.386087
C	-1.845568	2.360267	-0.044474
H	-2.035438	2.696295	2.110504
C	-2.444935	2.724117	-1.301984
H	-3.973000	3.773583	-2.380817
H	-1.974711	2.360747	-2.229018
C	-3.887507	-2.631003	-1.406767
C	-4.669243	-3.803949	-1.342104
C	-3.627152	-2.019440	-2.654691
C	-5.183849	-4.361847	-2.525330
H	-4.881717	-4.279128	-0.371692
C	-4.137380	-2.589035	-3.831389
H	-3.022174	-1.098457	-2.700930
C	-4.917335	-3.759053	-3.767206
H	-5.798618	-5.273858	-2.473996
H	-3.931251	-2.113631	-4.802897
H	-5.323612	-4.200009	-4.690818
C	-3.981336	-2.617269	1.542671
C	-3.550711	-3.850588	2.080325
C	-5.095719	-1.949539	2.095823
C	-4.244083	-4.414359	3.164139
H	-2.672129	-4.362718	1.656667
C	-5.784323	-2.522253	3.177258
H	-5.414004	-0.979015	1.680419
C	-5.359573	-3.753349	3.710244
H	-3.908946	-5.374269	3.586841
H	-6.652562	-2.002183	3.610750
H	-5.897944	-4.197492	4.562024
C	-1.395182	-2.466535	0.150160
C	-0.838999	-3.285382	-0.853503
C	-0.584733	-1.999327	1.211112
C	0.521395	-3.639398	-0.787091
H	-1.461236	-3.643868	-1.688012
C	0.768638	-2.357368	1.270014
H	-1.010166	-1.337901	1.983991
C	1.322400	-3.181096	0.270710
H	0.958783	-4.272731	-1.574323
H	1.402442	-1.975205	2.084401
H	2.389250	-3.449620	0.301825
Au	-2.964223	0.392556	0.040421
H	-4.040178	4.102780	1.990578
N	-5.277335	4.908755	-0.287471
C	-5.858412	5.478163	0.925002
H	-6.728087	6.103528	0.654925
H	-6.213497	4.686657	1.621247
H	-5.131932	6.120757	1.470605
C	-5.827902	5.278214	-1.588348
H	-6.155831	4.384443	-2.163452
H	-6.710769	5.925747	-1.441418
H	-5.092231	5.838882	-2.207269

[(PPh_3)Au(*para*-aniline-alkene)] Markovnikov

-1846.54317581 A.U.

H	2.309518	-3.094562	-0.056959
C	2.167604	-2.023673	-0.324349
C	3.099886	-1.122244	0.526766

C	5.117698	-2.316998	-0.569618
C	4.603671	-1.326019	0.290780
C	6.505791	-2.476472	-0.746098
C	5.526632	-0.497597	0.972697
C	7.408497	-1.646967	-0.062242
H	6.881307	-3.258544	-1.426141
C	6.910218	-0.653738	0.802749
H	5.141705	0.291185	1.640051
H	8.494601	-1.770845	-0.200670
H	7.606931	0.005564	1.345892
H	2.435663	-1.921323	-1.402231
H	2.920944	-1.382766	1.595729
H	4.425988	-2.978441	-1.111805
P	-1.965611	-0.459912	-0.032326
C	1.370997	2.274832	1.120989
C	1.691597	3.010769	-0.054513
C	1.878628	0.983844	1.317436
C	2.557700	2.384695	-0.996257
C	2.704153	0.346782	0.368821
H	1.610255	0.437498	2.237821
C	3.039686	1.084950	-0.783247
H	2.854157	2.911006	-1.914476
H	3.697702	0.626366	-1.539678
C	-1.971880	1.273705	-0.655859
C	-2.950929	2.206842	-0.246320
C	-0.973962	1.663598	-1.575274
C	-2.948154	3.506960	-0.779821
H	-3.710204	1.917650	0.498098
C	-0.980484	2.963137	-2.107438
H	-0.175293	0.955249	-1.849578
C	-1.969151	3.882183	-1.718599
H	-3.712238	4.232181	-0.457575
H	-0.194568	3.258466	-2.819073
H	-1.964403	4.903617	-2.131232
C	-2.628921	-0.282546	1.677737
C	-3.940814	-0.648938	2.042015
C	-1.756924	0.261434	2.648556
C	-4.376877	-0.466781	3.367435
H	-4.622260	-1.078086	1.290536
C	-2.200166	0.446559	3.966779
H	-0.730384	0.538671	2.359506
C	-3.511078	0.081777	4.329091
H	-5.402003	-0.756631	3.648134
H	-1.516257	0.871564	4.718530
H	-3.855937	0.221747	5.365867
C	-3.302203	-1.329642	-0.952950
C	-4.351315	-0.662331	-1.620584
C	-3.260346	-2.742470	-0.953784
C	-5.353790	-1.403848	-2.270118
H	-4.383074	0.438206	-1.640730
C	-4.269893	-3.477872	-1.595454
H	-2.422519	-3.259449	-0.456563
C	-5.318157	-2.809622	-2.254276
H	-6.167608	-0.877764	-2.794107
H	-4.230965	-4.578591	-1.590770
H	-6.105209	-3.386808	-2.765078
Au	0.164527	-1.428495	-0.163372
H	0.727305	2.712995	1.895987
N	1.177258	4.285651	-0.274555
C	0.232822	4.851422	0.668345
H	-0.189520	5.785673	0.251842
H	-0.619491	4.157664	0.839094
H	0.689796	5.090496	1.660173
C	1.723288	5.112186	-1.332331
H	1.533044	4.687084	-2.346172
H	1.249615	6.111610	-1.301319
H	2.826160	5.252080	-1.236333

[(PPh_3)Au(*ortho*-aniline)+(PPh_3)Au(alkene)]$^+$ adduct

3018.07337739 A.U.

P	3.730422	-0.984680	-0.017742
H	-0.940076	0.265887	-1.447460
C	-0.111877	0.991449	-1.420820
C	0.198307	1.591927	-0.188399

C	1.715065	3.469046	-0.972428
C	1.065250	2.748219	0.063489
C	2.569065	4.532697	-0.668264
C	1.300807	3.126433	1.408275
C	2.801911	4.894674	0.676592
H	3.066140	5.084692	-1.480761
C	2.167784	4.188505	1.711690
H	0.786301	2.581446	2.213986
H	3.475800	5.733022	0.912587
H	2.337339	4.474262	2.761074
C	5.049838	0.273180	-0.294629
C	6.341827	-0.070238	-0.748736
C	4.735031	1.631745	-0.052693
C	7.312148	0.931168	-0.927784
H	6.597712	-1.113727	-0.982934
C	5.712985	2.622715	-0.224085
H	3.719571	1.934587	0.247280
C	7.004947	2.275453	-0.657248
H	8.315561	0.654090	-1.286570
H	5.448777	3.673576	-0.030713
H	7.769351	3.055321	-0.798270
C	4.286329	-2.570211	-0.727775
C	5.427919	-3.244044	-0.229138
C	3.560307	-3.127292	-1.803806
C	5.827978	-4.462083	-0.801987
H	6.004127	-2.821394	0.609066
C	3.967396	-4.345547	-2.372288
H	2.670371	-2.604157	-2.189535
C	5.098593	-5.013721	-1.871352
H	6.715355	-4.983272	-0.410672
H	3.398450	-4.773915	-3.211912
H	5.415636	-5.969280	-2.317239
C	3.562191	-1.202612	1.809542
C	3.130471	-0.081155	2.556854
C	3.709887	-2.449380	2.452408
C	2.867196	-0.206230	3.928837
H	2.973217	0.892626	2.066416
C	3.438706	-2.568487	3.827800
H	4.017258	-3.340963	1.886781
C	3.018753	-1.450929	4.568430
H	2.532700	0.673284	4.500731
H	3.553935	-3.546841	4.319548
H	2.804533	-1.549651	5.643840
Au	1.690214	-0.142331	-0.746814
H	0.145381	1.472214	-2.378665
H	-0.308983	1.184972	0.704104
H	1.558508	3.181045	-2.022740
P	-3.385365	-1.266809	0.127750
C	-1.403700	4.921617	-0.356445
C	-2.114570	3.700899	-0.484323
C	-1.054813	5.425906	0.904607
C	-2.461753	2.957848	0.694317
C	-1.426591	4.732085	2.068439
H	-0.500582	6.374901	0.975250
C	-2.123521	3.514952	1.950031
H	-1.169674	5.132074	3.062207
H	-2.390519	2.965775	2.868104
C	-1.716001	-2.049076	0.242806
C	-1.174598	-2.847179	-0.786323
C	-0.959758	-1.807774	1.413829
C	0.104750	-3.413387	-0.634205
H	-1.753020	-3.028598	-1.705817
C	0.311156	-2.382810	1.566155
H	-1.373751	-1.164362	2.207914
C	0.842049	-3.190641	0.541450
H	0.525937	-4.038691	-1.436893
H	0.898076	-2.193646	2.477826
H	1.840340	-3.639151	0.654830
C	-3.920540	-1.594185	-1.601139
C	-4.652475	-2.747682	-1.954730
C	-3.543017	-0.668180	-2.601480
C	-4.993284	-2.976362	-3.299449
H	-4.963685	-3.465071	-1.179066
C	-3.880603	-0.907032	-3.943360

H	-2.998859	0.250435	-2.323505
C	-4.605388	-2.061177	-4.294203
H	-5.570119	-3.874532	-3.570145
H	-3.587792	-0.180949	-4.718070
H	-4.877777	-2.242567	-5.345697
C	-4.462953	-2.282728	1.203402
C	-4.185607	-3.639937	1.479534
C	-5.622873	-1.675407	1.733375
C	-5.074157	-4.385104	2.272804
H	-3.274106	-4.111667	1.078586
C	-6.508586	-2.428464	2.521353
H	-5.823106	-0.610168	1.530599
C	-6.235572	-3.782196	2.789942
H	-4.857889	-5.442958	2.489679
H	-7.412472	-1.953799	2.933677
H	-6.928796	-4.369651	3.412119
Au	-3.118630	1.013354	0.549849
H	-1.128369	5.501789	-1.248549
N	-2.452956	3.187183	-1.771528
C	-1.745628	3.735788	-2.920703
H	-1.902399	3.069862	-3.795071
H	-2.093663	4.758625	-3.216980
H	-0.658699	3.790118	-2.716435
C	-3.885573	3.032100	-2.054148
H	-4.412762	2.625051	-1.170983
H	-4.357692	4.009487	-2.325755
H	-4.037104	2.328165	-2.899028

[(PPh_3)Au(*ortho*-aniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3018.05945093 A.U.

P	3.793603	-1.066703	0.033770
H	-0.791026	-0.085087	-1.671775
C	0.044974	0.638843	-1.607723
C	-0.063085	1.572281	-0.480913
C	1.447464	3.407751	-1.371850
C	0.927940	2.661458	-0.287731
C	2.400683	4.412734	-1.152231
C	1.400744	2.941792	1.016804
C	2.857335	4.688233	0.151085
H	2.790988	4.989313	-2.005343
C	2.358301	3.943496	1.235801
H	1.029095	2.341279	1.861579
H	3.605558	5.478248	0.320292
H	2.723573	4.140982	2.256123
C	5.130101	0.145022	-0.340298
C	6.494210	-0.212407	-0.400016
C	4.751341	1.492608	-0.551037
C	7.466775	0.771227	-0.647943
H	6.806281	-1.259421	-0.270209
C	5.730885	2.471209	-0.782376
H	3.687397	1.783324	-0.548216
C	7.089614	2.113690	-0.830545
H	8.528371	0.483336	-0.700563
H	5.418347	3.515324	-0.937658
H	7.856809	2.879966	-1.022724
C	4.405450	-2.752191	-0.325860
C	5.432881	-3.362584	0.432788
C	3.816465	-3.457657	-1.399013
C	5.866146	-4.659044	0.111289
H	5.884375	-2.831213	1.285668
C	4.255631	-4.754221	-1.715936
H	3.008673	-2.983648	-1.980836
C	5.279689	-5.354513	-0.962594
H	6.665132	-5.130542	0.704498
H	3.794923	-5.298258	-2.555085
H	5.621844	-6.371508	-1.210233
C	3.551054	-0.973822	1.863296
C	3.391396	0.305073	2.444739
C	3.360722	-2.124443	2.658854
C	3.044272	0.426760	3.799049
H	3.531331	1.213074	1.838014
C	3.015630	-1.995309	4.016584
H	3.476271	-3.129005	2.224528
C	2.852295	-0.722187	4.589183

H	2.928637	1.428737	4.242037
H	2.873708	-2.899715	4.628646
H	2.582489	-0.624855	5.652334
Au	1.794809	-0.381111	-0.945271
H	0.250706	1.097983	-2.594256
H	-0.361555	1.094757	0.466106
H	1.089115	3.203914	-2.391024
P	-3.671221	-1.161998	0.012398
C	-1.500376	5.189986	-0.192080
C	-1.518427	5.443782	-1.559606
C	-1.668627	3.865211	0.326957
C	-1.702698	4.400790	-2.501275
C	-1.866430	2.773086	-0.622472
H	-1.378306	6.479328	-1.908883
C	-1.868665	3.110312	-2.021106
H	-1.704186	4.611213	-3.581340
H	-1.961100	2.282996	-2.745128
C	-4.455183	-2.015302	-1.404867
C	-5.131406	-3.243987	-1.239493
C	-4.328688	-1.445405	-2.691134
C	-5.671715	-3.897649	-2.359031
H	-5.242512	-3.685838	-0.236726
C	-4.866376	-2.108368	-3.806870
H	-3.814394	-0.477272	-2.812090
C	-5.537583	-3.333127	-3.641075
H	-6.204737	-4.852361	-2.228948
H	-4.769212	-1.661295	-4.808368
H	-5.965955	-3.847843	-4.515295
C	-4.655299	-1.562694	1.502468
C	-4.419166	-2.734988	2.254331
C	-5.692020	-0.678755	1.875851
C	-5.226099	-3.022300	3.368113
H	-3.600645	-3.417066	1.973988
C	-6.496231	-0.975181	2.988448
H	-5.862436	0.242227	1.293917
C	-6.264020	-2.145822	3.733774
H	-5.042351	-3.935913	3.954834
H	-7.304799	-0.286206	3.278182
H	-6.893162	-2.373971	4.608335
C	-2.037240	-1.988379	0.255047
C	-1.522131	-2.922044	-0.666011
C	-1.244648	-1.574605	1.352753
C	-0.225542	-3.439647	-0.486282
H	-2.129957	-3.243088	-1.526416
C	0.042953	-2.098571	1.531314
H	-1.641024	-0.835192	2.068375
C	0.555486	-3.031261	0.607488
H	0.178886	-4.162490	-1.211654
H	0.662025	-1.770209	2.380140
H	1.571579	-3.433734	0.736101
Au	-3.043194	1.049039	-0.289432
H	-1.358253	6.039932	0.486523
N	-1.558480	3.682629	1.689570
C	-1.886856	2.458739	2.402888
H	-2.474209	2.695326	3.314339
H	-2.502135	1.785481	1.765937
H	-0.978107	1.893208	2.711624
C	-1.111622	4.784794	2.542715
H	-1.891925	5.569601	2.663472
H	-0.870032	4.385911	3.545391
H	-0.189904	5.251609	2.138309

[(PPh_3)Au(*ortho*-aniline-alkene)Au(PPh_3)]$^+$ Intermediate Markovnikov

-3018.08738558 A.U.

P	3.949731	-0.911956	0.000301
H	-0.655439	0.047293	-1.596841
C	0.157522	0.800684	-1.459152
C	-0.267181	1.857018	-0.408387
C	0.966893	3.987205	-1.105070
C	0.822533	2.912394	-0.204751
C	2.016604	4.911571	-0.959466
C	1.748889	2.789219	0.853726
C	2.933043	4.780828	0.099291
H	2.117371	5.741566	-1.676622

C	2.792658	3.716633	1.008618
H	1.673369	1.935445	1.548498
H	3.751511	5.507965	0.218416
H	3.503306	3.605135	1.842734
C	5.321102	0.160670	-0.597722
C	6.642912	-0.302662	-0.767754
C	5.010887	1.514410	-0.870448
C	7.645329	0.585063	-1.195117
H	6.892545	-1.358196	-0.579526
C	6.021582	2.398250	-1.281254
H	3.976055	1.879451	-0.759583
C	7.339102	1.935064	-1.445931
H	8.674103	0.217432	-1.334004
H	5.769031	3.451062	-1.482828
H	8.129743	2.625460	-1.779325
C	4.438573	-2.656805	-0.277031
C	5.421171	-3.304044	0.507592
C	3.799231	-3.363871	-1.320222
C	5.761600	-4.640913	0.242878
H	5.910809	-2.765399	1.334714
C	4.145927	-4.700287	-1.581432
H	3.023226	-2.859051	-1.919638
C	5.126349	-5.338854	-0.801216
H	6.527073	-5.141668	0.856140
H	3.647299	-5.246046	-2.397723
H	5.395746	-6.387093	-1.004832
C	3.937151	-0.686833	1.833528
C	4.236986	0.577070	2.387289
C	3.485160	-1.722596	2.682266
C	4.075587	0.802688	3.764557
H	4.600889	1.388824	1.739128
C	3.328736	-1.492876	4.059840
H	3.265336	-2.719838	2.270097
C	3.617517	-0.228347	4.604264
H	4.319390	1.791018	4.185495
H	2.985161	-2.311143	4.712313
H	3.497751	-0.050887	5.684446
Au	1.901252	-0.178377	-0.850135
H	0.343627	1.280651	-2.445791
H	-0.361889	1.313781	0.550290
H	0.252357	4.102535	-1.936743
P	-3.634189	-1.282698	0.096611
C	-3.052395	4.547711	-0.275956
C	-3.494157	4.538041	-1.605685
C	-2.142566	3.575900	0.225541
C	-3.053464	3.555337	-2.505834
C	-1.619561	2.568815	-0.701058
H	-4.211320	5.306451	-1.935000
C	-2.120116	2.601742	-2.056621
H	-3.399187	3.540217	-3.549447
H	-1.649962	1.925139	-2.787465
C	-4.534678	-2.321329	-1.107982
C	-5.303159	-3.426333	-0.681303
C	-4.408079	-2.033685	-2.485469
C	-5.936825	-4.240380	-1.634592
H	-5.415173	-3.646687	0.391881
C	-5.038461	-2.858155	-3.431570
H	-3.818539	-1.161415	-2.813720
C	-5.802929	-3.959908	-3.006662
H	-6.541899	-5.098096	-1.302226
H	-4.939671	-2.633175	-4.504757
H	-6.303984	-4.599934	-3.749499
C	-4.516385	-1.363202	1.693367
C	-4.278207	-2.416833	2.604461
C	-5.475299	-0.369718	1.990553
C	-5.006802	-2.474544	3.804332
H	-3.518719	-3.182607	2.379619
C	-6.200601	-0.437348	3.190864
H	-5.646681	0.457147	1.281538
C	-5.967265	-1.488703	4.096452
H	-4.821414	-3.293839	4.516238
H	-6.948441	0.336716	3.422730
H	-6.534370	-1.537557	5.039112
C	-1.984068	-2.053887	0.348781

C	-1.472599	-3.003057	-0.559282
C	-1.167151	-1.565214	1.396193
C	-0.149788	-3.459728	-0.416959
H	-2.101349	-3.382062	-1.380062
C	0.148826	-2.026525	1.531579
H	-1.560844	-0.817672	2.103724
C	0.660008	-2.971703	0.620650
H	0.254017	-4.194507	-1.130339
H	0.790298	-1.635847	2.336351
H	1.699669	-3.320895	0.709241
Au	-3.084340	0.837233	-0.587877
H	-3.445135	5.318915	0.400805
N	-1.720787	3.629391	1.540296
C	-1.523085	2.431621	2.347911
H	-2.001047	2.578297	3.340060
H	-2.016775	1.558981	1.871259
H	-0.450394	2.190377	2.513238
C	-1.820721	4.873995	2.295037
H	-2.827274	5.031055	2.751194
H	-1.072180	4.856305	3.112163
H	-1.579707	5.739309	1.647910

[(PPh_3)Au(*ortho*-aniline-alkene)] Markovnikov

-1846.53785899 A.U.

P	2.263726	-0.178595	0.066794
H	-1.937032	-2.927194	0.551939
C	-1.749346	-1.997707	-0.029807
C	-2.728519	-0.877797	0.414002
C	-2.582228	0.780671	-1.534925
C	-2.306029	0.470329	-0.187210
C	-2.113278	1.976507	-2.108339
C	-1.531785	1.383422	0.562246
C	-1.348692	2.880723	-1.347036
H	-2.344107	2.202932	-3.162305
C	-1.054613	2.575401	-0.004746
H	-1.283496	1.140919	1.607954
H	-0.972567	3.811196	-1.801123
H	-0.437514	3.257313	0.602045
C	2.600090	0.481122	-1.618299
C	3.890663	0.540807	-2.183729
C	1.489138	0.972778	-2.342336
C	4.067651	1.095555	-3.464377
H	4.757918	0.153556	-1.625755
C	1.676230	1.536339	-3.613446
H	0.477198	0.920622	-1.908122
C	2.964321	1.597276	-4.177682
H	5.076093	1.136185	-3.906049
H	0.804442	1.923546	-4.164104
H	3.108436	2.032390	-5.179501
C	3.828494	-0.984096	0.594113
C	4.899769	-0.261465	1.163415
C	3.949995	-2.376562	0.391477
C	6.085220	-0.928188	1.517022
H	4.802341	0.822798	1.333419
C	5.139880	-3.036477	0.740896
H	3.100621	-2.937689	-0.032858
C	6.207525	-2.313500	1.303603
H	6.918030	-0.362533	1.964279
H	5.230103	-4.122591	0.581780
H	7.137258	-2.833426	1.584331
C	2.134802	1.343733	1.101550
C	2.581309	2.603293	0.650856
C	1.512602	1.234092	2.364958
C	2.406945	3.741449	1.457806
H	3.048982	2.697800	-0.341634
C	1.341538	2.372688	3.167661
H	1.138742	0.253339	2.702951
C	1.785169	3.629262	2.713859
H	2.751063	4.723707	1.097044
H	0.847159	2.281710	4.147724
H	1.639655	4.524076	3.339522
Au	0.236856	-1.347347	0.104148
H	-1.921921	-2.243328	-1.103340
H	-2.609153	-0.772980	1.515112

H	-3.184197	0.077027	-2.132420
C	-6.521733	-0.331697	-0.039960
C	-6.920523	-1.524842	-0.664742
C	-5.186225	-0.141848	0.380924
C	-5.982859	-2.548940	-0.865631
C	-4.210102	-1.156746	0.122517
H	-7.968491	-1.656225	-0.979604
C	-4.644031	-2.354226	-0.476667
H	-6.283362	-3.495030	-1.343351
H	-3.908994	-3.147632	-0.677037
H	-7.260774	0.463664	0.143369
N	-4.775952	1.069983	0.990709
C	-4.426029	1.058115	2.398553
H	-5.303504	1.283482	3.059392
H	-4.039729	0.064336	2.695172
H	-3.633599	1.812295	2.608684
C	-5.345304	2.317129	0.526505
H	-6.339307	2.569091	0.983049
H	-4.646756	3.147368	0.771993
H	-5.459665	2.289105	-0.575309

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ TS anti-Markovnikov

-3018.05850333 A.U.

P	-4.094414	-0.168498	-0.316174
H	0.484221	0.009355	-0.059308
C	0.130504	1.035261	0.161955
C	0.597090	2.003309	-0.793348
C	0.081027	0.183231	2.512906
C	0.072483	1.292556	1.629611
C	0.033689	0.362742	3.903015
C	-0.004070	2.591357	2.189089
C	-0.031005	1.659864	4.445837
H	0.054537	-0.516641	4.566470
C	-0.052341	2.770421	3.580486
H	-0.020774	3.470884	1.527775
H	-0.068132	1.805953	5.536551
H	-0.108104	3.788948	3.996405
C	-5.341688	0.944415	0.433402
C	-6.334464	0.458843	1.311913
C	-5.311113	2.313025	0.085075
C	-7.298559	1.341632	1.828261
H	-6.347999	-0.604545	1.599233
C	-6.280142	3.187093	0.602441
H	-4.521568	2.690337	-0.585843
C	-7.274048	2.702026	1.472740
H	-8.071910	0.963854	2.515158
H	-6.255501	4.253905	0.330954
H	-8.029968	3.390389	1.881878
C	-4.038025	-1.646416	0.780855
C	-4.558011	-2.898992	0.396714
C	-3.398758	-1.503018	2.035176
C	-4.441522	-4.000624	1.264730
H	-5.048384	-3.020351	-0.581889
C	-3.300159	-2.601882	2.901286
H	-2.960325	-0.534378	2.328530
C	-3.818449	-3.853692	2.516488
H	-4.843676	-4.978966	0.958879
H	-2.804148	-2.482259	3.877022
H	-3.731867	-4.718138	3.193092
C	-4.799075	-0.725887	-1.912619
C	-6.182156	-0.983263	-2.045669
C	-3.936573	-0.923450	-3.012964
C	-6.689605	-1.454433	-3.267558
H	-6.862762	-0.808172	-1.197154
C	-4.451034	-1.396494	-4.231618
H	-2.864152	-0.691731	-2.910308
C	-5.825664	-1.665286	-4.358369
H	-7.767796	-1.652938	-3.370504
H	-3.776979	-1.546452	-5.089365
H	-6.228761	-2.031089	-5.315620
Au	-1.933872	0.673157	-0.351265
H	0.364435	3.072808	-0.671438
H	0.681701	1.668095	-1.837478
H	0.121640	-0.831120	2.086024

P	3.147601	-1.933452	-0.095260
C	3.083228	4.501868	-1.869525
C	3.048053	5.297780	-0.674829
C	2.969365	3.119119	-1.807848
C	2.896340	4.604773	0.570631
C	2.783437	2.401632	-0.576558
H	2.998449	2.554258	-2.754751
C	2.784587	3.218370	0.607686
H	2.878657	5.159900	1.518298
H	2.680233	2.732678	1.590119
C	3.345692	-2.477779	1.645993
C	3.721141	-3.796822	1.980863
C	3.043830	-1.550189	2.668298
C	3.783759	-4.182907	3.330722
H	3.971558	-4.520810	1.189332
C	3.096134	-1.946641	4.014300
H	2.761474	-0.517037	2.408418
C	3.466712	-3.262334	4.346748
H	4.084498	-5.209994	3.590264
H	2.853691	-1.218180	4.803786
H	3.518129	-3.570464	5.402874
C	4.191191	-3.026602	-1.125878
C	3.738460	-4.292475	-1.560045
C	5.488702	-2.584617	-1.465741
C	4.588024	-5.113519	-2.320284
H	2.719959	-4.630883	-1.310260
C	6.333067	-3.412774	-2.223477
H	5.829432	-1.587626	-1.140822
C	5.884104	-4.676102	-2.649597
H	4.234816	-6.099769	-2.659943
H	7.344097	-3.066636	-2.488752
H	6.546058	-5.321588	-3.247879
C	1.403097	-2.368791	-0.528579
C	0.493700	-2.901053	0.408928
C	0.950766	-2.025631	-1.824850
C	-0.858040	-3.075761	0.057202
H	0.840950	-3.173462	1.417999
C	-0.394588	-2.213573	-2.173366
H	1.656741	-1.596285	-2.554788
C	-1.302775	-2.731183	-1.230012
H	-1.571620	-3.474362	0.794051
H	-0.737988	-1.948715	-3.185622
H	-2.362094	-2.864595	-1.496592
Au	3.228615	0.377147	-0.397710
H	3.212210	4.978314	-2.850691
N	3.160690	6.664327	-0.725931
C	3.346138	7.343047	-2.005172
H	3.411839	8.432746	-1.835269
H	4.281699	7.019360	-2.512830
H	2.495209	7.157151	-2.697229
C	3.131123	7.451790	0.502612
H	3.967439	7.183938	1.185945
H	3.226182	8.523924	0.253324
H	2.175823	7.313531	1.055759

[(PPh_3)Au(*para*-aniline-alkene)Au(PPh_3)]$^+$ Intermediate anti-Markovnikov

-3018.09912429 A.U.

P	-4.364515	0.137743	-0.343680
H	0.294346	0.534807	-0.316727
C	-0.172622	1.479101	0.057087
C	0.482451	2.640685	-0.720001
C	0.081495	0.254405	2.255371
C	-0.047879	1.484727	1.558445
C	0.169872	0.208974	3.655134
C	-0.099157	2.668631	2.335142
C	0.135584	1.397386	4.409070
H	0.273052	-0.765976	4.159369
C	-0.004748	2.625982	3.736926
H	-0.223695	3.642076	1.834175
H	0.206203	1.367322	5.507453
H	-0.047800	3.564895	4.312182
C	-5.684217	1.253587	0.273144
C	-6.721426	0.801725	1.117212
C	-5.649819	2.603588	-0.142419

C	-7.724275	1.695983	1.530616
H	-6.741237	-0.245635	1.458064
C	-6.658009	3.489151	0.270098
H	-4.824884	2.957540	-0.782956
C	-7.695820	3.036121	1.105677
H	-8.531430	1.342913	2.191427
H	-6.629316	4.540759	-0.055358
H	-8.482287	3.733877	1.433364
C	-4.402965	-1.310343	0.799185
C	-5.117468	-2.492032	0.509574
C	-3.686028	-1.205871	2.014490
C	-5.126776	-3.552468	1.434990
H	-5.664209	-2.590020	-0.441191
C	-3.705481	-2.263977	2.936151
H	-3.095569	-0.300003	2.232909
C	-4.427050	-3.438194	2.649942
H	-5.685716	-4.472631	1.203226
H	-3.143218	-2.172600	3.878406
H	-4.438852	-4.269387	3.372388
C	-4.972300	-0.486249	-1.960729
C	-6.349514	-0.670162	-2.216566
C	-4.025499	-0.808453	-2.958399
C	-6.768629	-1.193781	-3.451150
H	-7.094734	-0.395775	-1.452763
C	-4.450446	-1.334019	-4.189978
H	-2.954773	-0.622360	-2.769983
C	-5.821315	-1.530788	-4.435378
H	-7.843034	-1.333959	-3.648086
H	-3.708875	-1.580788	-4.965860
H	-6.154646	-1.937749	-5.402888
Au	-2.196476	1.015179	-0.306257
H	0.103936	3.624044	-0.365760
H	0.168355	2.572058	-1.781185
H	0.087816	-0.681885	1.676986
P	2.889563	-1.762294	-0.058822
C	4.101647	3.181253	-1.977703
C	4.818442	3.511489	-0.782381
C	2.763137	2.785136	-1.929243
C	4.109244	3.390577	0.456985
C	2.020564	2.679810	-0.698539
H	2.234019	2.587108	-2.875864
C	2.770271	2.994023	0.495752
H	4.607318	3.614553	1.408939
H	2.252493	2.957226	1.466143
C	3.739179	-2.119202	1.523808
C	4.667299	-3.173898	1.650347
C	3.408362	-1.322590	2.644896
C	5.259563	-3.430669	2.899885
H	4.930828	-3.792392	0.777938
C	3.996431	-1.594987	3.889106
H	2.680641	-0.499125	2.548999
C	4.923931	-2.646525	4.017546
H	5.987337	-4.251111	2.998325
H	3.730593	-0.977462	4.761227
H	5.389854	-2.853441	4.993697
C	3.737255	-2.719937	-1.363061
C	3.386657	-4.065643	-1.610097
C	4.783710	-2.112669	-2.090900
C	4.090596	-4.799563	-2.579700
H	2.562689	-4.534629	-1.048804
C	5.484197	-2.854784	-3.055308
H	5.039116	-1.056513	-1.902773
C	5.138510	-4.196802	-3.299170
H	3.816730	-5.847854	-2.775930
H	6.299282	-2.382027	-3.624919
H	5.685466	-4.775240	-4.060030
C	1.196141	-2.451532	0.110076
C	0.831078	-3.244836	1.219459
C	0.222405	-2.087923	-0.848871
C	-0.504853	-3.655763	1.370487
H	1.581950	-3.520244	1.975915
C	-1.108337	-2.500307	-0.686014
H	0.500243	-1.455551	-1.707590
C	-1.474333	-3.280344	0.425289

H	-0.794082	-4.262518	2.242441
H	-1.871628	-2.197299	-1.417812
H	-2.522557	-3.584905	0.559000
Au	2.692863	0.487893	-0.449773
H	4.591320	3.236171	-2.958237
N	6.128887	3.916005	-0.821450
C	6.811727	4.068258	-2.102166
H	7.852243	4.395026	-1.926051
H	6.849603	3.109309	-2.665222
H	6.319664	4.829422	-2.748228
C	6.825927	4.270528	0.411214
H	6.862324	3.415757	1.122148
H	7.866630	4.555306	0.173803
H	6.345691	5.131537	0.927744

[(PPh_3)Au(*para*-aniline-alkene)] anti-Markovnikov

-1846.53690951 A.U.

P	-2.645610	0.238531	-0.006971
H	2.062660	0.788508	-1.328058
C	1.751259	0.494183	-0.301260
C	2.564039	1.339985	0.710136
C	1.908139	-1.836156	-1.311554
C	1.861984	-1.004861	-0.163002
C	1.878566	-3.235357	-1.209950
C	1.819455	-1.653690	1.100139
C	1.819799	-3.858053	0.051151
H	1.905595	-3.848122	-2.125888
C	1.796214	-3.053272	1.206147
H	1.767195	-1.043494	2.015723
H	1.801746	-4.956533	0.133544
H	1.753565	-3.521538	2.203297
C	-3.389208	0.629012	1.629419
C	-4.345517	-0.198770	2.255675
C	-2.979623	1.826365	2.258380
C	-4.895485	0.178140	3.493406
H	-4.656103	-1.141396	1.778219
C	-3.537517	2.200806	3.491457
H	-2.211163	2.455626	1.778852
C	-4.496421	1.377505	4.109984
H	-5.638976	-0.472618	3.980515
H	-3.213815	3.134944	3.976935
H	-4.927880	1.667682	5.081120
C	-2.895829	-1.574761	-0.245998
C	-4.120281	-2.096254	-0.721134
C	-1.829508	-2.454874	0.051861
C	-4.279117	-3.483625	-0.879625
H	-4.947067	-1.414875	-0.979107
C	-1.994961	-3.839848	-0.111933
H	-0.855183	-2.065266	0.392579
C	-3.218453	-4.356397	-0.574031
H	-5.235343	-3.884037	-1.252432
H	-1.146657	-4.506030	0.110214
H	-3.344031	-5.442731	-0.708045
C	-3.778219	1.015663	-1.230905
C	-5.070821	1.475008	-0.900041
C	-3.310337	1.133140	-2.559439
C	-5.890570	2.036903	-1.895078
H	-5.435403	1.394984	0.136374
C	-4.136081	1.688553	-3.549219
H	-2.291520	0.791963	-2.808445
C	-5.427316	2.140964	-3.218521
H	-6.898445	2.396012	-1.632714
H	-3.766606	1.777065	-4.583052
H	-6.072020	2.582721	-3.994811
Au	-0.352769	0.688819	-0.188395
H	2.268385	1.097151	1.752816
H	2.298740	2.408225	0.562416
H	1.944728	-1.360675	-2.305787
C	6.155969	-0.027951	1.048178
C	6.871591	0.708715	0.061570
C	4.790269	0.198292	1.269672
C	6.134117	1.670564	-0.687979
C	4.059239	1.153900	0.534006
H	4.275111	-0.399713	2.038483

C	4.769109	1.876725	-0.447713
H	6.625951	2.270066	-1.466613
H	4.233812	2.629833	-1.051485
H	6.663715	-0.790849	1.654409
N	8.231408	0.499790	-0.160382
C	8.915234	-0.574990	0.532916
H	9.982156	-0.584068	0.239192
H	8.876371	-0.444227	1.638645
H	8.487772	-1.581489	0.302199
C	8.893745	1.180490	-1.256177
H	8.839587	2.288050	-1.148248
H	9.964917	0.902877	-1.269977
H	8.460439	0.922467	-2.253710

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^{+2}$ TS Markovnikov

-3018.34122123 A.U.

P	-3.873224	-0.286558	-0.080475
H	0.704221	-0.342593	-0.783791
C	0.553197	0.534289	-0.110281
C	0.702481	1.878639	-0.682954
C	-0.459141	3.145758	1.166113
C	0.121558	3.096746	-0.130008
C	-0.996387	4.340381	1.657781
C	0.158840	4.285764	-0.906829
C	-0.947417	5.514960	0.877754
H	-1.465941	4.359459	2.653209
C	-0.367698	5.484613	-0.403325
H	0.599244	4.256833	-1.915184
H	-1.371948	6.452837	1.268863
H	-0.341546	6.396474	-1.019571
C	-4.663537	1.112356	0.793955
C	-5.832883	0.917492	1.563626
C	-4.109478	2.406316	0.661609
C	-6.446150	2.017641	2.186716
H	-6.259083	-0.091253	1.683667
C	-4.729017	3.498205	1.288857
H	-3.187536	2.559585	0.076318
C	-5.897320	3.305670	2.049232
H	-7.357251	1.866453	2.785967
H	-4.292515	4.503740	1.185008
H	-6.381677	4.163136	2.541734
C	-4.252588	-1.797571	0.881700
C	-4.866339	-2.917220	0.283134
C	-3.832398	-1.854009	2.230849
C	-5.048576	-4.093867	1.032355
H	-5.204002	-2.871165	-0.764133
C	-4.028616	-3.027457	2.974547
H	-3.354017	-0.977313	2.697860
C	-4.629510	-4.151404	2.373396
H	-5.529312	-4.967721	0.566101
H	-3.711986	-3.068263	4.028306
H	-4.778851	-5.073004	2.956967
C	-4.677929	-0.478977	-1.709492
C	-6.053461	-0.196432	-1.862772
C	-3.929026	-0.976224	-2.799610
C	-6.674113	-0.421409	-3.102505
H	-6.638691	0.203851	-1.020069
C	-4.559166	-1.201025	-4.034534
H	-2.853161	-1.182667	-2.677053
C	-5.930555	-0.925492	-4.185556
H	-7.745296	-0.198284	-3.223960
H	-3.976977	-1.586110	-4.886066
H	-6.421963	-1.097812	-5.155652
Au	-1.589331	0.034020	-0.200104
H	0.599436	0.376289	0.985996
H	0.823772	1.890102	-1.778564
H	-0.514203	2.236047	1.783003
P	2.772154	-2.308303	0.075789
C	3.498958	4.279693	-1.440090
C	3.380384	5.024016	-0.212685
C	3.272923	2.911626	-1.467920
C	3.068594	4.284547	0.985187
C	2.866559	2.197447	-0.298703
H	3.374833	2.377720	-2.426631

C	2.839751	2.922061	0.934748
H	3.001360	4.795719	1.953858
H	2.572254	2.401775	1.869082
C	3.907062	-3.253058	-0.989993
C	3.536067	-4.531511	-1.470455
C	5.195195	-2.739271	-1.261965
C	4.454241	-5.283850	-2.221059
H	2.534687	-4.938557	-1.260033
C	6.105815	-3.501165	-2.010786
H	5.489773	-1.745892	-0.887804
C	5.735971	-4.770883	-2.491092
H	4.166051	-6.277939	-2.596148
H	7.108470	-3.099827	-2.223579
H	6.451360	-5.363761	-3.081784
C	1.062493	-2.818090	-0.356996
C	0.112932	-3.130575	0.640225
C	0.672080	-2.777756	-1.717641
C	-1.214500	-3.423333	0.274287
H	0.410239	-3.157574	1.700178
C	-0.654185	-3.072112	-2.072709
H	1.410081	-2.536041	-2.500489
C	-1.596546	-3.396512	-1.078327
H	-1.956152	-3.669772	1.049025
H	-0.950067	-3.058139	-3.133216
H	-2.636765	-3.624453	-1.354285
C	3.060450	-2.789227	1.812527
C	3.565295	-4.070606	2.126350
C	2.733655	-1.883107	2.847348
C	3.732467	-4.439465	3.471327
H	3.836874	-4.775390	1.324918
C	2.899077	-2.262267	4.189066
H	2.357669	-0.874568	2.605915
C	3.398083	-3.540401	4.500507
H	4.131893	-5.435583	3.716420
H	2.649192	-1.554730	4.994624
H	3.536335	-3.834234	5.552506
Au	2.892946	0.094328	-0.169267
H	3.779492	4.786176	-2.372738
N	3.560822	6.371712	-0.181538
C	3.895864	7.107949	-1.404110
H	3.995849	8.181631	-1.168405
H	4.858689	6.760834	-1.835589
H	3.101464	6.996806	-2.173030
C	3.430565	7.113421	1.076826
H	4.194114	6.794225	1.817978
H	3.575166	8.190187	0.881744
H	2.421752	6.975775	1.519793
H	4.465255	0.126539	-0.185611

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^{+2}$ Intermediate Markovnikov

-3018.37162533 A.U.

P	-3.962386	-0.046264	-0.075696
H	0.306142	-0.145676	-1.017099
C	0.561899	0.649262	-0.270421
C	0.767516	2.100488	-0.742314
C	-0.535392	3.087572	1.238283
C	-0.130867	3.158347	-0.114971
C	-1.340036	4.091314	1.802194
C	-0.561558	4.255321	-0.891588
C	-1.752611	5.184084	1.020271
H	-1.650199	4.018017	2.855836
C	-1.367300	5.260880	-0.330131
H	-0.262870	4.323588	-1.950728
H	-2.378572	5.973692	1.463507
H	-1.695101	6.108870	-0.951364
C	-4.784135	1.431153	0.612964
C	-5.932290	1.299297	1.427074
C	-4.303829	2.712326	0.259241
C	-6.604131	2.450393	1.871130
H	-6.298340	0.301735	1.717365
C	-4.988080	3.854491	0.703226
H	-3.392368	2.820564	-0.352726
C	-6.137154	3.725767	1.504765
H	-7.498147	2.349442	2.505646

H	-4.614903	4.851026	0.423885
H	-6.669470	4.625040	1.851663
C	-4.335588	-1.440730	1.051356
C	-5.000597	-2.599483	0.600741
C	-3.871977	-1.360598	2.384921
C	-5.189993	-3.679859	1.481893
H	-5.371735	-2.659730	-0.434424
C	-4.075308	-2.437722	3.260648
H	-3.354191	-0.452477	2.735309
C	-4.727394	-3.601849	2.807435
H	-5.710424	-4.584345	1.130925
H	-3.724848	-2.371519	4.302345
H	-4.882573	-4.448098	3.494442
C	-4.751858	-0.428788	-1.678914
C	-6.141237	-0.230342	-1.844945
C	-3.983175	-0.976196	-2.729765
C	-6.754418	-0.593939	-3.054930
H	-6.742806	0.212621	-1.035558
C	-4.605181	-1.337560	-3.935994
H	-2.897336	-1.111143	-2.599640
C	-5.989908	-1.149485	-4.097639
H	-7.836209	-0.437375	-3.185971
H	-4.006296	-1.759782	-4.757849
H	-6.475620	-1.428818	-5.045432
Au	-1.689182	0.233437	-0.221795
H	0.408827	0.432287	0.809680
H	0.582832	2.110106	-1.835571
H	-0.231954	2.234904	1.866826
P	2.563096	-2.164070	0.101820
C	4.315095	3.407497	-1.573382
C	4.822894	3.783824	-0.277849
C	3.101922	2.758970	-1.701796
C	4.015162	3.460090	0.871619
C	2.290659	2.398435	-0.559807
H	2.728237	2.513906	-2.709350
C	2.801906	2.814178	0.730877
H	4.346024	3.740088	1.879449
H	2.187121	2.635747	1.626627
C	3.656101	-3.203838	-0.912175
C	3.248776	-4.517045	-1.252797
C	4.941053	-2.741096	-1.274169
C	4.130962	-5.355127	-1.953377
H	2.250548	-4.886097	-0.970557
C	5.813535	-3.589490	-1.973466
H	5.254436	-1.717958	-1.013598
C	5.410156	-4.893823	-2.313888
H	3.815409	-6.375958	-2.218486
H	6.813344	-3.228034	-2.258709
H	6.096189	-5.554359	-2.866397
C	0.838883	-2.662873	-0.244102
C	-0.088796	-2.890360	0.797228
C	0.419341	-2.739196	-1.595258
C	-1.420224	-3.222738	0.485491
H	0.227044	-2.827713	1.849997
C	-0.910271	-3.074520	-1.893837
H	1.136910	-2.556976	-2.412134
C	-1.829038	-3.319238	-0.855430
H	-2.143652	-3.403328	1.294753
H	-1.228835	-3.153552	-2.944734
H	-2.872622	-3.575975	-1.090486
C	2.909121	-2.470040	1.864223
C	3.608168	-3.632116	2.258815
C	2.444870	-1.552546	2.836543
C	3.827575	-3.876646	3.624997
H	3.983362	-4.340988	1.504532
C	2.665597	-1.809445	4.198190
H	1.914843	-0.635728	2.529012
C	3.356459	-2.971303	4.592234
H	4.374083	-4.780926	3.933846
H	2.305467	-1.097086	4.956407
H	3.534752	-3.167523	5.660810
Au	2.720681	0.167229	-0.301217
H	4.883099	3.641626	-2.482484
N	6.012154	4.425557	-0.145897

C	6.811119	4.770919	-1.327694
H	7.752591	5.247210	-1.003844
H	7.070716	3.865736	-1.915685
H	6.272802	5.484708	-1.987188
C	6.498529	4.835241	1.176843
H	6.622023	3.959820	1.848691
H	7.482780	5.322526	1.067696
H	5.806570	5.560410	1.655705
H	4.329050	0.099841	-0.352950

[(PPh_3)Au(*para*-aniline-alkene)]$^+$ Markovnikov

-1846.89912989 A.U.

H	0.052107	2.420196	-0.921267
C	0.707665	1.772486	-0.308629
C	2.119133	1.533015	-0.873251
C	2.967442	3.751830	0.059261
C	3.242288	2.439703	-0.377236
C	4.006998	4.599699	0.480929
C	4.581844	1.993867	-0.382478
C	5.336987	4.145623	0.474135
H	3.774864	5.622357	0.817902
C	5.621748	2.838763	0.039187
H	4.817722	0.970865	-0.720773
H	6.150898	4.808159	0.807462
H	6.661295	2.474754	0.028614
H	0.713754	2.138182	0.740375
H	2.064532	1.638762	-1.980535
H	1.929194	4.120234	0.063139
P	-2.141044	-0.018372	0.034892
C	3.313028	-2.124082	-1.398719
C	3.589350	-2.549794	-0.053788
C	2.742461	-0.887799	-1.653544
C	3.264065	-1.641374	1.011604
C	2.385158	0.025993	-0.599650
H	2.564378	-0.579491	-2.696304
C	2.701110	-0.404341	0.743887
H	3.472819	-1.907543	2.055299
H	2.521676	0.298231	1.573348
C	-3.242850	-1.163478	-0.866918
C	-4.543585	-0.733511	-1.220893
C	-2.837654	-2.489778	-1.130794
C	-5.430057	-1.634398	-1.833049
H	-4.863480	0.300440	-1.018658
C	-3.732909	-3.381602	-1.742516
H	-1.817635	-2.810284	-0.865118
C	-5.027162	-2.956578	-2.093784
H	-6.441476	-1.298527	-2.109535
H	-3.414263	-4.414464	-1.951954
H	-5.724319	-3.657889	-2.578260
C	-2.688773	1.668265	-0.397567
C	-3.220024	2.552926	0.563562
C	-2.541045	2.083106	-1.741995
C	-3.605573	3.848719	0.174995
H	-3.339145	2.233471	1.610220
C	-2.932864	3.375049	-2.120373
H	-2.117227	1.392765	-2.490021
C	-3.463358	4.259834	-1.161118
H	-4.023287	4.538669	0.924450
H	-2.820813	3.696210	-3.167475
H	-3.766538	5.275475	-1.459279
C	-2.433445	-0.253911	1.822729
C	-3.515189	-1.031758	2.287213
C	-1.563374	0.378181	2.741973
C	-3.726273	-1.168547	3.670231
H	-4.189574	-1.529129	1.572953
C	-1.787251	0.240409	4.120017
H	-0.715061	0.978612	2.375008
C	-2.867529	-0.533746	4.584633
H	-4.569408	-1.776190	4.033593
H	-1.113381	0.736173	4.835830
H	-3.038280	-0.644564	5.666762
Au	0.141383	-0.307373	-0.350023
H	3.549745	-2.776634	-2.248433
N	4.147306	-3.768512	0.201314

C	4.511439	-4.663366	-0.898125
H	4.942828	-5.592054	-0.484901
H	3.624685	-4.940472	-1.508031
H	5.269380	-4.201943	-1.567848
C	4.437078	-4.178444	1.575964
H	3.518463	-4.179218	2.200937
H	4.844901	-5.204583	1.572279
H	5.188101	-3.512022	2.053789
H	-0.005491	-1.946669	-0.419674

[(PPh_3)Au(*para*-aniline-alkene) + AnilineH]$^+$ Intermediate Markovnikov

-2212.94218385 A.U.

H	2.725882	-1.223383	-1.612307
C	2.062252	-0.346535	-1.471517
C	2.682369	0.604113	-0.412113
C	4.219018	2.267887	-1.624697
C	4.057572	1.078835	-0.884064
C	5.485591	2.646450	-2.102288
C	5.192685	0.279049	-0.629413
C	6.610275	1.842800	-1.843303
H	5.596497	3.580065	-2.676436
C	6.460002	0.656050	-1.103283
H	5.074807	-0.653111	-0.051550
H	7.602988	2.142949	-2.213809
H	7.336822	0.023306	-0.891333
H	2.023508	0.161558	-2.463074
H	2.877160	-0.010878	0.496027
H	3.343828	2.908941	-1.817405
P	-2.231301	-0.680029	-0.418781
C	0.991104	3.283369	1.787430
C	-0.064880	3.779898	0.964213
C	1.862374	2.291627	1.317442
C	-0.143161	3.263396	-0.363613
C	1.755475	1.737894	0.023937
H	2.673256	1.944498	1.981943
C	0.751388	2.280651	-0.808976
H	-0.916666	3.615103	-1.059748
H	0.650206	1.933113	-1.848645
C	-2.350851	-0.311612	1.378507
C	-2.908505	-1.205847	2.316814
C	-1.770184	0.901680	1.817491
C	-2.881162	-0.883657	3.687874
H	-3.376764	-2.144052	1.977619
C	-1.764623	1.223587	3.182480
H	-1.316831	1.592960	1.088787
C	-2.315148	0.329307	4.121839
H	-3.320594	-1.579881	4.419446
H	-1.310688	2.173532	3.504626
H	-2.307402	0.579418	5.194260
C	-3.331948	-2.110224	-0.717260
C	-4.735372	-2.006393	-0.589318
C	-2.744582	-3.348611	-1.056838
C	-5.539381	-3.139511	-0.789505
H	-5.200153	-1.039196	-0.340780
C	-3.555034	-4.480338	-1.253330
H	-1.650769	-3.412814	-1.183737
C	-4.950502	-4.375826	-1.117727
H	-6.633292	-3.057635	-0.694018
H	-3.096602	-5.444067	-1.524553
H	-5.586071	-5.260732	-1.277716
C	-2.978973	0.805683	-1.206328
C	-3.977030	1.566250	-0.557978
C	-2.497103	1.215472	-2.469370
C	-4.487093	2.722322	-1.171737
H	-4.340116	1.270854	0.439083
C	-3.007273	2.374896	-3.076317
H	-1.709544	0.632421	-2.974722
C	-4.000700	3.130139	-2.427700
H	-5.266384	3.311235	-0.663347
H	-2.622858	2.691956	-4.058087
H	-4.396841	4.041503	-2.902036
Au	0.063877	-0.785611	-1.013848
H	1.132559	3.667322	2.806819
N	-0.985906	4.699351	1.437340

C	-0.802491	5.304440	2.745699
H	-1.606322	6.040985	2.928305
H	-0.848021	4.551524	3.567393
H	0.172731	5.836612	2.833643
C	-2.054046	5.162486	0.565679
H	-2.661145	4.313054	0.179173
H	-2.729778	5.829195	1.132711
H	-1.672475	5.731098	-0.314874
C	3.617734	-2.285879	2.280615
C	2.582149	-2.529581	1.366057
C	4.918473	-2.718540	1.965582
C	2.823860	-3.194358	0.151080
C	5.175327	-3.380903	0.754080
H	5.736421	-2.525475	2.675948
C	4.126444	-3.617621	-0.152249
H	2.006606	-3.347884	-0.570402
H	4.322290	-4.124053	-1.109305
H	3.440600	-1.760134	3.228243
N	1.188149	-2.085165	1.630815
C	1.028811	-1.042434	2.689555
H	-0.026850	-0.723031	2.694462
H	1.295296	-1.464718	3.675534
H	1.661035	-0.172001	2.440378
C	0.255175	-3.238949	1.865036
H	0.560474	-3.762797	2.790094
H	-0.772617	-2.840327	1.962355
H	0.309304	-3.929437	1.005400
H	0.848235	-1.614201	0.698240
H	6.197606	-3.707782	0.511125

[(PPh_3)Au(*para*-aniline-alkene)--H--Aniline]$^+$ TS Markovnikov

H	2.895516	-1.232650	-1.348718
C	2.096514	-0.497317	-1.108757
C	2.692168	0.713152	-0.329038
C	3.714042	2.420918	-1.976910
C	3.857727	1.305476	-1.127161
C	4.803287	2.887996	-2.734247
C	5.119424	0.674721	-1.044650
C	6.052198	2.248499	-2.651473
H	4.675614	3.765202	-3.388179
C	6.207573	1.139772	-1.800018
H	5.249772	-0.191652	-0.375903
H	6.904769	2.618384	-3.242239
H	7.184862	0.638066	-1.717567
H	1.778300	-0.176808	-2.131904
H	3.149893	0.300175	0.593709
H	2.748381	2.946059	-2.035448
P	-2.337814	-0.732786	-0.352757
C	0.695199	3.108396	1.928836
C	-0.366176	3.565601	1.088874
C	1.657157	2.209581	1.450094
C	-0.380011	3.078888	-0.253463
C	1.638932	1.712401	0.130355
H	2.466743	1.893563	2.130298
C	0.599444	2.185340	-0.706321
H	-1.169447	3.384090	-0.952558
H	0.549261	1.865029	-1.759844
C	-2.506943	-0.544017	1.465533
C	-3.354621	-1.357170	2.245026
C	-1.716527	0.456079	2.079644
C	-3.411892	-1.163546	3.638030
H	-3.967301	-2.139470	1.769833
C	-1.784941	0.644299	3.466992
H	-1.043104	1.084700	1.475063
C	-2.631836	-0.165528	4.248788
H	-4.073304	-1.797993	4.248393
H	-1.164609	1.426273	3.933176
H	-2.682219	-0.020218	5.339279
C	-3.353571	-2.172192	-0.838704
C	-4.753321	-2.058271	-0.991255
C	-2.723370	-3.424175	-1.012263
C	-5.514110	-3.196644	-1.304487
H	-5.247514	-1.080971	-0.873929
C	-3.491278	-4.558473	-1.322162

H	-1.627683	-3.501584	-0.915771
C	-4.885802	-4.445179	-1.466842
H	-6.604587	-3.106996	-1.427377
H	-2.998201	-5.533047	-1.461080
H	-5.486372	-5.333816	-1.716084
C	-3.118949	0.763756	-1.067429
C	-4.143270	1.448796	-0.379291
C	-2.684866	1.223137	-2.329843
C	-4.738044	2.580265	-0.963767
H	-4.465751	1.107695	0.617348
C	-3.277036	2.359508	-2.903574
H	-1.873362	0.694877	-2.856728
C	-4.305391	3.036744	-2.222325
H	-5.540135	3.112397	-0.429107
H	-2.933564	2.719317	-3.885772
H	-4.769109	3.928044	-2.672891
Au	-0.079962	-0.829123	-0.805489
H	0.776925	3.459035	2.966163
N	-1.338401	4.429776	1.554417
C	-1.271774	4.931023	2.917652
H	-2.139501	5.587742	3.111643
H	-1.306980	4.103618	3.662685
H	-0.346992	5.523180	3.110664
C	-2.337840	4.955271	0.636985
H	-2.952964	4.144458	0.188585
H	-3.019699	5.632141	1.183730
H	-1.879980	5.534024	-0.198760
C	4.205925	-1.539004	2.269715
C	3.520826	-2.215685	1.238648
C	5.611365	-1.522300	2.290286
C	4.266992	-2.880620	0.239510
C	6.350725	-2.181368	1.295673
H	6.129118	-0.986298	3.100515
C	5.669597	-2.862873	0.272143
H	3.761900	-3.410701	-0.580536
H	6.232494	-3.382710	-0.518074
H	3.660314	-1.013878	3.063948
N	2.067358	-2.181700	1.135645
C	1.357461	-1.490351	2.236461
H	0.274248	-1.491972	2.009990
H	1.523494	-1.995949	3.210937
H	1.673752	-0.433299	2.293082
C	1.449390	-3.507548	0.874715
H	1.627766	-4.199179	1.724262
H	0.359756	-3.362665	0.734762
H	1.855081	-3.951415	-0.051394
H	1.758962	-1.408169	-0.030464
H	7.450703	-2.164754	1.316967

[(PPh_3)Au(*para*-aniline-alkeneH) + Aniline]$^+$ Intermediate Markovnikov

-2212.97229653 A.U.

H	3.256016	-0.959021	-2.573206
C	2.516691	-0.301337	-2.073704
C	3.082595	0.221913	-0.740979
C	4.360190	2.298301	-1.539463
C	4.377465	1.009419	-0.964492
C	5.555504	2.998329	-1.769848
C	5.622136	0.442025	-0.623032
C	6.791950	2.421432	-1.425489
H	5.523040	4.004839	-2.216606
C	6.821800	1.140082	-0.849817
H	5.645996	-0.564108	-0.174276
H	7.728987	2.972258	-1.602657
H	7.784430	0.680844	-0.573726
H	2.274436	0.523132	-2.775016
H	3.355223	-0.663692	-0.133638
H	3.396994	2.766753	-1.798748
P	-2.123043	-0.074028	-0.605267
C	1.269827	1.772762	2.284571
C	0.298898	2.632605	1.689133
C	2.133554	1.007896	1.487334
C	0.253456	2.661626	0.266799
C	2.072925	1.018987	0.075821
H	2.907908	0.391679	1.974085

C	1.108228	1.867475	-0.507231
H	-0.453680	3.320476	-0.250169
H	1.013889	1.923535	-1.601954
C	-3.104046	0.993116	0.516995
C	-4.320808	1.552707	0.058772
C	-2.696977	1.191231	1.853120
C	-5.103798	2.326876	0.927940
H	-4.663281	1.370336	-0.972496
C	-3.498824	1.948479	2.723166
H	-1.745398	0.762377	2.205944
C	-4.694393	2.523237	2.261342
H	-6.046769	2.766903	0.568349
H	-3.178884	2.097932	3.765346
H	-5.318106	3.121175	2.944020
C	-3.333986	-1.297984	-1.255327
C	-3.968034	-1.108194	-2.502247
C	-3.676455	-2.410184	-0.453745
C	-4.938433	-2.026940	-2.939173
H	-3.700960	-0.249395	-3.137579
C	-4.648745	-3.320773	-0.895043
H	-3.177087	-2.560670	0.518038
C	-5.280066	-3.130541	-2.138662
H	-5.428420	-1.877994	-3.913918
H	-4.913043	-4.186280	-0.267772
H	-6.039035	-3.848775	-2.485788
C	-1.608359	0.896598	-2.067227
C	-1.916593	2.262650	-2.225719
C	-0.839013	0.227502	-3.044650
C	-1.429333	2.960883	-3.343848
H	-2.519327	2.787601	-1.469785
C	-0.361087	0.928533	-4.161676
H	-0.604938	-0.842442	-2.925481
C	-0.646827	2.299034	-4.306889
H	-1.661253	4.030736	-3.460834
H	0.245755	0.405484	-4.916542
H	-0.261432	2.852217	-5.177317
Au	-0.453195	-1.158654	0.520209
H	1.380638	1.727076	3.376859
N	-0.564882	3.404165	2.450180
C	-0.473567	3.377318	3.898999
H	-1.268417	4.013529	4.330556
H	-0.615502	2.345944	4.297880
H	0.506062	3.752153	4.278029
C	-1.434184	4.370033	1.796588
H	-2.122556	3.875749	1.074445
H	-2.064719	4.867860	2.555516
H	-0.860998	5.154666	1.250347
C	3.289915	-2.505341	1.914499
C	2.100333	-2.722828	1.195884
C	4.532233	-2.755295	1.301038
C	2.166551	-3.186766	-0.135097
C	4.598133	-3.225149	-0.019187
H	5.456336	-2.573742	1.870826
C	3.406890	-3.438345	-0.736278
H	1.240261	-3.335350	-0.712710
H	3.441521	-3.791260	-1.778015
H	3.276857	-2.140350	2.949223
N	0.769128	-2.503669	1.793516
C	0.804167	-1.889873	3.152066
H	-0.236583	-1.738999	3.494289
H	1.322642	-2.555801	3.875618
H	1.304164	-0.906980	3.105033
C	0.032413	-3.811068	1.884692
H	0.596582	-4.511874	2.537590
H	-0.972586	-3.630594	2.311527
H	-0.080973	-4.260664	0.882898
H	1.587937	-0.884890	-1.897399
H	5.572624	-3.414360	-0.493743

[(PPh_3)Au(*para*-aniline-alkeneH)]$^+$ Markovnikov

-1846.96572674 A.U.

H	-2.579978	-3.504234	1.496102
C	-2.324132	-2.428079	1.554698
C	-2.751094	-1.719036	0.256191

C	-5.189199	-1.161351	0.805369
C	-4.255765	-1.860794	0.010365
C	-6.568657	-1.309915	0.588923
C	-4.735212	-2.707386	-1.009735
C	-7.036515	-2.159650	-0.430283
H	-7.284377	-0.758415	1.218852
C	-6.116006	-2.858184	-1.229620
H	-4.017504	-3.260316	-1.638823
H	-8.118166	-2.275320	-0.601065
H	-6.473028	-3.525204	-2.030027
H	-2.853917	-2.018931	2.439120
H	-2.237226	-2.225716	-0.589963
H	-4.835588	-0.486318	1.602290
P	2.187298	-0.205875	-0.052994
C	-2.667935	1.839415	-1.167456
C	-2.673994	2.665976	0.007754
C	-2.527182	0.459789	-1.073970
C	-2.504163	2.010494	1.271238
C	-2.362591	-0.226551	0.187240
H	-2.592458	-0.148582	-1.990667
C	-2.365338	0.624681	1.353401
H	-2.484915	2.590380	2.202577
H	-2.288195	0.162391	2.349512
C	2.817916	0.188868	-1.725275
C	3.972473	-0.447117	-2.231705
C	2.162647	1.182034	-2.486805
C	4.469054	-0.082005	-3.494734
H	4.479580	-1.227773	-1.642872
C	2.667770	1.542509	-3.745872
H	1.253714	1.666945	-2.093072
C	3.820285	0.911353	-4.249823
H	5.367063	-0.580219	-3.891705
H	2.156375	2.315037	-4.340832
H	4.211253	1.191167	-5.240443
C	2.810037	-1.877921	0.358892
C	3.993395	-2.053146	1.108232
C	2.105469	-3.002006	-0.128507
C	4.468225	-3.351668	1.362758
H	4.540971	-1.179522	1.495427
C	2.589447	-4.294193	0.126904
H	1.175685	-2.863069	-0.705224
C	3.770204	-4.469522	0.872790
H	5.389334	-3.488974	1.950099
H	2.039807	-5.169351	-0.252809
H	4.145017	-5.484477	1.077275
C	3.009775	0.949694	1.105716
C	4.149358	1.689292	0.724155
C	2.503079	1.053946	2.421199
C	4.781120	2.524616	1.662373
H	4.542469	1.615918	-0.301923
C	3.143520	1.885718	3.352229
H	1.606356	0.481954	2.712956
C	4.282483	2.621411	2.973254
H	5.669636	3.102752	1.364659
H	2.750686	1.963764	4.377876
H	4.781368	3.276818	3.704053
Au	-0.108864	-0.110747	0.083125
H	-2.788491	2.284601	-2.163214
N	-2.832129	4.021716	-0.077798
C	-3.047118	4.659843	-1.375224
H	-3.145481	5.750764	-1.233813
H	-2.192828	4.482899	-2.064637
H	-3.975084	4.293125	-1.866584
C	-2.858341	4.838436	1.134177
H	-1.913432	4.740106	1.711812
H	-2.975416	5.901058	0.856700
H	-3.705936	4.562966	1.799898
H	-1.229672	-2.338443	1.727993

[(PPh_3)Au(*para*-aniline-alkeneH)]$^+$ Anti-Markovnikov

-1846.98198153 A.U.

H	2.607137	4.011588	-1.677702
C	0.862642	4.305208	-0.429116
C	1.717308	3.422411	-1.360573

C	-0.701811	3.582555	1.452805
C	-0.421946	3.670215	0.071127
C	-1.910290	3.029497	1.913123
C	-1.389368	3.173548	-0.838652
C	-2.860068	2.543678	0.997901
H	-2.113253	2.982776	2.994728
C	-2.598122	2.620203	-0.380367
H	-1.204751	3.243555	-1.923159
H	-3.804442	2.106107	1.355464
H	-3.336290	2.241212	-1.103310
H	0.611779	5.232710	-0.989009
H	1.158641	3.205529	-2.296373
H	0.032825	3.969445	2.178327
P	-1.052319	-0.991439	-0.034651
C	3.630158	0.095829	-1.246575
C	4.003975	-0.023594	0.132050
C	2.772398	1.109016	-1.673621
C	3.479535	0.954161	1.040326
C	2.226780	2.101259	-0.778530
H	2.537682	1.188739	-2.747722
C	2.632677	1.972810	0.598900
H	3.726294	0.912669	2.108687
H	2.280213	2.717562	1.328596
C	-0.414549	-2.554524	-0.754957
C	-1.285354	-3.500323	-1.338292
C	0.969195	-2.828189	-0.665589
C	-0.771568	-4.716300	-1.822366
H	-2.362455	-3.284563	-1.421230
C	1.471646	-4.047897	-1.144065
H	1.651532	-2.077916	-0.230366
C	0.603359	-4.992394	-1.723185
H	-1.451126	-5.451110	-2.281268
H	2.549432	-4.263066	-1.071564
H	1.001766	-5.945440	-2.104506
C	-2.663277	-0.670976	-0.840221
C	-3.869230	-0.644630	-0.111835
C	-2.659556	-0.367237	-2.220457
C	-5.068103	-0.307256	-0.765406
H	-3.871935	-0.873271	0.965103
C	-3.860831	-0.042571	-2.867673
H	-1.711873	-0.375099	-2.783882
C	-5.065579	-0.005328	-2.138453
H	-6.009995	-0.280301	-0.195839
H	-3.858030	0.191996	-3.943405
H	-6.006466	0.260454	-2.644842
C	-1.397938	-1.346771	1.727154
C	-1.867115	-2.618601	2.125694
C	-1.233818	-0.321002	2.682793
C	-2.178602	-2.852972	3.474955
H	-1.982291	-3.427000	1.386255
C	-1.551330	-0.563102	4.029466
H	-0.863380	0.666710	2.365576
C	-2.024031	-1.826943	4.425889
H	-2.541619	-3.844770	3.786261
H	-1.424292	0.238994	4.773225
H	-2.268346	-2.016690	5.482757
Au	0.457340	0.707254	-0.345033
H	4.000820	-0.618709	-1.992096
N	4.811179	-1.042927	0.565684
C	5.333665	-2.019752	-0.385207
H	5.922950	-2.780569	0.156994
H	4.512260	-2.544459	-0.921989
H	5.997097	-1.549712	-1.144938
C	5.213373	-1.118839	1.968153
H	4.333685	-1.217769	2.641462
H	5.853376	-2.006608	2.117583
H	5.794194	-0.223264	2.281563
H	1.470210	4.642082	0.437043

[(PPh_3)Au(alkene)-(aniline)]$^+$ Adduct

-1846.50270633 A.U.

P	1.144108	0.987342	0.063582
H	-0.894629	-3.268427	-1.261654
C	0.966896	-2.227780	-1.768937

C	-0.400262	-2.502186	-1.882123
C	1.446458	-3.593031	0.317712
C	1.881151	-2.752568	-0.742188
C	2.344090	-4.039089	1.298900
C	3.251317	-2.383758	-0.775786
C	3.697640	-3.651012	1.258694
H	1.980469	-4.687598	2.112086
C	4.143254	-2.819429	0.214501
H	3.609301	-1.724755	-1.582746
H	4.397990	-3.992168	2.037071
H	5.196619	-2.499654	0.172007
C	1.737970	0.756093	1.788400
C	1.996996	1.837025	2.658339
C	1.975788	-0.565992	2.222053
C	2.495760	1.590906	3.949633
H	1.807223	2.870485	2.327812
C	2.487105	-0.804106	3.507079
H	1.764602	-1.411749	1.551227
C	2.745734	0.272996	4.374284
H	2.691507	2.436455	4.628232
H	2.677386	-1.840992	3.825613
H	3.138301	0.085836	5.386537
C	0.544985	2.726642	0.015028
C	1.362859	3.806016	-0.382798
C	-0.784310	2.966964	0.431193
C	0.851978	5.116087	-0.364212
H	2.398786	3.620318	-0.708504
C	-1.284129	4.278610	0.455939
H	-1.426176	2.117807	0.719836
C	-0.468715	5.354123	0.056683
H	1.491381	5.955929	-0.679878
H	-2.321629	4.458232	0.779206
H	-0.865927	6.381658	0.068627
C	2.692838	0.996073	-0.933989
C	3.977059	0.911634	-0.356631
C	2.562199	0.985525	-2.342087
C	5.113914	0.807944	-1.178787
H	4.087998	0.907509	0.738500
C	3.699209	0.891967	-3.158584
H	1.557529	1.033714	-2.794743
C	4.979190	0.794451	-2.577400
H	6.112034	0.730354	-0.719136
H	3.587242	0.882648	-4.254358
H	5.870494	0.705345	-3.218332
Au	-0.536075	-0.558889	-0.617414
H	1.449374	-1.639347	-2.568837
H	-0.939897	-2.232546	-2.803757
H	0.386900	-3.884049	0.382187
C	-4.772390	0.669733	-0.446442
C	-5.461300	-0.412053	0.171014
C	-3.384617	0.616615	-0.662351
C	-4.684127	-1.552295	0.520928
C	-2.599738	-0.504594	-0.301060
H	-2.907083	1.489305	-1.140234
C	-3.299656	-1.585718	0.285404
H	-5.157988	-2.430889	0.981684
H	-2.753415	-2.500259	0.574702
H	-5.317094	1.570825	-0.763435
N	-6.834980	-0.358620	0.420062
C	-7.612378	0.747795	-0.102339
H	-8.668820	0.636951	0.209236
H	-7.251822	1.724486	0.293072
H	-7.588328	0.813296	-1.218783
C	-7.521966	-1.542507	0.898260
H	-7.108230	-1.892324	1.871207
H	-8.591356	-1.307752	1.061681
H	-7.464389	-2.402715	0.185437

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov

-1846.45044194 A.U.

P	-1.662362	-0.256028	0.157793
H	0.218454	2.522807	-3.526684
C	0.330311	2.719857	-2.446986

C	1.590154	2.297942	-1.841888
C	1.369366	3.720861	0.246386
C	2.165223	2.962560	-0.648737
C	1.930177	4.300300	1.396637
C	3.543307	2.819319	-0.355085
C	3.301589	4.151869	1.670934
H	1.289206	4.878599	2.081799
C	4.106916	3.412009	0.783256
H	4.169014	2.208111	-1.025028
H	3.741989	4.610040	2.570748
H	5.182287	3.286919	0.987657
C	-1.037812	-0.117148	1.890167
C	-1.123134	-1.189097	2.805693
C	-0.404966	1.082070	2.286100
C	-0.592781	-1.054684	4.100236
H	-1.579733	-2.143104	2.497854
C	0.126959	1.211192	3.578415
H	-0.294511	1.908259	1.565508
C	0.032079	0.143884	4.489491
H	-0.659741	-1.897766	4.806287
H	0.635410	2.146207	3.861901
H	0.456086	0.241299	5.501609
C	-1.516554	-2.048364	-0.227930
C	-2.576623	-2.800209	-0.776690
C	-0.249590	-2.646840	-0.046740
C	-2.365979	-4.144532	-1.133711
H	-3.565220	-2.337741	-0.924607
C	-0.047749	-3.988440	-0.401153
H	0.581253	-2.059215	0.370974
C	-1.105227	-4.740168	-0.946840
H	-3.195307	-4.729768	-1.562015
H	0.949582	-4.432490	-0.253097
H	-0.947039	-5.793009	-1.230536
C	-3.478163	0.061131	0.243088
C	-4.286061	-0.519860	1.245915
C	-4.062718	0.890774	-0.735334
C	-5.668266	-0.273605	1.262103
H	-3.835587	-1.162026	2.018894
C	-5.448579	1.128371	-0.718801
H	-3.408691	1.352431	-1.496475
C	-6.251297	0.548587	0.278772
H	-6.294889	-0.723954	2.048380
H	-5.900687	1.776460	-1.486323
H	-7.336008	0.740987	0.295819
Au	-0.413332	1.075958	-1.210885
H	-0.108373	3.678545	-2.123046
H	2.332377	1.824677	-2.502135
H	0.292826	3.841595	0.047113
C	2.748150	-2.028785	-1.528070
C	3.200639	-2.250391	-0.195863
C	2.039571	-0.861493	-1.859397
C	2.986939	-1.203259	0.749336
C	1.770585	0.137376	-0.906050
H	1.675249	-0.747488	-2.897565
C	2.289856	-0.036979	0.387579
H	3.346391	-1.300170	1.783689
H	2.142311	0.744955	1.153123
H	2.917642	-2.781872	-2.310591
N	3.808752	-3.454700	0.173537
C	4.196159	-4.400193	-0.857844
H	4.634843	-5.300326	-0.386164
H	3.316566	-4.733580	-1.452696
H	4.945780	-3.985418	-1.576413
C	4.407549	-3.575522	1.490454
H	5.251836	-2.861552	1.658323
H	3.657300	-3.397833	2.292182
H	4.796560	-4.603107	1.625097

[(PPh_3)Au(alkene)-(*para*-aniline)]$^+$ Intermediate Markovnikov

--1846.54997316 A.U.

P	1.615984	-0.422655	-0.036813
H	-2.018276	-0.358857	-3.285314
C	-2.006516	-1.080118	-2.438049
C	-3.103653	-0.655935	-1.419713

C	-2.672230	-2.868972	-0.141995
C	-3.407897	-1.679970	-0.321808
C	-2.951131	-3.743873	0.926414
C	-4.453586	-1.408924	0.592175
C	-3.979656	-3.449458	1.835713
H	-2.355022	-4.663675	1.044524
C	-4.737225	-2.275222	1.658165
H	-5.034918	-0.479492	0.472548
H	-4.197965	-4.132105	2.672804
H	-5.552965	-2.033053	2.358624
C	0.883908	-0.522113	1.657296
C	1.063650	0.485598	2.627738
C	0.023413	-1.608870	1.935631
C	0.385694	0.407245	3.857618
H	1.712494	1.349158	2.413502
C	-0.660586	-1.677510	3.158723
H	-0.159620	-2.379421	1.169831
C	-0.482712	-0.666914	4.121418
H	0.524104	1.202959	4.606922
H	-1.362771	-2.507060	3.336191
H	-1.031693	-0.710544	5.075376
C	2.165776	1.329898	-0.182449
C	3.409434	1.782377	0.310380
C	1.268148	2.248979	-0.771189
C	3.741348	3.146201	0.230478
H	4.120270	1.067689	0.755548
C	1.607220	3.609422	-0.849526
H	0.300311	1.898589	-1.164132
C	2.839857	4.060756	-0.345288
H	4.712304	3.495317	0.616609
H	0.897847	4.314546	-1.307575
H	3.105004	5.128265	-0.408898
C	3.167971	-1.403342	0.053290
C	3.837449	-1.660368	1.269443
C	3.698549	-1.899720	-1.157899
C	5.036147	-2.394769	1.268193
H	3.414695	-1.289825	2.217180
C	4.899345	-2.628034	-1.153827
H	3.156435	-1.718715	-2.101054
C	5.569527	-2.875201	0.058514
H	5.555079	-2.595666	2.218993
H	5.308810	-3.013555	-2.100901
H	6.507322	-3.453175	0.061437
Au	-0.121818	-0.942447	-1.523773
H	-2.232272	-2.081166	-2.869503
H	-4.060597	-0.518040	-1.981495
H	-1.855180	-3.110747	-0.837713
C	-2.404234	3.132127	-1.095197
C	-1.745687	3.233187	0.163552
C	-2.882629	1.896232	-1.560553
C	-1.644591	2.043774	0.938308
C	-2.744654	0.710193	-0.812969
H	-3.363998	1.855112	-2.552436
C	-2.130527	0.824815	0.452492
H	-1.166570	2.051638	1.926140
H	-2.011053	-0.071348	1.078143
H	-2.534674	4.018477	-1.731741
N	-1.196695	4.431602	0.610814
C	-1.422797	5.655165	-0.130635
H	-0.964281	6.505382	0.408805
H	-0.974423	5.626774	-1.154142
H	-2.508357	5.877895	-0.255703
C	-0.426336	4.451292	1.840048
H	-1.048326	4.244011	2.744138
H	0.394409	3.698359	1.812889
H	0.039884	5.446499	1.968051

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS anti-Markovnikov

-1846.45504741 A.U.

P	0.631301	1.275045	0.051083
H	1.782995	-2.368048	-2.734832
C	1.330157	-2.618739	-1.761200
C	-0.091868	-2.935866	-1.736855
C	3.660409	-2.806340	-0.842311

C	2.253894	-2.958176	-0.670507
C	4.558068	-3.058778	0.202372
C	1.806370	-3.393273	0.612662
C	4.094060	-3.482403	1.465888
H	5.638699	-2.922512	0.031274
C	2.709271	-3.649162	1.654408
H	0.727096	-3.497603	0.804032
H	4.801222	-3.679709	2.286824
H	2.322408	-3.971073	2.635165
C	1.523560	1.036039	1.644163
C	1.237816	1.819961	2.783282
C	2.527670	0.041661	1.707843
C	1.958009	1.614253	3.973284
H	0.446264	2.585006	2.742734
C	3.241631	-0.156970	2.899826
H	2.742726	-0.594898	0.832774
C	2.959648	0.628368	4.032630
H	1.729409	2.225286	4.861083
H	4.006238	-0.948510	2.934346
H	3.516774	0.465904	4.969200
C	-0.921438	2.183361	0.479880
C	-1.009901	3.593136	0.485410
C	-2.064157	1.410384	0.782932
C	-2.230072	4.216871	0.801324
H	-0.128970	4.204490	0.232313
C	-3.280981	2.037970	1.094161
H	-2.009179	0.311655	0.753372
C	-3.365259	3.442281	1.104496
H	-2.295551	5.316736	0.801735
H	-4.166355	1.415026	1.302300
H	-4.321320	3.937441	1.338968
C	1.623149	2.511586	-0.884593
C	2.504463	3.405147	-0.239759
C	1.470769	2.567294	-2.287112
C	3.221525	4.350308	-0.995154
H	2.635976	3.356034	0.852905
C	2.180612	3.519698	-3.034993
H	0.802278	1.847058	-2.788042
C	3.057923	4.412076	-2.390056
H	3.914930	5.040470	-0.488734
H	2.057616	3.558643	-4.128921
H	3.622486	5.152140	-2.979151
Au	0.343142	-0.732795	-0.949017
H	-0.420812	-3.736949	-1.053595
H	-0.598842	-2.962465	-2.715094
H	4.040157	-2.460658	-1.818083
C	-3.962661	-0.857635	-1.268810
C	-4.384909	-1.202018	0.048062
C	-2.661365	-1.150179	-1.705634
C	-3.472740	-1.948324	0.850789
C	-1.722016	-1.787958	-0.870168
H	-2.365794	-0.831509	-2.721736
C	-2.174311	-2.222793	0.393155
H	-3.761750	-2.291709	1.854199
H	-1.488179	-2.768668	1.065204
H	-4.642515	-0.332763	-1.954454
N	-5.628491	-0.803565	0.540581
C	-6.565423	-0.130895	-0.341657
H	-7.460883	0.171158	0.234198
H	-6.118212	0.792991	-0.771211
H	-6.903279	-0.769462	-1.194519
C	-6.104787	-1.336371	1.805502
H	-6.215087	-2.448061	1.795903
H	-5.418756	-1.075491	2.642118
H	-7.092787	-0.896931	2.040135

[(PPh_3)Au(alkene)-(*para*-aniline)]$^+$ Intermediate anti-Markovnikov

-1846.54542765 A.U.

P	1.363795	0.940601	0.014354
H	-0.067496	-3.014919	-2.615992
C	-0.545764	-2.655099	-1.680538
C	-2.087044	-2.640059	-1.880964
C	1.259145	-4.101481	-0.634198
C	-0.002735	-3.454959	-0.523746

C	1.846003	-4.763242	0.454659
C	-0.655990	-3.530525	0.735113
C	1.185596	-4.815051	1.697869
H	2.828077	-5.248723	0.331005
C	-0.070685	-4.194737	1.825114
H	-1.619965	-3.019955	0.868213
H	1.642150	-5.337689	2.553531
H	-0.601756	-4.220726	2.790792
C	2.030289	0.267004	1.598119
C	2.300127	1.117035	2.695211
C	2.241181	-1.124958	1.725023
C	2.794916	0.581280	3.895530
H	2.106922	2.199008	2.615100
C	2.730001	-1.654546	2.931098
H	1.999624	-1.808271	0.893254
C	3.011507	-0.804606	4.014474
H	3.001491	1.248903	4.747158
H	2.867475	-2.743627	3.015456
H	3.388953	-1.222942	4.961281
C	0.224637	2.279885	0.559329
C	0.611407	3.636280	0.617673
C	-1.077749	1.900821	0.955609
C	-0.296990	4.603340	1.083538
H	1.620802	3.936321	0.293306
C	-1.976394	2.869812	1.429543
H	-1.396796	0.848382	0.876146
C	-1.587087	4.220683	1.493476
H	0.006374	5.661699	1.125046
H	-2.993971	2.559848	1.716482
H	-2.296720	4.981340	1.856787
C	2.754592	1.818645	-0.806099
C	3.985796	2.093968	-0.175223
C	2.548860	2.221403	-2.145659
C	4.995157	2.778356	-0.876132
H	4.159854	1.768436	0.862129
C	3.555619	2.913348	-2.836303
H	1.595731	1.977374	-2.644078
C	4.780882	3.192987	-2.202037
H	5.956653	2.986912	-0.380577
H	3.388323	3.225506	-3.879267
H	5.574374	3.727904	-2.747633
Au	0.324389	-0.784142	-1.155920
H	-2.507243	-3.624754	-1.570977
H	-2.270233	-2.562002	-2.974313
H	1.793709	-4.054491	-1.597893
C	-3.558170	0.838337	-1.123010
C	-4.343479	0.624189	0.045138
C	-2.847139	-0.211822	-1.715199
C	-4.402722	-0.704233	0.546335
C	-2.881620	-1.530286	-1.207121
H	-2.243431	-0.000402	-2.613545
C	-3.689843	-1.744131	-0.074572
H	-5.016472	-0.945150	1.424797
H	-3.783991	-2.763610	0.335835
H	-3.485496	1.838001	-1.571336
N	-5.022480	1.681228	0.670160
C	-5.202540	2.923867	-0.065756
H	-5.759122	3.644281	0.564077
H	-4.223657	3.390358	-0.309499
H	-5.764377	2.788440	-1.022556
C	-5.980759	1.374247	1.719258
H	-5.494427	0.829063	2.556232
H	-6.384911	2.317683	2.134277
H	-6.840741	0.752852	1.364721

Using CH_2=CHPh(Me on para) as alkene:

[(PPh_3)Au(alkene)]$^+$
-1520.24685521 A.U.

P	1.228543	0.203736	0.007402
H	-1.285824	-4.175936	-0.273809
C	-1.755633	-3.221388	-0.562953
C	-2.394434	-2.448722	0.414955
C	-3.595514	-0.762379	-1.054879

C	-3.251941	-1.271797	0.225479
C	-4.328401	0.418737	-1.173218
C	-3.686717	-0.559410	1.372242
C	-4.755579	1.140861	-0.028708
H	-4.579391	0.801625	-2.175309
C	-4.422385	0.625767	1.244243
H	-3.427895	-0.935924	2.375181
H	-4.744549	1.164677	2.149323
C	0.337817	1.771437	-0.321656
C	0.992542	2.839845	-0.973223
C	-0.998206	1.919131	0.116546
C	0.312827	4.053284	-1.173511
H	2.029087	2.723320	-1.327202
C	-1.666669	3.136204	-0.085976
H	-1.525215	1.085034	0.609475
C	-1.013139	4.203411	-0.729108
H	0.823094	4.885460	-1.682671
H	-2.706520	3.244689	0.257049
H	-1.541519	5.155911	-0.890603
C	2.591836	0.099699	-1.204912
C	3.902532	0.493372	-0.859735
C	2.300577	-0.336945	-2.517004
C	4.916360	0.453193	-1.832643
H	4.131943	0.825992	0.164830
C	3.318811	-0.370573	-3.481752
H	1.276972	-0.651113	-2.781848
C	4.626209	0.024232	-3.139862
H	5.939972	0.757426	-1.564790
H	3.093442	-0.712220	-4.503783
H	5.424810	-0.008471	-3.897163
C	1.992882	0.346940	1.661367
C	2.143373	1.601929	2.289795
C	2.478335	-0.825633	2.283702
C	2.787292	1.678289	3.537096
H	1.759115	2.515026	1.808914
C	3.123499	-0.737857	3.526769
H	2.352008	-1.805341	1.793350
C	3.277967	0.513453	4.153189
H	2.905015	2.655746	4.029938
H	3.503539	-1.650271	4.011623
H	3.780195	0.579250	5.130873
Au	-0.263254	-1.565920	-0.121055
H	-1.975322	-3.093460	-1.637303
H	-3.272405	-1.289219	-1.965704
H	-2.293706	-2.784489	1.465026
C	-5.558308	2.406726	-0.179300
H	-5.164833	3.042484	-0.999537
H	-6.613058	2.167915	-0.439503
H	-5.575668	3.002675	0.754344

[(PPh_3)Au(alkene)Cl]

-1980.59126364 A.U.

P	-0.944771	0.513818	-0.016280
H	0.559359	-3.953627	-1.573405
C	1.098718	-3.280789	-0.886778
C	1.529663	-2.005717	-1.350912
C	3.264940	-1.518091	0.453832
C	2.587756	-1.162131	-0.737128
C	4.175115	-0.636039	1.055426
C	2.889368	0.094842	-1.315768
C	4.442167	0.636256	0.502924
H	4.678749	-0.936853	1.988840
C	3.788764	0.975507	-0.702823
H	2.379234	0.398474	-2.243418
H	3.974648	1.958864	-1.165140
C	-0.246782	1.363868	1.455051
C	-0.948749	2.360301	2.164784
C	1.067992	1.019596	1.839908
C	-0.330839	3.011852	3.247144
H	-1.977261	2.624877	1.872975
C	1.682625	1.681984	2.913019
H	1.614915	0.233496	1.297821
C	0.984217	2.678984	3.619300
H	-0.883134	3.785494	3.803850

H	2.710058	1.405545	3.198223
H	1.462803	3.193397	4.467794
C	-2.729236	0.931654	-0.043053
C	-3.204346	2.119103	-0.644145
C	-3.627445	0.045242	0.592670
C	-4.575668	2.421329	-0.601854
H	-2.501853	2.803090	-1.146839
C	-4.996313	0.361142	0.631750
H	-3.253007	-0.896257	1.035010
C	-5.471291	1.544534	0.038209
H	-4.946825	3.345460	-1.072919
H	-5.696860	-0.331930	1.123706
H	-6.546533	1.783211	0.067587
C	-0.219998	1.432049	-1.439783
C	0.552954	2.600733	-1.284988
C	-0.396064	0.878572	-2.728626
C	1.150975	3.202221	-2.407298
H	0.706208	3.030537	-0.283148
C	0.194284	1.486801	-3.846694
H	-0.982655	-0.047844	-2.847081
C	0.976690	2.647393	-3.686595
H	1.762835	4.108963	-2.277225
H	0.054604	1.047500	-4.847039
H	1.452600	3.116607	-4.562069
Au	-0.319058	-1.778932	-0.125903
H	1.587487	-3.779686	-0.033461
H	1.258307	-1.713455	-2.382278
H	3.058760	-2.486647	0.934137
Cl	-1.874780	-2.977651	1.326480
C	5.358443	1.621766	1.189815
H	5.951364	1.143511	1.995137
H	6.065938	2.091166	0.474501
H	4.771046	2.446720	1.650481

[(PPh_3)Au(alkene)(*para*-aniline)]$^+$

-1886.24440731 A.U.

P	-0.116786	0.856962	-0.251686
H	0.981245	-3.556742	-2.269214
C	1.428072	-3.134446	-1.353778
C	2.213959	-1.967174	-1.445486
C	3.481866	-2.145991	0.750318
C	3.169781	-1.455598	-0.446348
C	4.325906	-1.568520	1.707737
C	3.761869	-0.185771	-0.659281
C	4.882945	-0.282512	1.517407
H	4.557864	-2.126658	2.629263
C	4.592251	0.389315	0.307840
H	3.543755	0.363509	-1.588430
H	5.021895	1.387308	0.124622
C	0.553811	1.334746	1.388407
C	0.313229	2.616851	1.937650
C	1.410398	0.437854	2.060661
C	0.928323	2.988288	3.144191
H	-0.352624	3.326682	1.422347
C	2.024559	0.816774	3.265291
H	1.617020	-0.556872	1.635806
C	1.785062	2.090594	3.808890
H	0.738306	3.987029	3.567277
H	2.696490	0.108819	3.774401
H	2.264027	2.386360	4.755409
C	-1.720708	1.744511	-0.402982
C	-2.093464	2.367623	-1.614016
C	-2.587534	1.806511	0.710685
C	-3.318562	3.049801	-1.705467
H	-1.420050	2.341286	-2.484522
C	-3.794983	2.515227	0.620171
H	-2.306802	1.314024	1.654775
C	-4.166689	3.133879	-0.587223
H	-3.600733	3.536099	-2.652157
H	-4.452907	2.584326	1.499980
H	-5.115321	3.688953	-0.654143
C	1.002886	1.664157	-1.478266
C	1.896396	2.692150	-1.112501
C	1.006637	1.177634	-2.806169

C	2.786028	3.220369	-2.064339
H	1.921952	3.064571	-0.077677
C	1.890696	1.715024	-3.755743
H	0.325384	0.359305	-3.094624
C	2.787881	2.733451	-3.383267
H	3.488525	4.015170	-1.768859
H	1.886758	1.330234	-4.787458
H	3.491588	3.145453	-4.123082
Au	0.066106	-1.471603	-0.654925
H	1.557293	-3.840806	-0.516145
H	2.244064	-1.445387	-2.419762
H	3.061608	-3.145841	0.939834
C	-3.714528	-1.553115	-0.637372
C	-3.884331	-1.186688	0.737342
C	-2.708044	-2.434112	-1.023751
C	-2.927107	-1.684505	1.680944
C	-1.781193	-2.966818	-0.077270
H	-2.643757	-2.747307	-2.077730
C	-1.920859	-2.563529	1.284071
H	-2.995032	-1.410637	2.741638
H	-1.192284	-3.862491	-0.328871
H	-1.238852	-2.976786	2.043709
H	-4.400130	-1.169398	-1.403046
N	-4.937200	-0.401506	1.135660
C	-5.941018	0.022326	0.164952
H	-6.701754	0.641674	0.673023
H	-5.488629	0.641196	-0.640166
H	-6.458881	-0.846043	-0.300060
C	-5.128695	-0.093213	2.547197
H	-4.259385	0.458188	2.970380
H	-6.021341	0.547061	2.664601
H	-5.283268	-1.010397	3.158748
C	5.736780	0.372141	2.574392
H	6.039798	-0.341042	3.365907
H	6.655255	0.816260	2.137921
H	5.178999	1.202271	3.061713

[(PPh_3)Au(alkene)(*ortho*-aniline)]$^+$

-1886.24966838 A.U.

P	-0.270180	1.047592	0.017867
H	-0.036651	-2.961967	-2.944497
C	0.625661	-2.763784	-2.085872
C	1.493894	-1.651893	-2.128015
C	3.073151	-2.317347	-0.249941
C	2.640568	-1.394351	-1.234075
C	4.084734	-1.972987	0.655871
C	3.283903	-0.132198	-1.295588
C	4.696074	-0.698122	0.625533
H	4.407142	-2.708781	1.410215
C	4.281938	0.208387	-0.377951
H	2.969078	0.599732	-2.055782
H	4.746814	1.205785	-0.433064
C	0.697376	1.198105	1.568225
C	0.698596	2.389901	2.332333
C	1.532277	0.126305	1.949235
C	1.518667	2.493526	3.467924
H	0.060530	3.239640	2.042937
C	2.352973	0.238357	3.082508
H	1.552327	-0.800102	1.355650
C	2.345436	1.418656	3.845552
H	1.512360	3.421089	4.061229
H	3.002830	-0.604649	3.363540
H	2.985023	1.504301	4.737929
C	-1.846816	1.964486	0.269527
C	-2.516449	2.521251	-0.843180
C	-2.429156	2.069853	1.552518
C	-3.749032	3.173576	-0.671492
H	-2.072305	2.463126	-1.848661
C	-3.657276	2.732355	1.718836
H	-1.919955	1.640190	2.426888
C	-4.321368	3.283436	0.609015
H	-4.259286	3.609084	-1.544564
H	-4.095086	2.819784	2.725527
H	-5.282365	3.803991	0.741817

C	0.667745	2.024095	-1.240157
C	1.670504	2.947013	-0.877130
C	0.419787	1.771184	-2.609431
C	2.413472	3.605834	-1.872268
H	1.896736	3.134487	0.182761
C	1.155013	2.441720	-3.600222
H	-0.335250	1.022584	-2.902696
C	2.158910	3.356609	-3.232281
H	3.202128	4.316459	-1.579759
H	0.953009	2.239226	-4.663568
H	2.746972	3.871367	-4.007776
Au	-0.321774	-1.182094	-0.778614
H	0.840561	-3.631528	-1.440937
H	1.402495	-0.956701	-2.982237
H	2.613177	-3.315714	-0.187328
C	-1.823610	-2.719721	0.428003
C	-2.891730	-1.779348	0.684427
C	-0.836980	-2.974533	1.429377
C	-2.852222	-1.072736	1.927954
C	-0.819279	-2.258462	2.626617
H	-0.083265	-3.753524	1.233425
C	-1.840679	-1.308450	2.858539
H	-3.632057	-0.339081	2.162868
H	-0.038108	-2.435702	3.379299
H	-1.845955	-0.740077	3.802216
H	-1.918407	-3.442552	-0.395114
N	-3.887074	-1.569767	-0.236655
C	-3.776231	-2.174808	-1.554278
H	-4.644006	-1.883859	-2.172409
H	-2.842377	-1.844297	-2.077119
H	-3.756616	-3.284350	-1.500315
C	-4.865178	-0.503567	-0.029701
H	-4.392832	0.503807	-0.032912
H	-5.617279	-0.539329	-0.838315
H	-5.405635	-0.635718	0.930563
C	5.737845	-0.296735	1.639277
H	6.060202	-1.150698	2.266861
H	6.637440	0.130340	1.149160
H	5.335875	0.489869	2.315155

[(PPh_3)Au(*para*-aniline)+(PPh_3)Au(alkene)]$^+$ adduct

-3057.37015216 A.U.

P	3.932148	-0.739968	0.049221
H	-0.747222	-0.211571	-1.098365
C	-0.146945	0.716042	-1.090421
C	-0.340768	1.566475	0.030226
C	0.490222	3.735679	-0.940582
C	0.000037	2.962574	0.152045
C	0.797099	5.084588	-0.779697
C	-0.179858	3.621513	1.399196
C	0.617150	5.738658	0.467349
H	1.175986	5.661107	-1.639262
C	0.142765	4.972845	1.555633
H	-0.582547	3.051473	2.250758
H	0.000938	5.454034	2.536430
C	5.205455	0.047483	-1.009412
C	6.308115	-0.680350	-1.507252
C	5.085252	1.427914	-1.286159
C	7.287561	-0.024260	-2.272829
H	6.397433	-1.759616	-1.305450
C	6.070352	2.075915	-2.047945
H	4.215720	1.990971	-0.907341
C	7.171114	1.351102	-2.541357
H	8.145551	-0.593136	-2.663649
H	5.975264	3.151465	-2.263719
H	7.939435	1.860378	-3.143762
C	4.055821	-2.540285	-0.283206
C	4.444882	-3.470694	0.701430
C	3.661576	-2.991114	-1.564173
C	4.430286	-4.846245	0.406377
H	4.752117	-3.126017	1.701046
C	3.662291	-4.363243	-1.855861
H	3.343412	-2.264067	-2.329399
C	4.040212	-5.293466	-0.867970

H	4.727261	-5.571658	1.179591
H	3.356853	-4.710256	-2.855152
H	4.029936	-6.371070	-1.093900
C	4.489033	-0.480801	1.776648
C	5.852565	-0.629168	2.117546
C	3.545591	-0.147311	2.772055
C	6.259584	-0.464854	3.451222
H	6.595946	-0.865605	1.339467
C	3.960363	0.016628	4.104394
H	2.487937	-0.011499	2.495729
C	5.314926	-0.145939	4.444867
H	7.322121	-0.580411	3.715948
H	3.223048	0.279269	4.878943
H	5.639614	-0.014735	5.488878
Au	1.791028	0.034394	-0.410923
H	-0.000790	1.170630	-2.087085
H	-0.763027	1.095956	0.935363
H	0.627171	3.262668	-1.924456
P	-3.139902	-2.098447	0.025729
C	-3.163924	4.448694	0.938267
C	-2.699605	5.079421	-0.255921
C	-3.467566	3.082623	0.959183
C	-2.630692	4.274635	-1.432455
C	-3.334435	2.254832	-0.186028
H	-3.808759	2.645689	1.912240
C	-2.933124	2.910510	-1.382201
H	-2.322177	4.712760	-2.391223
H	-2.832670	2.327798	-2.313084
C	-4.216039	-3.076012	1.141215
C	-3.735351	-4.185239	1.871959
C	-5.574852	-2.701991	1.237090
C	-4.616050	-4.920670	2.683083
H	-2.672536	-4.469712	1.811408
C	-6.449694	-3.444791	2.046735
H	-5.940385	-1.822951	0.680597
C	-5.971540	-4.553636	2.768529
H	-4.240856	-5.784489	3.254033
H	-7.508347	-3.151157	2.120557
H	-6.657819	-5.131183	3.407512
C	-1.429992	-2.345170	0.684182
C	-0.475588	-3.172150	0.055484
C	-1.080881	-1.645714	1.862867
C	0.810585	-3.309940	0.609418
H	-0.736766	-3.710021	-0.869325
C	0.201007	-1.790805	2.414369
H	-1.823397	-0.989577	2.346979
C	1.147550	-2.624872	1.789351
H	1.555201	-3.953864	0.117388
H	0.462334	-1.254872	3.340472
H	2.153602	-2.736333	2.220910
C	-3.135120	-2.977865	-1.587004
C	-3.440967	-4.351679	-1.693653
C	-2.767364	-2.248603	-2.740329
C	-3.369772	-4.989422	-2.944113
H	-3.742023	-4.922076	-0.800818
C	-2.691516	-2.893358	-3.985744
H	-2.553865	-1.169551	-2.659269
C	-2.992342	-4.264013	-4.088508
H	-3.616472	-6.059664	-3.025062
H	-2.409673	-2.319939	-4.882728
H	-2.943071	-4.766684	-5.067163
Au	-3.489727	0.214762	-0.098447
H	-3.283181	5.030060	1.862701
N	-2.311059	6.410804	-0.265736
C	-2.534347	7.238405	0.910145
H	-2.098991	8.240484	0.741388
H	-3.616559	7.362646	1.148317
H	-2.036445	6.802183	1.802181
C	-2.007863	7.063738	-1.530267
H	-2.882284	7.082504	-2.221634
H	-1.698992	8.107964	-1.338898
H	-1.169555	6.552457	-2.050326
C	0.971320	7.194757	0.625969
H	0.473842	7.647531	1.506129

H	2.067779	7.321869	0.764311
H	0.691759	7.778837	-0.274544

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3057.35146844 A.U.

P	3.458935	-1.801716	-0.020118
H	-0.949560	-0.043586	-1.494951
C	-0.019892	0.552271	-1.395686
C	-0.025701	1.438242	-0.199541
C	1.821025	3.001553	-0.999558
C	1.146636	2.332387	0.045722
C	2.901528	3.858180	-0.731687
C	1.606157	2.547880	1.366458
C	3.354535	4.078014	0.585950
H	3.413441	4.359122	-1.569797
C	2.691024	3.393057	1.631122
H	1.098567	2.032873	2.198333
H	3.033759	3.529260	2.670102
C	4.950932	-0.728404	-0.192609
C	6.261426	-1.245109	-0.282634
C	4.750676	0.672425	-0.230139
C	7.357087	-0.371168	-0.386240
H	6.435488	-2.331072	-0.290933
C	5.851700	1.538647	-0.322957
H	3.732247	1.094110	-0.206452
C	7.156243	1.020413	-0.398859
H	8.375263	-0.783754	-0.462321
H	5.678110	2.624951	-0.352406
H	8.018278	1.700780	-0.481696
C	3.893185	-3.486529	-0.584789
C	4.823097	-4.305795	0.099348
C	3.263016	-3.972103	-1.752497
C	5.119062	-5.589392	-0.387284
H	5.307286	-3.946911	1.021458
C	3.565540	-5.256654	-2.235516
H	2.532486	-3.334798	-2.277902
C	4.492853	-6.064683	-1.554617
H	5.842236	-6.223524	0.148963
H	3.073150	-5.627942	-3.147732
H	4.727883	-7.071967	-1.932620
C	3.144123	-1.914568	1.798262
C	2.999940	-0.697862	2.505268
C	2.871891	-3.133019	2.455865
C	2.595683	-0.704316	3.848517
H	3.188538	0.262165	1.999217
C	2.468277	-3.132674	3.803911
H	2.958042	-4.089997	1.919602
C	2.326415	-1.921737	4.502523
H	2.488777	0.249643	4.388841
H	2.258737	-4.089470	4.307211
H	2.007358	-1.925690	5.556397
Au	1.583499	-0.742159	-0.917945
H	0.186318	1.072948	-2.352551
H	-0.331101	0.912507	0.722488
H	1.502241	2.842545	-2.039374
P	-3.984107	-0.884507	0.063336
C	-0.831227	4.804092	0.946418
C	-0.424428	5.392973	-0.299983
C	-1.372280	3.532510	0.967863
C	-0.811175	4.719789	-1.512569
C	-1.565616	2.738249	-0.223525
H	-1.587396	3.075885	1.948454
C	-1.356290	3.449997	-1.459406
H	-0.615512	5.178907	-2.490633
H	-1.548659	2.922387	-2.408452
C	-4.909869	-1.514221	-1.386720
C	-5.869629	-2.542565	-1.269783
C	-4.603938	-0.974698	-2.656445
C	-6.513852	-3.028147	-2.420177
H	-6.119829	-2.959037	-0.281412
C	-5.245979	-1.471036	-3.802559
H	-3.862873	-0.162189	-2.740569
C	-6.201619	-2.496775	-3.684702
H	-7.267238	-3.825856	-2.327078

H	-5.006170	-1.048420	-4.790658
H	-6.711281	-2.879410	-4.582790
C	-4.994038	-1.232685	1.547550
C	-4.961343	-2.494051	2.182992
C	-5.844429	-0.215998	2.034565
C	-5.786631	-2.735533	3.293934
H	-4.285368	-3.281117	1.812027
C	-6.669060	-0.466611	3.143576
H	-5.851086	0.771677	1.544479
C	-6.641270	-1.725094	3.771948
H	-5.761009	-3.718142	3.790493
H	-7.331969	0.326504	3.522941
H	-7.285324	-1.917929	4.644187
C	-2.488386	-1.959230	0.205678
C	-2.112152	-2.864588	-0.806661
C	-1.635151	-1.754725	1.316909
C	-0.889484	-3.555006	-0.707713
H	-2.767328	-3.026935	-1.676708
C	-0.421146	-2.448462	1.412666
H	-1.922914	-1.040959	2.106672
C	-0.043860	-3.346215	0.394192
H	-0.593310	-4.255489	-1.503890
H	0.245198	-2.280307	2.272199
H	0.916887	-3.879176	0.459656
Au	-3.021455	1.220681	-0.116876
H	-0.658044	5.330276	1.894109
N	0.343547	6.518868	-0.328554
C	0.870522	7.080060	0.916074
H	1.547292	7.920118	0.679023
H	0.058846	7.470222	1.566833
H	1.446144	6.315866	1.482983
C	0.810123	7.061418	-1.603126
H	-0.038819	7.330508	-2.265997
H	1.395766	7.979341	-1.417739
H	1.459296	6.332221	-2.137441
C	4.509700	5.004702	0.885651
H	5.294888	4.491582	1.480381
H	4.980483	5.392551	-0.039582
H	4.179317	5.879549	1.487213

[(PPh_3)Au(*para*-aniline-alkene)] Markovnikov

-1885.83233447 A.U.

P	2.516617	-0.396880	-0.022716
H	-1.985801	-2.662738	0.306215
C	-1.714727	-1.655232	-0.079572
C	-2.506677	-0.554340	0.680002
C	-2.078438	1.474892	-0.829646
C	-1.886324	0.817503	0.403407
C	-1.373657	2.651260	-1.136898
C	-1.006533	1.411278	1.332735
C	-0.453670	3.216418	-0.224762
H	-1.528737	3.136042	-2.115984
C	-0.299082	2.583020	1.026128
H	-0.839121	0.915570	2.303096
H	0.407487	2.997298	1.763486
C	2.855739	0.535707	-1.572946
C	4.119142	0.570484	-2.198798
C	1.783769	1.286163	-2.107218
C	4.308915	1.361653	-3.346416
H	4.955067	-0.019097	-1.790164
C	1.984776	2.084664	-3.243511
H	0.792755	1.253015	-1.625021
C	3.246796	2.123570	-3.865672
H	5.295653	1.383983	-3.835810
H	1.145172	2.674582	-3.644015
H	3.401889	2.745154	-4.761893
C	3.968079	-1.499545	0.207508
C	5.162811	-1.064288	0.821643
C	3.868767	-2.823357	-0.274584
C	6.250546	-1.946006	0.942262
H	5.237499	-0.035700	1.209564
C	4.961530	-3.698192	-0.157101
H	2.924532	-3.163210	-0.732043
C	6.152487	-3.260643	0.450827

H	7.180114	-1.604634	1.424933
H	4.878934	-4.730082	-0.533280
H	7.006127	-3.949972	0.549197
C	2.693037	0.891600	1.286157
C	3.234939	2.168145	1.029479
C	2.209373	0.584468	2.577365
C	3.295129	3.126036	2.057188
H	3.593642	2.421603	0.019743
C	2.277227	1.541431	3.601624
H	1.755085	-0.401991	2.767237
C	2.817911	2.815406	3.342543
H	3.709384	4.124807	1.847351
H	1.891284	1.298023	4.604045
H	2.857851	3.570390	4.143565
Au	0.347611	-1.282417	-0.014998
H	-1.995955	-1.636345	-1.158681
H	-2.364443	-0.744560	1.769102
H	-2.781674	1.044617	-1.561004
C	-6.205229	0.531974	0.777656
C	-6.880118	-0.479091	0.031882
C	-4.819269	0.483726	0.963098
C	-6.077191	-1.519537	-0.512685
C	-4.019208	-0.550515	0.426572
H	-4.334573	1.290748	1.537792
C	-4.687583	-1.545187	-0.312458
H	-6.533258	-2.326030	-1.103459
H	-4.113666	-2.374485	-0.752594
H	-6.764370	1.369729	1.217020
N	-8.259585	-0.446120	-0.154893
C	-9.028200	0.682018	0.334399
H	-10.098988	0.527931	0.101623
H	-8.940951	0.798302	1.439474
H	-8.715171	1.650090	-0.127080
C	-8.896461	-1.448339	-0.987098
H	-8.734022	-2.478767	-0.594345
H	-9.988424	-1.270615	-1.010273
H	-8.525680	-1.433594	-2.040949
C	0.394656	4.411150	-0.595643
H	-0.081237	5.031945	-1.382300
H	0.599874	5.059003	0.281359
H	1.380713	4.076244	-0.990879

[(PPh_3)Au(*ortho*-aniline)+(PPh_3)Au(alkene)]$^+$ adduct

-3057.36619731 A.U.

P	3.621505	-1.272460	-0.034759
H	-1.000983	0.165724	-1.463752
C	-0.134630	0.845873	-1.457218
C	0.208186	1.458335	-0.238547
C	1.808145	3.248607	-1.057407
C	1.133009	2.569887	-0.010557
C	2.726874	4.259904	-0.773122
C	1.416634	2.947624	1.325074
C	3.021974	4.632385	0.563207
H	3.241824	4.772276	-1.601452
C	2.351977	3.953205	1.603277
H	0.889594	2.439721	2.146968
H	2.557255	4.228255	2.650157
C	4.995171	-0.078606	-0.330371
C	6.267257	-0.482787	-0.790415
C	4.742983	1.294295	-0.095720
C	7.280267	0.472985	-0.982438
H	6.474070	-1.538215	-1.019568
C	5.763317	2.239227	-0.279644
H	3.744157	1.644522	0.208346
C	7.035449	1.831459	-0.718744
H	8.267840	0.148967	-1.345851
H	5.548325	3.302121	-0.091827
H	7.833308	2.575076	-0.869904
C	4.095948	-2.892310	-0.727213
C	5.210957	-3.613472	-0.234227
C	3.324696	-3.432506	-1.780278
C	5.539904	-4.860208	-0.790439
H	5.820681	-3.206216	0.587768
C	3.660661	-4.679674	-2.332108

H	2.455213	-2.872956	-2.161513
C	4.765580	-5.394288	-1.836964
H	6.406418	-5.418351	-0.403322
H	3.056394	-5.094463	-3.153671
H	5.026781	-6.372819	-2.269041
C	3.452338	-1.460682	1.795566
C	3.075193	-0.312266	2.531082
C	3.545211	-2.705762	2.451417
C	2.812284	-0.409710	3.905374
H	2.959443	0.661097	2.028505
C	3.273529	-2.797106	3.828849
H	3.809784	-3.616069	1.894005
C	2.908593	-1.653085	4.558252
H	2.520433	0.490456	4.468458
H	3.344940	-3.774217	4.331269
H	2.693835	-1.730000	5.635344
Au	1.617818	-0.352130	-0.770492
H	0.140283	1.293826	-2.426203
H	-0.316463	1.092557	0.662189
H	1.622276	2.966106	-2.104506
P	-3.505562	-1.150149	0.163106
C	-1.198462	4.903366	-0.484405
C	-1.983159	3.725715	-0.572187
C	-0.796207	5.412062	0.759518
C	-2.350929	3.029510	0.627624
C	-1.185984	4.765915	1.944353
H	-0.184596	6.327207	0.799298
C	-1.956377	3.590559	1.864674
H	-0.885626	5.169144	2.924531
H	-2.237496	3.077133	2.799101
C	-1.882233	-2.022617	0.282150
C	-1.394833	-2.870260	-0.734173
C	-1.104399	-1.802929	1.443428
C	-0.148175	-3.504704	-0.579545
H	-1.989802	-3.037394	-1.645702
C	0.132720	-2.446898	1.598872
H	-1.474868	-1.122579	2.228252
C	0.609769	-3.302324	0.586570
H	0.230048	-4.168453	-1.372690
H	0.736389	-2.273947	2.502827
H	1.581772	-3.804561	0.702453
C	-4.074585	-1.485332	-1.553442
C	-4.855427	-2.615412	-1.877219
C	-3.674234	-0.592433	-2.574735
C	-5.221745	-2.854594	-3.213281
H	-5.184862	-3.306012	-1.084915
C	-4.037784	-0.842028	-3.907966
H	-3.091403	0.308991	-2.320001
C	-4.811008	-1.973052	-4.229140
H	-5.836569	-3.734137	-3.460552
H	-3.726838	-0.141668	-4.699119
H	-5.103426	-2.162320	-5.273850
C	-4.626768	-2.082022	1.270682
C	-4.419196	-3.444473	1.580398
C	-5.746797	-1.400135	1.796057
C	-5.336666	-4.119645	2.403087
H	-3.539033	-3.975095	1.183050
C	-6.661844	-2.083432	2.613573
H	-5.893354	-0.331370	1.567437
C	-6.457860	-3.442092	2.916310
H	-5.174412	-5.181446	2.646230
H	-7.534015	-1.550041	3.022413
H	-7.173499	-3.974857	3.561898
Au	-3.115024	1.121312	0.532616
H	-0.904942	5.446327	-1.394044
N	-2.377031	3.203681	-1.841139
C	-1.653267	3.674230	-3.013891
H	-1.870413	3.000494	-3.869283
H	-1.933534	4.711842	-3.330835
H	-0.561866	3.656779	-2.827694
C	-3.821777	3.144993	-2.096550
H	-4.360248	2.796658	-1.195399
H	-4.229102	4.147048	-2.383496
H	-4.037961	2.434254	-2.921593

C	3.996478	5.743861	0.864308
H	4.709692	5.908753	0.031724
H	3.454636	6.702517	1.022624
H	4.574753	5.544338	1.789301

[(PPh_3)Au(*ortho*-aniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3057.34910658 A.U.

P	3.638292	-1.356934	-0.107095
H	-0.846482	0.316429	-1.495119
C	0.038008	0.948574	-1.284112
C	-0.069849	1.681313	-0.006062
C	1.724349	3.417526	-0.511836
C	1.042401	2.590524	0.405709
C	2.810378	4.205957	-0.102647
C	1.477377	2.596319	1.751007
C	3.261397	4.195309	1.235516
H	3.328781	4.837951	-0.841913
C	2.571230	3.372568	2.155245
H	0.958972	1.955840	2.483268
H	2.900702	3.342707	3.206914
C	5.080125	-0.219413	-0.284055
C	6.395543	-0.671301	-0.524086
C	4.830433	1.169169	-0.169467
C	7.449042	0.253741	-0.624895
H	6.606473	-1.743113	-0.652385
C	5.890002	2.085170	-0.260435
H	3.803952	1.546479	-0.029408
C	7.201347	1.630649	-0.485568
H	8.471151	-0.107399	-0.818596
H	5.677684	3.161152	-0.169502
H	8.030498	2.350848	-0.566462
C	4.081207	-2.978396	-0.828937
C	5.100609	-3.799840	-0.289958
C	3.363325	-3.414244	-1.965267
C	5.396612	-5.035397	-0.888422
H	5.655840	-3.481436	0.606528
C	3.665549	-4.650765	-2.560160
H	2.563179	-2.776788	-2.376250
C	4.681544	-5.460752	-2.023340
H	6.189824	-5.671023	-0.464892
H	3.104410	-4.982921	-3.447444
H	4.917234	-6.430329	-2.489258
C	3.431516	-1.618090	1.710931
C	3.234441	-0.464749	2.505822
C	3.300898	-2.894156	2.298711
C	2.915934	-0.589820	3.866214
H	3.309410	0.538520	2.057878
C	2.982038	-3.012694	3.664189
H	3.432765	-3.805442	1.696413
C	2.786540	-1.864427	4.450083
H	2.764892	0.316345	4.474011
H	2.882567	-4.013547	4.112541
H	2.534494	-1.961775	5.517540
Au	1.699601	-0.303407	-0.864772
H	0.280132	1.580022	-2.162601
H	-0.396032	1.041975	0.832173
H	1.409815	3.430234	-1.565904
P	-3.778391	-1.020368	0.212498
C	-1.152026	5.125212	-0.811111
C	-1.528579	3.775102	-1.095469
C	-1.064492	5.597605	0.495138
C	-1.742761	2.858664	0.026710
C	-1.333493	4.755176	1.602075
H	-0.788800	6.651146	0.662302
C	-1.662553	3.433220	1.354066
H	-1.264255	5.140374	2.630166
H	-1.807623	2.756338	2.212777
C	-2.192652	-1.965988	0.271223
C	-1.777783	-2.815773	-0.773461
C	-1.326218	-1.720576	1.363912
C	-0.505139	-3.414987	-0.722220
H	-2.443191	-3.009567	-1.629060
C	-0.063422	-2.326895	1.413404
H	-1.645016	-1.049286	2.178761

C	0.349008	-3.173488	0.365557
H	-0.178583	-4.074016	-1.541678
H	0.612223	-2.129784	2.259579
H	1.344225	-3.641421	0.396037
C	-4.708230	-1.684368	-1.220934
C	-5.700811	-2.676319	-1.074008
C	-4.384333	-1.197588	-2.507899
C	-6.360674	-3.176447	-2.209939
H	-5.963714	-3.054326	-0.073769
C	-5.039510	-1.709669	-3.638730
H	-3.614548	-0.417154	-2.619747
C	-6.030170	-2.698055	-3.490164
H	-7.140085	-3.945257	-2.091903
H	-4.782882	-1.329519	-4.639832
H	-6.551109	-3.092452	-4.376514
C	-4.697395	-1.486138	1.721941
C	-4.564832	-2.771203	2.294329
C	-5.575761	-0.541118	2.295926
C	-5.318103	-3.107048	3.431305
H	-3.868900	-3.503200	1.854100
C	-6.328262	-0.886494	3.430650
H	-5.660762	0.465497	1.854016
C	-6.200163	-2.167724	3.997133
H	-5.214582	-4.107537	3.879613
H	-7.012627	-0.149419	3.878579
H	-6.787213	-2.434672	4.889826
Au	-3.025477	1.166450	0.057297
H	-0.962751	5.831912	-1.629497
N	-1.568712	3.367081	-2.414567
C	-1.005198	4.212191	-3.466518
H	-0.823404	3.587835	-4.363160
H	-1.687897	5.043114	-3.760886
H	-0.034229	4.643509	-3.155109
C	-2.449295	2.328651	-2.939588
H	-2.983567	1.819694	-2.110337
H	-3.207653	2.779158	-3.619729
H	-1.878650	1.561038	-3.502301
C	4.441379	5.025505	1.683275
H	4.898406	5.583502	0.841996
H	4.141687	5.765793	2.455634
H	5.228741	4.388186	2.139378

[(PPh_3)Au(*ortho*-aniline-alkene)Au(PPh_3)]$^+$ Intermediate Markovnikov

-3057.37875780 A.U.

P	3.824913	-1.181945	-0.011539
H	-0.768542	-0.046038	-1.559393
C	0.089461	0.659642	-1.451853
C	-0.241465	1.754654	-0.406766
C	1.208472	3.711780	-1.188359
C	0.933521	2.718923	-0.229222
C	2.354200	4.519919	-1.082941
C	1.829085	2.573993	0.852379
C	3.253997	4.377230	-0.005110
H	2.554531	5.278270	-1.857689
C	2.961708	3.392561	0.965330
H	1.662981	1.776121	1.596285
H	3.644836	3.257045	1.819818
C	5.232346	-0.146640	-0.595614
C	6.565421	-0.610309	-0.608209
C	4.947552	1.180762	-0.993275
C	7.602456	0.250207	-1.005768
H	6.798382	-1.646775	-0.319664
C	5.991363	2.038547	-1.378332
H	3.907473	1.545993	-0.998982
C	7.318889	1.575271	-1.385189
H	8.640171	-0.118179	-1.020447
H	5.756653	3.070294	-1.682638
H	8.136248	2.245147	-1.695355
C	4.256220	-2.941018	-0.299093
C	5.190476	-3.638513	0.501167
C	3.619444	-3.606742	-1.370833
C	5.488973	-4.982411	0.221642
H	5.673252	-3.135055	1.354053
C	3.923837	-4.950469	-1.646553

H	2.879676	-3.063157	-1.982113
C	4.858702	-5.638184	-0.852189
H	6.217244	-5.521958	0.847203
H	3.427489	-5.463442	-2.485193
H	5.095189	-6.691998	-1.067581
C	3.829727	-0.966542	1.821436
C	4.217982	0.271187	2.378609
C	3.309540	-1.973024	2.666622
C	4.075063	0.501873	3.757122
H	4.632822	1.057443	1.729511
C	3.172897	-1.738957	4.045370
H	3.020989	-2.951139	2.250426
C	3.549106	-0.498986	4.593604
H	4.386305	1.469488	4.181753
H	2.775822	-2.534250	4.695887
H	3.444190	-0.318209	5.674798
Au	1.798039	-0.386052	-0.855110
H	0.278673	1.112483	-2.450702
H	-0.366382	1.231199	0.559128
H	0.525319	3.848249	-2.042939
P	-3.785583	-1.148928	0.105702
C	-2.803862	4.653391	-0.244162
C	-3.268850	4.673666	-1.566459
C	-1.968004	3.613323	0.246326
C	-2.925713	3.654435	-2.467540
C	-1.535863	2.570086	-0.685733
H	-3.928632	5.495117	-1.887533
C	-2.059445	2.632429	-2.030773
H	-3.292181	3.661245	-3.504163
H	-1.653101	1.920161	-2.766374
C	-4.739032	-2.126219	-1.109967
C	-5.549091	-3.206304	-0.696769
C	-4.610362	-1.819679	-2.483130
C	-6.223301	-3.975759	-1.659259
H	-5.660895	-3.441660	0.373263
C	-5.281664	-2.599612	-3.438740
H	-3.986347	-0.967593	-2.800500
C	-6.088427	-3.675967	-3.027223
H	-6.860650	-4.813919	-1.337494
H	-5.181215	-2.359582	-4.508511
H	-6.621246	-4.281111	-3.777172
C	-4.671536	-1.206111	1.701252
C	-4.476920	-2.276646	2.602740
C	-5.592000	-0.178971	2.005548
C	-5.210730	-2.317790	3.800107
H	-3.747125	-3.068932	2.371603
C	-6.322886	-0.230180	3.203229
H	-5.730492	0.660573	1.304219
C	-6.133176	-1.298453	4.099263
H	-5.059333	-3.150631	4.504304
H	-7.040968	0.569956	3.440585
H	-6.704769	-1.334460	5.039780
C	-2.178535	-2.010476	0.347080
C	-1.728718	-2.991163	-0.560286
C	-1.327006	-1.564839	1.386051
C	-0.432373	-3.520666	-0.426694
H	-2.384190	-3.338058	-1.374329
C	-0.037285	-2.097284	1.511910
H	-1.673198	-0.794543	2.093955
C	0.413273	-3.072637	0.600431
H	-0.076922	-4.279653	-1.140340
H	0.633182	-1.736675	2.307003
H	1.434860	-3.474252	0.679053
Au	-3.128942	0.943622	-0.568305
H	-3.121608	5.455309	0.436420
N	-1.526031	3.629707	1.556478
C	-1.442678	2.419647	2.365700
H	-1.911582	2.609226	3.355240
H	-2.009773	1.594311	1.886551
H	-0.397387	2.082902	2.538580
C	-1.512141	4.877014	2.312680
H	-2.495696	5.115638	2.784044
H	-0.755432	4.796491	3.118658
H	-1.211071	5.720847	1.662373

C	4.484726	5.244985	0.125531
H	4.711841	5.783507	-0.816173
H	4.354820	6.009976	0.921991
H	5.375174	4.641535	0.400327

[(PPh_3)Au(*ortho*-aniline-alkene)] Markovnikov

-1885.82982587 A.U.

P	2.256574	-0.285620	0.055599
H	-1.940807	-3.095020	0.189856
C	-1.758021	-2.087871	-0.245492
C	-2.744990	-1.048765	0.354556
C	-2.481911	0.892290	-1.301702
C	-2.289427	0.371347	-0.006187
C	-1.927166	2.130194	-1.671219
C	-1.540477	1.144037	0.906759
C	-1.152304	2.889112	-0.765766
H	-2.085400	2.510377	-2.695134
C	-0.982301	2.375692	0.538423
H	-1.369278	0.754993	1.923630
H	-0.380063	2.937368	1.271013
C	2.592157	0.564978	-1.542294
C	3.887255	0.728908	-2.076275
C	1.477969	1.117426	-2.214446
C	4.065087	1.450496	-3.270696
H	4.757633	0.294881	-1.559064
C	1.665094	1.848065	-3.397797
H	0.462764	0.984257	-1.805559
C	2.957911	2.015491	-3.928734
H	5.077407	1.573509	-3.687476
H	0.790201	2.282714	-3.906729
H	3.102703	2.583570	-4.861439
C	3.818142	-1.157017	0.476917
C	4.893688	-0.515762	1.129586
C	3.933293	-2.513366	0.100352
C	6.077486	-1.226110	1.392493
H	4.800673	0.538871	1.434902
C	5.121478	-3.216259	0.359868
H	3.080296	-3.013326	-0.388352
C	6.193706	-2.573726	1.005446
H	6.913890	-0.724399	1.904659
H	5.206867	-4.273993	0.064896
H	7.122262	-3.128179	1.214979
C	2.152636	1.111008	1.256245
C	2.561480	2.421941	0.934721
C	1.589486	0.846687	2.524321
C	2.410050	3.456422	1.875061
H	2.982243	2.640241	-0.059120
C	1.442956	1.881510	3.460979
H	1.241888	-0.172066	2.762485
C	1.850390	3.189554	3.136773
H	2.723052	4.479787	1.614309
H	0.995467	1.669497	4.444804
H	1.723610	4.003729	3.867735
Au	0.226341	-1.448898	-0.029368
H	-1.925906	-2.170749	-1.344471
H	-2.651630	-1.130958	1.460519
H	-3.074664	0.313453	-2.028681
C	-6.520549	-0.403978	-0.134666
C	-6.906794	-1.498387	-0.925513
C	-5.197244	-0.284260	0.347525
C	-5.969543	-2.495886	-1.233311
C	-4.219361	-1.264595	-0.016089
H	-7.945448	-1.576031	-1.285870
C	-4.642649	-2.367424	-0.782174
H	-6.260576	-3.366977	-1.841715
H	-3.906393	-3.134231	-1.064119
H	-7.261175	0.365675	0.132453
N	-4.802224	0.829626	1.130006
C	-4.500398	0.616852	2.533061
H	-5.408775	0.700924	3.185409
H	-4.072975	-0.391915	2.691143
H	-3.753461	1.363927	2.884853
C	-5.363713	2.129541	0.830060
H	-6.370993	2.315957	1.289319

H	-4.675260	2.917117	1.208579
H	-5.448475	2.255942	-0.267654
C	-0.457522	4.161981	-1.192385
H	-0.976162	4.655108	-2.040303
H	-0.385748	4.891425	-0.359294
H	0.582877	3.943613	-1.524950

[(PPh_3)Au(*para*-aniline-alkene)Au(PPh_3)]$^+$ Intermediate anti-Markovnikov

-3057.38948798 A.U.

P	4.382921	-0.062083	-0.402330
H	-0.294973	-0.428371	-0.299717
C	0.173629	-1.414963	-0.062129
C	-0.427700	-2.440704	-1.050171
C	-0.341135	-0.599082	2.277890
C	-0.046481	-1.674150	1.405223
C	-0.561955	-0.801732	3.649420
C	0.041799	-2.963523	1.985869
C	-0.499168	-2.090616	4.220829
H	-0.796885	0.065409	4.290156
C	-0.184757	-3.164828	3.355841
H	0.291751	-3.829034	1.351219
H	-0.112730	-4.185100	3.769006
C	5.696468	-1.256365	0.065095
C	6.824318	-0.878935	0.826035
C	5.563704	-2.589163	-0.384796
C	7.815865	-1.829722	1.123785
H	6.925125	0.155303	1.191712
C	6.561080	-3.531658	-0.088282
H	4.671392	-2.885272	-0.961060
C	7.687281	-3.153031	0.665622
H	8.693447	-1.534259	1.719980
H	6.454749	-4.569724	-0.440038
H	8.465248	-3.895347	0.903376
C	4.569064	1.325924	0.793874
C	5.150142	2.564643	0.451589
C	4.087076	1.115769	2.107056
C	5.258023	3.580064	1.420725
H	5.518842	2.740285	-0.570993
C	4.207330	2.128048	3.071225
H	3.609460	0.157482	2.369864
C	4.793229	3.362393	2.730084
H	5.711162	4.546184	1.148611
H	3.833988	1.955277	4.092624
H	4.883203	4.158288	3.485903
C	4.901714	0.617410	-2.028708
C	6.265294	0.781000	-2.359567
C	3.905736	1.007483	-2.951263
C	6.623949	1.347938	-3.593828
H	7.047022	0.457456	-1.653904
C	4.270374	1.576647	-4.183082
H	2.843540	0.842119	-2.704969
C	5.628637	1.750229	-4.503538
H	7.688029	1.471444	-3.849221
H	3.490513	1.876310	-4.900630
H	5.914184	2.191117	-5.471473
Au	2.196699	-0.891938	-0.315838
H	-0.045235	-3.463799	-0.843929
H	-0.073248	-2.196773	-2.072459
H	-0.378986	0.421073	1.866690
P	-2.882790	1.814027	0.059176
C	-3.982774	-2.844812	-2.526055
C	-4.736792	-3.362841	-1.424417
C	-2.656178	-2.437119	-2.363738
C	-4.078492	-3.417815	-0.152527
C	-1.964686	-2.504581	-1.100599
H	-2.095930	-2.092619	-3.248431
C	-2.752362	-3.008662	0.000440
H	-4.606862	-3.792657	0.733329
H	-2.272021	-3.111373	0.985387
C	-3.802027	1.999297	1.631870
C	-4.631011	3.113681	1.880159
C	-3.614450	1.014935	2.629215
C	-5.265837	3.241530	3.128263
H	-4.783870	3.878607	1.102583

C	-4.243820	1.157738	3.875139
H	-2.963879	0.145663	2.436202
C	-5.071110	2.268901	4.125196
H	-5.916721	4.108474	3.321214
H	-4.088665	0.392824	4.651929
H	-5.570152	2.375338	5.101109
C	-3.644385	2.942438	-1.159495
C	-3.231227	4.290085	-1.248250
C	-4.684702	2.461929	-1.984605
C	-3.867382	5.152747	-2.156696
H	-2.410523	4.660180	-0.613158
C	-5.317500	3.332122	-2.886577
H	-4.987446	1.403459	-1.921789
C	-4.909833	4.676315	-2.972352
H	-3.544427	6.202902	-2.229797
H	-6.127873	2.958155	-3.531381
H	-5.403457	5.355445	-3.684929
C	-1.187737	2.442627	0.384652
C	-0.843058	3.038433	1.616809
C	-0.192293	2.219570	-0.594911
C	0.494471	3.393999	1.866611
H	-1.611978	3.201922	2.387584
C	1.138684	2.577307	-0.334918
H	-0.455270	1.735754	-1.549775
C	1.485175	3.159271	0.898145
H	0.766189	3.847650	2.832242
H	1.917111	2.385739	-1.088766
H	2.533108	3.420654	1.105050
Au	-2.679764	-0.374196	-0.599113
H	-4.433170	-2.760797	-3.523268
N	-6.035030	-3.780117	-1.577184
C	-6.661289	-3.761250	-2.895077
H	-7.696818	-4.137571	-2.813982
H	-6.706970	-2.731853	-3.315090
H	-6.119207	-4.407439	-3.621301
C	-6.774068	-4.315203	-0.437843
H	-6.849712	-3.572392	0.386698
H	-7.801089	-4.570483	-0.755172
H	-6.303327	-5.238124	-0.030822
C	-0.727440	-2.321822	5.697470
H	-1.448142	-3.147863	5.875610
H	0.216482	-2.606408	6.211786
H	-1.117953	-1.414350	6.200688

[(PPh_3)Au(*para*-aniline-alkene)] anti-Markovnikov

-1885.82701285 A.U.

P	2.685547	-0.320526	-0.007711
H	-2.010936	-0.957673	-1.386938
C	-1.701188	-0.659435	-0.360801
C	-2.494539	-1.518206	0.654527
C	-1.853231	1.674599	-1.365047
C	-1.831024	0.837796	-0.219848
C	-1.820770	3.071241	-1.259492
C	-1.817047	1.490250	1.039849
C	-1.785101	3.714567	-0.001643
H	-1.821050	3.682383	-2.178262
C	-1.791999	2.890158	1.143774
H	-1.782041	0.886115	1.960163
H	-1.765735	3.355247	2.144095
C	3.409342	-0.797035	1.614912
C	4.293619	0.031312	2.338118
C	3.056129	-2.064395	2.131161
C	4.828620	-0.412937	3.560284
H	4.559525	1.026532	1.948545
C	3.599702	-2.505610	3.348171
H	2.342962	-2.696920	1.576498
C	4.486809	-1.680536	4.064048
H	5.515563	0.238647	4.123395
H	3.320480	-3.494254	3.745337
H	4.906440	-2.023694	5.023013
C	2.893863	1.509978	-0.126301
C	4.115028	2.090367	-0.537586
C	1.799576	2.343093	0.202619
C	4.242056	3.488450	-0.602811

H	4.964618	1.447124	-0.818171
C	1.933934	3.739400	0.134315
H	0.828107	1.908514	0.493223
C	3.153637	4.313998	-0.264992
H	5.195700	3.934949	-0.926666
H	1.066694	4.370766	0.381955
H	3.254908	5.409468	-0.324395
C	3.862764	-0.990291	-1.253131
C	5.162656	-1.429481	-0.923344
C	3.422501	-1.046137	-2.595022
C	6.017157	-1.909041	-1.932085
H	5.505120	-1.399150	0.123222
C	4.282848	-1.519048	-3.598205
H	2.397858	-0.723221	-2.844234
C	5.581250	-1.950824	-3.268242
H	7.030661	-2.252670	-1.670656
H	3.934896	-1.559538	-4.642461
H	6.253095	-2.328092	-4.055477
Au	0.407299	-0.817161	-0.245159
H	-2.190531	-1.276038	1.695018
H	-2.217687	-2.582581	0.499967
H	-1.863699	1.204769	-2.362664
C	-6.077679	-1.887682	-0.701450
C	-6.821076	-0.949786	0.072167
C	-4.705854	-2.072970	-0.483669
C	-6.103687	-0.212423	1.056768
C	-3.994323	-1.351108	0.497603
H	-4.166545	-2.808791	-1.104918
C	-4.731225	-0.417810	1.255693
H	-6.615575	0.533811	1.680029
H	-4.216067	0.178489	2.025672
H	-6.570354	-2.485149	-1.481113
N	-8.188398	-0.764478	-0.124658
C	-8.854686	-1.441083	-1.220600
H	-9.932265	-1.189162	-1.209681
H	-8.446236	-1.155961	-2.221379
H	-8.772461	-2.548583	-1.132948
C	-8.879082	0.292802	0.588381
H	-8.476162	1.309108	0.355798
H	-9.951719	0.282354	0.316203
H	-8.815514	0.156072	1.692149
C	-1.764174	5.223598	0.103312
H	-2.766841	5.660713	-0.101956
H	-1.461433	5.561050	1.116028
H	-1.063646	5.675711	-0.631150

[(PPh_3)Au(*para*-aniline-alkene)]$^+$ Markovnikov

-1885.83233447 A.U.

P	2.516617	-0.396880	-0.022716
H	-1.985801	-2.662738	0.306215
C	-1.714727	-1.655232	-0.079572
C	-2.506677	-0.554340	0.680002
C	-2.078438	1.474892	-0.829646
C	-1.886324	0.817503	0.403407
C	-1.373657	2.651260	-1.136898
C	-1.006533	1.411278	1.332735
C	-0.453670	3.216418	-0.224762
H	-1.528737	3.136042	-2.115984
C	-0.299082	2.583020	1.026128
H	-0.839121	0.915570	2.303096
H	0.407487	2.997298	1.763486
C	2.855739	0.535707	-1.572946
C	4.119142	0.570484	-2.198798
C	1.783769	1.286163	-2.107218
C	4.308915	1.361653	-3.346416
H	4.955067	-0.019097	-1.790164
C	1.984776	2.084664	-3.243511
H	0.792755	1.253015	-1.625021
C	3.246796	2.123570	-3.865672
H	5.295653	1.383983	-3.835810
H	1.145172	2.674582	-3.644015
H	3.401889	2.745154	-4.761893
C	3.968079	-1.499545	0.207508
C	5.162811	-1.064288	0.821643

C	3.868767	-2.823357	-0.274584
C	6.250546	-1.946006	0.942262
H	5.237499	-0.035700	1.209564
C	4.961530	-3.698192	-0.157101
H	2.924532	-3.163210	-0.732043
C	6.152487	-3.260643	0.450827
H	7.180114	-1.604634	1.424933
H	4.878934	-4.730082	-0.533280
H	7.006127	-3.949972	0.549197
C	2.693037	0.891600	1.286157
C	3.234939	2.168145	1.029479
C	2.209373	0.584468	2.577365
C	3.295129	3.126036	2.057188
H	3.593642	2.421603	0.019743
C	2.277227	1.541431	3.601624
H	1.755085	-0.401991	2.767237
C	2.817911	2.815406	3.342543
H	3.709384	4.124807	1.847351
H	1.891284	1.298023	4.604045
H	2.857851	3.570390	4.143565
Au	0.347611	-1.282417	-0.014998
H	-1.995955	-1.636345	-1.158681
H	-2.364443	-0.744560	1.769102
H	-2.781674	1.044617	-1.561004
C	-6.205229	0.531974	0.777656
C	-6.880118	-0.479091	0.031882
C	-4.819269	0.483726	0.963098
C	-6.077191	-1.519537	-0.512685
C	-4.019208	-0.550515	0.426572
H	-4.334573	1.290748	1.537792
C	-4.687583	-1.545187	-0.312458
H	-6.533258	-2.326030	-1.103459
H	-4.113666	-2.374485	-0.752594
H	-6.764370	1.369729	1.217020
N	-8.259585	-0.446120	-0.154893
C	-9.028200	0.682018	0.334399
H	-10.098988	0.527931	0.101623
H	-8.940951	0.798302	1.439474
H	-8.715171	1.650090	-0.127080
C	-8.896461	-1.448339	-0.987098
H	-8.734022	-2.478767	-0.594345
H	-9.988424	-1.270615	-1.010273
H	-8.525680	-1.433594	-2.040949
C	0.394656	4.411150	-0.595643
H	-0.081237	5.031945	-1.382300
H	0.599874	5.059003	0.281359
H	1.380713	4.076244	-0.990879

Using CH_2=CHPh(OMe on para) as alkene:

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

-1595.40785425 A.U.

P	1.334553	0.256632	0.010449
H	-0.711867	-4.330162	-0.662326
C	-1.271105	-3.395666	-0.833993
C	-1.966650	-2.813421	0.237940
C	-3.348630	-1.089022	-0.996645
C	-2.930462	-1.716314	0.206628
C	-4.148373	0.053251	-0.980743
C	-3.387638	-1.170400	1.440076
C	-4.557568	0.608193	0.261338
H	-4.440714	0.519721	-1.930835
C	-4.185505	-0.030569	1.472183
H	-3.085282	-1.645259	2.387384
H	-4.531835	0.405074	2.420749
C	0.259819	1.733741	-0.163363
C	0.748929	2.916170	-0.760519
C	-1.055179	1.693020	0.353820
C	-0.075196	4.052932	-0.829251
H	1.769304	2.948964	-1.173755
C	-1.868096	2.835727	0.288532
H	-1.451921	0.768167	0.804652

C	-1.378686	4.015620	-0.302483
H	0.306308	4.973768	-1.296938
H	-2.890070	2.799740	0.696941
H	-2.017607	4.911030	-0.355570
C	2.696617	0.439670	-1.194491
C	3.921912	1.030057	-0.815300
C	2.489146	0.024918	-2.529225
C	4.932002	1.208006	-1.776143
H	4.088851	1.344229	0.227100
C	3.502948	0.209357	-3.482045
H	1.535473	-0.446416	-2.820354
C	4.723504	0.800851	-3.105890
H	5.889613	1.664334	-1.481373
H	3.343294	-0.116778	-4.521358
H	5.520003	0.938421	-3.853603
C	2.087765	0.337663	1.674618
C	2.091978	1.536582	2.419600
C	2.717288	-0.820830	2.183921
C	2.733299	1.572189	3.670117
H	1.596471	2.438194	2.026612
C	3.357567	-0.773744	3.431582
H	2.706542	-1.757423	1.601808
C	3.365589	0.422044	4.174602
H	2.737143	2.506049	4.253319
H	3.849154	-1.675294	3.828598
H	3.864770	0.455284	5.155476
Au	0.067556	-1.662298	-0.283265
H	-1.548518	-3.185003	-1.881784
H	-3.021314	-1.489542	-1.968204
H	-1.790823	-3.248310	1.240363
C	-5.695222	2.452914	-0.778960
H	-4.821948	2.801279	-1.373691
H	-6.356712	1.826594	-1.415896
H	-6.263752	3.327671	-0.414576
O	-5.273765	1.742515	0.391627

[(PPh_3)Au(alkene)(*para*-aniline)]$^+$

-1960.94445311 A.U.

P	2.075556	-0.175709	-0.219169
H	0.791132	-2.960710	2.559576
C	0.067331	-2.823014	1.738712
C	-1.193420	-2.194221	2.027104
C	-2.503036	-3.033394	0.009871
C	-2.450015	-2.377302	1.260657
C	-3.695088	-3.130306	-0.725478
C	-3.655581	-1.814409	1.751636
C	-4.884590	-2.563368	-0.214621
H	-3.683485	-3.645381	-1.696216
C	-4.851594	-1.905517	1.035886
H	-3.640113	-1.272599	2.710887
H	-5.783430	-1.461773	1.417376
C	2.752610	1.396249	0.450966
C	2.918135	2.559171	-0.327439
C	3.019353	1.438643	1.838890
C	3.343846	3.754091	0.280070
H	2.696831	2.536833	-1.405685
C	3.452214	2.630725	2.437931
H	2.864051	0.535171	2.451660
C	3.610318	3.793328	1.659282
H	3.461714	4.662688	-0.331472
H	3.652880	2.657815	3.520586
H	3.936619	4.733183	2.132096
C	1.770694	0.150098	-2.004122
C	2.651822	-0.294690	-3.014197
C	0.607775	0.876639	-2.355250
C	2.372780	-0.012104	-4.362725
H	3.556758	-0.863100	-2.748258
C	0.343253	1.160759	-3.704623
H	-0.087902	1.211751	-1.568405
C	1.221606	0.717146	-4.710371
H	3.062479	-0.364371	-5.146372
H	-0.563425	1.728228	-3.967414
H	1.007241	0.937173	-5.768473
C	3.514369	-1.325281	-0.196873

C	4.851029	-0.868698	-0.205102
C	3.250195	-2.711987	-0.193793
C	5.908744	-1.794361	-0.212253
H	5.061022	0.212740	-0.203973
C	4.310134	-3.633066	-0.213633
H	2.204427	-3.057688	-0.160124
C	5.640745	-3.175515	-0.220044
H	6.949891	-1.433988	-0.213289
H	4.096757	-4.713758	-0.212237
H	6.472420	-3.897947	-0.224320
Au	0.077152	-0.750158	0.966985
H	0.131875	-3.585541	0.943210
H	-1.344929	-1.803983	3.049699
H	-1.585025	-3.464567	-0.418992
C	-3.025707	2.149819	-0.238459
C	-2.516850	3.446451	0.056009
C	-2.287077	0.994880	0.069602
C	-1.248529	3.507853	0.699728
C	-1.009926	1.043913	0.682091
H	-2.736184	0.019055	-0.183834
C	-0.526827	2.338085	0.991278
H	-0.807776	4.476255	0.977042
H	0.455121	2.455877	1.477931
H	-4.012217	2.029024	-0.708844
N	-3.229008	4.603835	-0.271173
C	-4.589532	4.490265	-0.759143
H	-4.989388	5.499369	-0.976972
H	-4.638813	3.903717	-1.704592
H	-5.278646	3.997477	-0.028787
C	-2.748417	5.891410	0.189595
H	-1.726322	6.108051	-0.195698
H	-3.416934	6.690800	-0.184156
H	-2.705256	5.972636	1.304618
C	-6.182493	-3.223249	-2.114217
H	-5.526060	-2.731822	-2.870109
H	-5.917809	-4.305531	-2.065154
H	-7.236087	-3.128592	-2.440762
O	-6.097044	-2.594936	-0.846044

[(PPh_3)Au(*para*-aniline)+(PPh_3)Au(alkene)]$^+$ adduct

-3132.52910522 A.U.

P	3.799141	-1.171785	0.040515
H	-0.797076	-0.206315	-1.222150
C	-0.111180	0.659170	-1.167430
C	-0.250966	1.480997	-0.014625
C	0.746107	3.624990	-0.875796
C	0.201014	2.831759	0.175158
C	1.192151	4.926714	-0.652263
C	0.092613	3.430556	1.464890
C	1.075288	5.496666	0.642994
H	1.606943	5.506827	-1.487628
C	0.534944	4.725775	1.703445
H	-0.350327	2.846764	2.286588
H	0.463423	5.185970	2.699671
C	5.163628	-0.543421	-1.013042
C	6.207692	-1.385398	-1.453606
C	5.174857	0.830003	-1.344013
C	7.259785	-0.849845	-2.216568
H	6.195100	-2.459255	-1.208357
C	6.231664	1.357481	-2.102566
H	4.350224	1.481712	-1.009859
C	7.274029	0.518753	-2.539041
H	8.072169	-1.507733	-2.562601
H	6.238844	2.427847	-2.360872
H	8.099092	0.933386	-3.138976
C	3.771459	-2.985896	-0.228690
C	4.095021	-3.914000	0.781450
C	3.335682	-3.442692	-1.493901
C	3.973716	-5.292594	0.527497
H	4.433156	-3.565270	1.769659
C	3.230062	-4.818751	-1.744805
H	3.065544	-2.715676	-2.277569
C	3.542857	-5.745815	-0.731504
H	4.219218	-6.015591	1.320784

H	2.891747	-5.170551	-2.731751
H	3.448966	-6.825631	-0.925306
C	4.344362	-0.894862	1.769672
C	5.680972	-1.154222	2.148693
C	3.418113	-0.430382	2.728247
C	6.076516	-0.968737	3.483149
H	6.413693	-1.493916	1.399366
C	3.821274	-0.245928	4.061424
H	2.382817	-0.209579	2.423249
C	5.147736	-0.518456	4.440095
H	7.118253	-1.171037	3.776930
H	3.097276	0.119256	4.806477
H	5.463478	-0.370925	5.484682
Au	1.748224	-0.214765	-0.487308
H	0.087541	1.140074	-2.142658
H	-0.720286	1.007634	0.865219
H	0.823117	3.203873	-1.889075
P	-3.320041	-1.926921	0.036068
C	-2.773721	4.597938	0.895071
C	-2.259343	5.162984	-0.309744
C	-3.218061	3.271356	0.934179
C	-2.297067	4.346618	-1.479310
C	-3.188097	2.422809	-0.203838
H	-3.590089	2.880948	1.895948
C	-2.742897	3.022092	-1.412215
H	-1.958600	4.740679	-2.447110
H	-2.719155	2.424777	-2.338851
C	-4.473340	-2.838756	1.130825
C	-4.074617	-3.976931	1.866201
C	-5.807329	-2.380300	1.206987
C	-5.012237	-4.657288	2.661517
H	-3.030683	-4.326844	1.822388
C	-6.739551	-3.068365	2.000813
H	-6.108101	-1.478428	0.648327
C	-6.343234	-4.206251	2.726941
H	-4.700735	-5.543848	3.235922
H	-7.778723	-2.708967	2.059076
H	-7.074283	-4.740732	3.353625
C	-1.640062	-2.290297	0.717146
C	-0.749307	-3.205664	0.118975
C	-1.248877	-1.598362	1.887180
C	0.513180	-3.438470	0.694645
H	-1.042417	-3.741361	-0.797502
C	0.011247	-1.834078	2.457418
H	-1.941449	-0.875871	2.350440
C	0.893092	-2.756674	1.863078
H	1.204615	-4.154936	0.226891
H	0.305633	-1.300588	3.375038
H	1.883260	-2.938762	2.307649
C	-3.347499	-2.800266	-1.580431
C	-3.721137	-4.156844	-1.694199
C	-2.933232	-2.088078	-2.728678
C	-3.667741	-4.795301	-2.945149
H	-4.060156	-4.713196	-0.806137
C	-2.876373	-2.733434	-3.974839
H	-2.669225	-1.020624	-2.643129
C	-3.242302	-4.087607	-4.083837
H	-3.966172	-5.851897	-3.031182
H	-2.557890	-2.172669	-4.867567
H	-3.206932	-4.590544	-5.062974
Au	-3.505840	0.403913	-0.092873
H	-2.817906	5.197380	1.814458
N	-1.723776	6.444604	-0.341247
C	-1.805281	7.295815	0.837132
H	-1.244042	8.230582	0.653356
H	-2.854886	7.562324	1.104915
H	-1.337476	6.802307	1.714166
C	-1.453305	7.066827	-1.629145
H	-2.364462	7.139152	-2.268154
H	-1.068150	8.091117	-1.468926
H	-0.685546	6.498234	-2.197566
C	2.022909	7.595422	-0.031703
H	2.251032	8.555419	0.467040
H	2.963321	7.167450	-0.444457

H	1.306810	7.775756	-0.862960
O	1.457485	6.751549	0.970303

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3132.51063184 A.U.

P	3.322250	-2.054460	-0.014028
H	-1.008371	-0.008751	-1.212399
C	-0.055336	0.556521	-1.179110
C	0.009442	1.512710	-0.033672
C	1.914367	2.884709	-1.014631
C	1.225113	2.369250	0.103913
C	3.069146	3.672582	-0.875873
C	1.728906	2.693942	1.387128
C	3.558382	3.971471	0.414827
H	3.585519	4.031531	-1.776826
C	2.875390	3.473673	1.549343
H	1.209045	2.308803	2.279117
H	3.281177	3.701708	2.546048
C	4.628688	-1.017136	0.756270
C	5.582387	-1.586356	1.632740
C	4.657260	0.372107	0.495826
C	6.567683	-0.776601	2.219817
H	5.541094	-2.661271	1.871892
C	5.640882	1.177858	1.095527
H	3.895008	0.830549	-0.156526
C	6.598334	0.604550	1.950462
H	7.309064	-1.224382	2.900033
H	5.642606	2.263180	0.911584
H	7.365560	1.238756	2.421871
C	4.095757	-3.099636	-1.310086
C	5.468752	-3.424157	-1.321036
C	3.242962	-3.617434	-2.312206
C	5.978880	-4.269729	-2.320844
H	6.144669	-3.008814	-0.557851
C	3.757106	-4.472050	-3.301069
H	2.176128	-3.336642	-2.315699
C	5.125344	-4.798658	-3.305912
H	7.052189	-4.515912	-2.330612
H	3.089170	-4.874715	-4.078535
H	5.530351	-5.461296	-4.086720
C	2.822369	-3.222111	1.319378
C	2.461652	-2.677977	2.574059
C	2.667282	-4.604030	1.086939
C	1.952242	-3.510755	3.582327
H	2.578510	-1.597393	2.757189
C	2.144611	-5.431371	2.097891
H	2.954450	-5.037662	0.115981
C	1.785349	-4.888601	3.343574
H	1.679433	-3.082005	4.559394
H	2.024467	-6.509789	1.909984
H	1.379287	-5.540159	4.132886
Au	1.507491	-0.785179	-0.731380
H	0.115179	1.024624	-2.170080
H	-0.258775	1.045074	0.930410
H	1.553363	2.651183	-2.026477
P	-4.122565	-0.707592	0.077922
C	-0.691431	4.856408	1.078798
C	-0.241584	5.402162	-0.173553
C	-1.289575	3.611448	1.114971
C	-0.665453	4.738426	-1.379138
C	-1.494747	2.801495	-0.065919
H	-1.534934	3.180356	2.100100
C	-1.269187	3.497138	-1.310949
H	-0.450734	5.178453	-2.361974
H	-1.485858	2.968074	-2.253865
C	-5.302580	-1.037832	-1.286216
C	-6.157993	-2.161222	-1.254294
C	-5.320684	-0.169579	-2.399260
C	-7.020290	-2.412707	-2.333096
H	-6.157155	-2.835367	-0.383292
C	-6.184437	-0.428909	-3.477342
H	-4.659613	0.712946	-2.413266
C	-7.033530	-1.548919	-3.444526
H	-7.689888	-3.286451	-2.304612

H	-6.198808	0.251799	-4.342729
H	-7.714599	-1.747846	-4.286768
C	-4.979451	-1.141837	1.637243
C	-5.014238	-2.465390	2.130346
C	-5.652439	-0.112451	2.332038
C	-5.727122	-2.753242	3.306394
H	-4.473963	-3.267225	1.602256
C	-6.366831	-0.409054	3.504284
H	-5.608567	0.921965	1.952659
C	-6.404914	-1.728264	3.991315
H	-5.752389	-3.784990	3.690642
H	-6.891215	0.395092	4.043583
H	-6.961740	-1.958241	4.913189
C	-2.768885	-1.946400	-0.124042
C	-2.537064	-2.576116	-1.364512
C	-1.862078	-2.146785	0.944042
C	-1.410368	-3.402312	-1.531340
H	-3.234800	-2.420829	-2.202479
C	-0.749529	-2.984634	0.775719
H	-2.028410	-1.643747	1.910597
C	-0.519435	-3.609239	-0.465155
H	-1.232534	-3.887705	-2.503685
H	-0.047174	-3.144348	1.607238
H	0.362440	-4.255917	-0.590615
Au	-2.999683	1.325911	0.025349
H	-0.502773	5.391321	2.018710
N	0.596325	6.475720	-0.213330
C	1.139415	7.032259	1.027397
H	1.859017	7.833296	0.782157
H	0.341517	7.473665	1.661930
H	1.672844	6.251338	1.611565
C	1.113759	6.959314	-1.492342
H	0.294278	7.280649	-2.169109
H	1.765317	7.833507	-1.315370
H	1.711035	6.172612	-2.005126
C	5.425601	5.218768	-0.428918
H	6.281347	5.768615	0.005430
H	5.811629	4.408225	-1.087936
H	4.815778	5.921843	-1.041247
O	4.684646	4.697928	0.670446

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ Intermediate Markovnikov

-3132.54068887 A.U.

P	3.977238	-0.899242	-0.090532
H	-0.747502	0.075556	-1.138920
C	0.028507	0.868353	-1.004827
C	-0.372884	1.833049	0.140417
C	0.770321	3.973337	-0.686642
C	0.655194	2.954939	0.276198
C	1.815037	4.915104	-0.643578
C	1.605612	2.924342	1.321722
C	2.774709	4.846210	0.390084
H	1.874354	5.687189	-1.423280
C	2.649706	3.851673	1.386456
H	1.539182	2.133023	2.086864
H	3.401600	3.815806	2.188238
C	5.159872	0.411531	0.419405
C	6.278352	0.120188	1.235066
C	4.909185	1.744212	0.024185
C	7.146485	1.151476	1.627817
H	6.456847	-0.910201	1.582643
C	5.773249	2.774600	0.433452
H	4.014080	1.980322	-0.574202
C	6.893550	2.477724	1.228849
H	8.017144	0.921226	2.261842
H	5.544092	3.816580	0.161481
H	7.566593	3.286471	1.554667
C	4.771911	-1.900048	-1.412002
C	6.170810	-2.060101	-1.511874
C	3.924015	-2.557118	-2.332668
C	6.712395	-2.880811	-2.515613
H	6.841019	-1.534978	-0.813890
C	4.471431	-3.382278	-3.329327
H	2.833451	-2.406693	-2.268346

C	5.865298	-3.545988	-3.420766
H	7.804623	-2.998177	-2.593551
H	3.806979	-3.890274	-4.045899
H	6.294662	-4.186699	-4.206925
C	3.916830	-2.013953	1.374374
C	3.467189	-1.457161	2.594445
C	4.201429	-3.392107	1.299089
C	3.302401	-2.273871	3.723412
H	3.243460	-0.379164	2.651073
C	4.021553	-4.209338	2.430873
H	4.562921	-3.828393	0.354381
C	3.571121	-3.654540	3.640965
H	2.958293	-1.833664	4.672572
H	4.242404	-5.286308	2.365479
H	3.434804	-4.296599	4.525154
Au	1.865809	-0.046219	-0.625122
H	0.093335	1.423589	-1.968130
H	-0.340333	1.264687	1.096105
H	0.038985	4.033296	-1.509348
P	-3.353171	-1.805536	0.100340
C	-3.556142	3.792535	1.127470
C	-4.125115	4.153331	-0.138306
C	-2.445227	2.955295	1.204081
C	-3.519997	3.595712	-1.311492
C	-1.811974	2.394759	0.037360
H	-1.997644	2.745518	2.189511
C	-2.409153	2.756240	-1.222349
H	-3.921841	3.822317	-2.307366
H	-1.946374	2.376734	-2.146813
C	-4.296131	-2.390174	-1.355793
C	-5.060876	-3.575352	-1.303564
C	-4.199491	-1.662720	-2.563699
C	-5.719627	-4.029540	-2.458604
H	-5.149059	-4.140333	-0.362379
C	-4.853863	-2.128695	-3.715268
H	-3.610864	-0.730672	-2.598467
C	-5.614399	-3.311263	-3.663219
H	-6.320611	-4.951121	-2.415230
H	-4.775025	-1.561946	-4.655976
H	-6.133024	-3.671701	-4.565259
C	-4.134166	-2.522480	1.588045
C	-3.783112	-3.814597	2.039063
C	-5.133491	-1.783212	2.257905
C	-4.439467	-4.362879	3.153626
H	-2.993430	-4.384894	1.524737
C	-5.786657	-2.340829	3.368729
H	-5.389878	-0.768824	1.909967
C	-5.440580	-3.629257	3.816009
H	-4.165101	-5.368607	3.508155
H	-6.564797	-1.764249	3.892458
H	-5.950379	-4.062037	4.690901
C	-1.677054	-2.547835	-0.029093
C	-1.236729	-3.176448	-1.211565
C	-0.791436	-2.391263	1.063104
C	0.082988	-3.657090	-1.292407
H	-1.918927	-3.292976	-2.067769
C	0.517783	-2.884836	0.977909
H	-1.127237	-1.878711	1.979475
C	0.955210	-3.517390	-0.201352
H	0.427223	-4.146284	-2.216894
H	1.210873	-2.764711	1.823419
H	1.988569	-3.889427	-0.264006
Au	-2.985442	0.457375	0.130374
H	-3.985285	4.176667	2.061700
N	-5.209153	4.989323	-0.221155
C	-5.783746	5.571215	0.988260
H	-6.642140	6.210466	0.714519
H	-6.153530	4.787672	1.686058
H	-5.048000	6.202999	1.534087
C	-5.756787	5.355822	-1.523708
H	-6.100013	4.462458	-2.090745
H	-6.629170	6.018322	-1.380615
H	-5.014103	5.899686	-2.149282
C	4.017972	6.720917	-0.444857

H	4.933828	7.268172	-0.152110
H	4.146927	6.327599	-1.479422
H	3.156143	7.426383	-0.432209
O	3.856735	5.674209	0.505353

[(PPh_3)Au(*para*-aniline-alkene)] Markovnikov

-1960.98644672 A.U.

P	2.595258	-0.535862	-0.031544
H	-2.054055	-2.363135	-0.231667
C	-1.750944	-1.314586	-0.446439
C	-2.524581	-0.368590	0.515877
C	-1.641157	1.689543	-0.757039
C	-2.071939	1.087993	0.442477
C	-1.187766	3.022517	-0.801985
C	-2.055599	1.886039	1.609088
C	-1.153771	3.786239	0.382480
H	-0.842152	3.437834	-1.758907
C	-1.601939	3.209223	1.590558
H	-2.392677	1.446549	2.562474
H	-1.565224	3.817293	2.507184
C	2.862949	0.997718	0.953066
C	4.037466	1.205411	1.710395
C	1.870125	2.002694	0.906894
C	4.222561	2.416261	2.399301
H	4.805461	0.417177	1.763650
C	2.064874	3.214752	1.591963
H	0.937027	1.835469	0.343466
C	3.240725	3.422151	2.335591
H	5.138334	2.573002	2.991437
H	1.286890	3.992609	1.545881
H	3.388479	4.369847	2.877827
C	3.482165	-0.230164	-1.618146
C	4.446733	0.787534	-1.777414
C	3.171982	-1.075759	-2.707357
C	5.101155	0.947860	-3.011761
H	4.683577	1.459074	-0.937134
C	3.833400	-0.915242	-3.935434
H	2.400198	-1.854480	-2.587589
C	4.798977	0.096805	-4.089549
H	5.851043	1.746062	-3.131340
H	3.586339	-1.577999	-4.779803
H	5.312083	0.227011	-5.055636
C	3.622720	-1.805884	0.819871
C	3.027139	-2.514310	1.887603
C	4.960112	-2.077458	0.459992
C	3.769196	-3.471601	2.597711
H	1.974425	-2.316027	2.150021
C	5.696338	-3.041899	1.170852
H	5.423877	-1.536027	-0.379952
C	5.104447	-3.736375	2.240714
H	3.299256	-4.021289	3.428511
H	6.739179	-3.252392	0.884756
H	5.683347	-4.492760	2.794144
Au	0.319599	-1.059044	-0.283160
H	-2.067407	-1.123186	-1.498185
H	-2.301669	-0.708012	1.551407
H	-1.624695	1.097959	-1.684911
C	-6.134192	-1.678898	0.885887
C	-6.859366	-0.942133	-0.094351
C	-4.762447	-1.464162	1.077727
C	-6.129198	0.023029	-0.846610
C	-4.036230	-0.517439	0.326599
H	-4.235952	-2.058458	1.844386
C	-4.757881	0.219099	-0.634975
H	-6.633104	0.637917	-1.605335
H	-4.236780	0.984636	-1.232406
H	-6.639730	-2.427660	1.511505
N	-8.219914	-1.151657	-0.303751
C	-8.944038	-2.085072	0.536660
H	-10.001946	-2.128117	0.215045
H	-8.531006	-3.118042	0.464335
H	-8.927887	-1.796129	1.615719
C	-8.938988	-0.328569	-1.256459
H	-8.520699	-0.420776	-2.285621

H	-9.996778	-0.650715	-1.298682
H	-8.923809	0.755748	-0.987988
C	-0.146749	5.671542	-0.699193
H	0.196320	6.682564	-0.406509
H	0.718534	5.100466	-1.110344
H	-0.919643	5.770811	-1.496206
O	-0.668083	5.068441	0.474748

[(PPh_3)Au(*ortho*-aniline)+(PPh_3)Au(alkene)]$^+$ adduct

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P	3.497190	-1.536971	-0.063676
H	-1.078296	0.047299	-1.474951
C	-0.181380	0.685945	-1.504717
C	0.188896	1.352357	-0.320110
C	1.867230	3.012113	-1.240135
C	1.168668	2.417972	-0.151430
C	2.879490	3.935571	-1.020477
C	1.512015	2.822896	1.161236
C	3.243046	4.297217	0.306195
H	3.433549	4.392713	-1.853242
C	2.542827	3.742713	1.400603
H	0.959969	2.394099	2.011184
H	2.785231	4.025245	2.433637
C	4.919161	-0.409208	-0.392567
C	6.169288	-0.871982	-0.857146
C	4.724194	0.976630	-0.181152
C	7.217027	0.039686	-1.076039
H	6.331569	-1.938430	-1.070167
C	5.777975	1.879135	-0.392557
H	3.740388	1.365594	0.124545
C	7.028173	1.411429	-0.835878
H	8.187208	-0.329411	-1.443347
H	5.610308	2.955046	-0.228943
H	7.852389	2.120329	-1.010775
C	3.893049	-3.190991	-0.725323
C	4.992096	-3.942392	-0.241801
C	3.072228	-3.729129	-1.741342
C	5.259123	-5.214262	-0.773654
H	5.637098	-3.539179	0.554853
C	3.345894	-5.001996	-2.268572
H	2.213294	-3.147305	-2.113295
C	4.437342	-5.744726	-1.785360
H	6.114009	-5.795317	-0.394429
H	2.703455	-5.414576	-3.061799
H	4.650352	-6.742877	-2.198602
C	3.339109	-1.686511	1.771352
C	3.011642	-0.513230	2.491089
C	3.391024	-2.923472	2.446694
C	2.757491	-0.578736	3.868966
H	2.927214	0.454611	1.971663
C	3.128163	-2.982665	3.827585
H	3.616445	-3.851732	1.901665
C	2.812663	-1.814300	4.541253
H	2.503135	0.340138	4.419923
H	3.166812	-3.953684	4.345177
H	2.603760	-1.866042	5.620993
Au	1.525840	-0.554803	-0.804433
H	0.098394	1.079507	-2.496226
H	-0.340217	1.048584	0.600991
H	1.621510	2.722408	-2.272614
P	-3.619390	-1.014796	0.231061
C	-1.059040	4.853292	-0.698246
C	-1.919735	3.727657	-0.686556
C	-0.562265	5.393092	0.498349
C	-2.266490	3.112486	0.561723
C	-0.932420	4.831131	1.730977
H	0.108301	6.266268	0.462339
C	-1.777742	3.704989	1.748802
H	-0.558499	5.260588	2.674203
H	-2.041245	3.254236	2.720049
C	-2.045524	-1.973275	0.357260
C	-1.623078	-2.881053	-0.635911
C	-1.238575	-1.760602	1.499869
C	-0.413314	-3.581881	-0.476196

H	-2.239809	-3.043106	-1.533645
C	-0.037644	-2.468970	1.660247
H	-1.557209	-1.033103	2.265004
C	0.374007	-3.383706	0.671116
H	-0.086113	-4.292016	-1.251643
H	0.589676	-2.299065	2.548523
H	1.318394	-3.935564	0.789924
C	-4.199474	-1.324498	-1.487704
C	-5.016268	-2.428244	-1.814225
C	-3.770159	-0.441580	-2.506390
C	-5.389519	-2.652626	-3.150924
H	-5.367454	-3.109742	-1.023289
C	-4.141967	-0.676822	-3.840121
H	-3.158458	0.440699	-2.249607
C	-4.950582	-1.781866	-4.164415
H	-6.031908	-3.511543	-3.400678
H	-3.808941	0.015489	-4.629428
H	-5.248609	-1.959144	-5.209667
C	-4.791786	-1.886960	1.335452
C	-4.648699	-3.254597	1.658197
C	-5.882689	-1.150127	1.847759
C	-5.601149	-3.880194	2.480483
H	-3.790784	-3.827820	1.271515
C	-6.833086	-1.783887	2.664825
H	-5.978692	-0.077720	1.609657
C	-6.693296	-3.147767	2.980498
H	-5.488848	-4.946085	2.733741
H	-7.682504	-1.207788	3.063530
H	-7.436504	-3.641569	3.625934
Au	-3.120173	1.240619	0.563758
H	-0.779314	5.331458	-1.648071
N	-2.418832	3.172639	-1.905550
C	-1.711255	3.510746	-3.131958
H	-2.025162	2.813047	-3.936936
H	-1.912409	4.550330	-3.499049
H	-0.618132	3.404025	-2.987946
C	-3.873911	3.247770	-2.090103
H	-4.394591	3.001082	-1.145986
H	-4.196016	4.270041	-2.412258
H	-4.201533	2.520829	-2.862833
C	4.706716	5.588833	1.703408
H	5.545687	6.288688	1.535173
H	3.889788	6.120211	2.239475
H	5.060889	4.734612	2.322792
O	4.285574	5.155730	0.408345

[(PPh_3)Au(*ortho*-aniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3132.50765533 A.U.

P	3.456302	-1.632232	-0.144005
H	-0.959782	0.257816	-1.432246
C	-0.030580	0.846615	-1.300457
C	-0.040288	1.667390	-0.065631
C	1.847489	3.207600	-0.803904
C	1.140529	2.532255	0.221452
C	3.015703	3.918777	-0.532429
C	1.636804	2.636939	1.537142
C	3.526256	3.973617	0.787652
H	3.576743	4.428157	-1.329777
C	2.821169	3.333736	1.831223
H	1.098557	2.129026	2.353912
H	3.186618	3.364366	2.866698
C	4.973257	-0.604774	-0.367292
C	6.239108	-1.140493	-0.687046
C	4.830936	0.794490	-0.206699
C	7.350495	-0.288825	-0.814641
H	6.366207	-2.219407	-0.857583
C	5.947649	1.638021	-0.320935
H	3.839676	1.236847	-0.016306
C	7.210445	1.096534	-0.621754
H	8.332956	-0.715229	-1.070948
H	5.820890	2.723724	-0.187504
H	8.085276	1.757947	-0.722121
C	3.767834	-3.303611	-0.821466
C	4.781977	-4.154779	-0.319715

C	2.938564	-3.755215	-1.872856
C	4.964492	-5.433045	-0.872169
H	5.423208	-3.825755	0.513202
C	3.125904	-5.035476	-2.420772
H	2.140604	-3.096528	-2.253753
C	4.138591	-5.873795	-1.922839
H	5.755237	-6.090244	-0.477942
H	2.477663	-5.379067	-3.241915
H	4.284978	-6.876980	-2.352853
C	3.258650	-1.831452	1.685711
C	3.056011	-0.651968	2.440464
C	3.146943	-3.085457	2.321717
C	2.757032	-0.729942	3.808739
H	3.108284	0.334172	1.953322
C	2.843433	-3.157339	3.694079
H	3.278840	-4.016697	1.751044
C	2.647216	-1.983401	4.440587
H	2.601526	0.196011	4.384798
H	2.756165	-4.142249	4.178794
H	2.406962	-2.044130	5.513451
Au	1.574347	-0.474807	-0.894383
H	0.191334	1.414144	-2.226751
H	-0.347643	1.095618	0.827418
H	1.483088	3.147898	-1.839904
P	-3.868158	-0.868644	0.277227
C	-0.961604	5.113988	-0.941185
C	-1.418968	3.779675	-1.180010
C	-0.823318	5.616142	0.349068
C	-1.650128	2.904112	-0.028301
C	-1.117984	4.820603	1.484561
H	-0.486959	6.656977	0.481131
C	-1.519739	3.511685	1.280507
H	-1.012996	5.231788	2.499593
H	-1.684433	2.867626	2.160780
C	-2.340498	-1.902381	0.368033
C	-1.993382	-2.832218	-0.632509
C	-1.448074	-1.657666	1.439607
C	-0.763455	-3.512522	-0.557350
H	-2.678109	-3.026208	-1.472477
C	-0.228938	-2.345835	1.514370
H	-1.711288	-0.920701	2.216732
C	0.114645	-3.273622	0.511469
H	-0.489366	-4.233651	-1.343118
H	0.466893	-2.149685	2.344243
H	1.076780	-3.804641	0.560675
C	-4.817544	-1.497885	-1.159160
C	-5.916981	-2.368532	-1.007461
C	-4.407790	-1.099550	-2.452494
C	-6.597527	-2.837683	-2.144762
H	-6.246910	-2.675519	-0.002811
C	-5.084744	-1.581144	-3.583634
H	-3.552775	-0.413940	-2.568967
C	-6.182308	-2.448829	-3.430343
H	-7.459918	-3.511439	-2.023172
H	-4.760374	-1.271736	-4.589466
H	-6.719442	-2.818625	-4.317630
C	-4.834156	-1.260456	1.777837
C	-4.780180	-2.542107	2.369949
C	-5.670986	-0.261710	2.321927
C	-5.570300	-2.820612	3.497360
H	-4.116902	-3.316271	1.951845
C	-6.461213	-0.549973	3.446901
H	-5.694117	0.740976	1.863753
C	-6.411407	-1.827689	4.033407
H	-5.528248	-3.818393	3.961387
H	-7.113607	0.228740	3.871499
H	-7.027920	-2.049913	4.918455
Au	-3.013723	1.275788	0.075155
H	-0.749417	5.786694	-1.782288
N	-1.517318	3.340810	-2.485429
C	-0.934663	4.122962	-3.575358
H	-0.802112	3.461846	-4.454197
H	-1.582459	4.976359	-3.883801
H	0.062131	4.515680	-3.297244

C	-2.466718	2.338438	-2.958605
H	-3.026962	1.901230	-2.105732
H	-3.199321	2.807378	-3.653921
H	-1.951989	1.511394	-3.490673
C	5.308621	4.678290	2.229444
H	6.249382	5.247772	2.113157
H	4.660535	5.197859	2.970387
H	5.544451	3.655134	2.601011
O	4.705022	4.637807	0.938491

[(PPh_3)Au(*ortho*-aniline-alkene)Au(PPh_3)]$^+$ Intermediate Markovnikov

-3132.52781657 A.U.

P	3.507495	-1.436543	-0.137380
H	-1.074001	0.322211	-0.971928
C	-0.129560	0.911052	-0.955673
C	-0.165757	1.922319	0.216625
C	1.591169	3.513420	-0.794112
C	1.121190	2.744727	0.297046
C	2.831584	4.154780	-0.744542
C	1.939603	2.656016	1.439302
C	3.651785	4.041515	0.402952
H	3.207774	4.740097	-1.597130
C	3.193918	3.290441	1.506677
H	1.614084	2.035864	2.291299
H	3.806642	3.177250	2.411665
C	4.960983	-0.433780	-0.669789
C	6.236846	-0.995835	-0.889977
C	4.778835	0.962928	-0.802129
C	7.320006	-0.165501	-1.223739
H	6.390016	-2.083091	-0.813188
C	5.870438	1.789859	-1.118258
H	3.780269	1.408529	-0.659948
C	7.141272	1.226187	-1.328891
H	8.311660	-0.610327	-1.401737
H	5.717626	2.877366	-1.197441
H	7.995518	1.872209	-1.586040
C	3.774164	-3.154890	-0.719027
C	4.721301	-4.029167	-0.136867
C	2.985008	-3.603764	-1.802013
C	4.873109	-5.334003	-0.635549
H	5.332077	-3.695162	0.717015
C	3.144380	-4.907736	-2.299557
H	2.237100	-2.923296	-2.241529
C	4.086513	-5.773986	-1.716150
H	5.610250	-6.011655	-0.177062
H	2.528884	-5.250107	-3.146262
H	4.208647	-6.797585	-2.103687
C	3.641208	-1.476657	1.705198
C	3.943984	-0.270704	2.377200
C	3.294372	-2.618509	2.460378
C	3.901178	-0.211860	3.779179
H	4.205089	0.630679	1.801484
C	3.256348	-2.554725	3.864722
H	3.054972	-3.566623	1.955327
C	3.556353	-1.351985	4.528018
H	4.142418	0.733273	4.291243
H	2.993762	-3.454782	4.442823
H	3.527786	-1.305146	5.627831
Au	1.502443	-0.362144	-0.684722
H	-0.048109	1.439684	-1.925636
H	-0.175100	1.316319	1.148232
H	0.971081	3.581569	-1.699152
P	-3.641924	-1.100689	0.109148
C	-2.915874	4.661708	-0.275452
C	-1.938883	3.712351	-0.645461
C	-3.467058	4.725597	1.020490
C	-1.419132	2.815058	0.355260
C	-3.045265	3.818481	1.992672
H	-4.234506	5.479571	1.253688
C	-2.029796	2.870445	1.663101
H	-3.453279	3.841956	3.014170
H	-1.518351	2.345074	2.490559
C	-2.100712	-2.090990	0.223177
C	-1.755162	-3.042904	-0.761400

C	-1.240749	-1.876625	1.324456
C	-0.555378	-3.765272	-0.641299
H	-2.412540	-3.214258	-1.627474
C	-0.049013	-2.606552	1.440231
H	-1.492472	-1.119968	2.085462
C	0.295168	-3.550260	0.455493
H	-0.277421	-4.495666	-1.416749
H	0.629214	-2.417841	2.285760
H	1.241833	-4.106605	0.526106
C	-4.189281	-1.157584	-1.638102
C	-5.526703	-1.463723	-1.967241
C	-3.267418	-0.820335	-2.657545
C	-5.937684	-1.431418	-3.311507
H	-6.246823	-1.729085	-1.177522
C	-3.687605	-0.793336	-3.995603
H	-2.219016	-0.592808	-2.406783
C	-5.022919	-1.095186	-4.324353
H	-6.981041	-1.673581	-3.566420
H	-2.966306	-0.535761	-4.786733
H	-5.349704	-1.071731	-5.375582
C	-4.928192	-1.940557	1.096254
C	-4.961642	-3.350977	1.165833
C	-5.917944	-1.171759	1.746095
C	-5.990304	-3.984658	1.881241
H	-4.181626	-3.950303	0.669625
C	-6.946565	-1.814673	2.454749
H	-5.877565	-0.070681	1.699080
C	-6.982304	-3.219052	2.522180
H	-6.015978	-5.083748	1.941373
H	-7.718617	-1.215826	2.962084
H	-7.785404	-3.721306	3.083743
Au	-3.120215	1.036626	0.782291
H	-3.279386	5.365326	-1.039345
N	-1.460672	3.645409	-1.984018
C	-1.267701	4.919931	-2.672036
H	-0.644129	4.746536	-3.574140
H	-2.217352	5.402112	-3.018055
H	-0.728039	5.627723	-2.012386
C	-2.186089	2.672749	-2.807995
H	-2.371496	1.748350	-2.233425
H	-3.177503	3.070616	-3.145504
H	-1.590560	2.409565	-3.707237
C	5.773855	4.499431	1.415034
H	6.687800	5.058480	1.140062
H	5.365355	4.919402	2.362038
H	6.036101	3.427547	1.571245
O	4.865770	4.659493	0.330513

[(PPh_3)Au(*ortho*-aniline-alkene)] Markovnikov

-1960.97929492 A.U.

P	2.211017	-0.548736	-0.024482
H	-2.375423	-2.668143	0.022902
C	-2.063226	-1.636676	-0.254330
C	-2.720594	-0.601279	0.701781
C	-2.400785	1.460954	-0.810063
C	-2.175206	0.802934	0.420947
C	-1.755837	2.663857	-1.118249
C	-1.296209	1.415538	1.334363
C	-0.834181	3.233923	-0.210360
H	-1.913873	3.165820	-2.085346
C	-0.614013	2.609041	1.034202
H	-1.085160	0.918467	2.295043
H	0.109489	3.005875	1.760247
C	2.640591	0.643308	-1.359001
C	3.924052	0.756954	-1.931456
C	1.618722	1.544423	-1.734127
C	4.182571	1.780799	-2.861957
H	4.722500	0.053553	-1.646237
C	1.889722	2.579712	-2.641384
H	0.610846	1.441368	-1.301418
C	3.173426	2.698117	-3.207339
H	5.184261	1.866491	-3.312656
H	1.091657	3.296770	-2.888634
H	3.387876	3.506315	-3.924738

C	3.636040	-1.703579	0.080961
C	4.817861	-1.391332	0.788186
C	3.528466	-2.938938	-0.595127
C	5.885234	-2.305206	0.807633
H	4.898533	-0.434612	1.328884
C	4.601181	-3.845851	-0.577431
H	2.593002	-3.186321	-1.124293
C	5.779397	-3.530045	0.123316
H	6.804426	-2.060636	1.363412
H	4.512375	-4.808524	-1.105133
H	6.616811	-4.245499	0.143084
C	2.334806	0.513508	1.484415
C	3.008620	1.753107	1.476357
C	1.670695	0.091100	2.656898
C	3.010379	2.563246	2.625394
H	3.516435	2.094562	0.560883
C	1.676710	0.901599	3.803531
H	1.120647	-0.864264	2.655104
C	2.340005	2.142801	3.787705
H	3.531413	3.533752	2.608064
H	1.145889	0.569852	4.709774
H	2.331680	2.784293	4.683124
Au	0.016155	-1.360186	-0.206741
H	-2.391472	-1.449600	-1.297045
H	-2.358062	-0.852456	1.721420
H	-3.065089	0.978690	-1.541262
C	-6.584656	-0.559622	0.077819
C	-5.202878	-0.609288	-0.220412
C	-7.057820	-0.522593	1.397229
C	-4.253526	-0.626557	0.841879
C	-6.133024	-0.550530	2.452552
H	-8.140550	-0.479526	1.597347
C	-4.761613	-0.604086	2.163049
H	-6.475325	-0.526034	3.499508
H	-4.038029	-0.610484	2.995686
H	-7.306032	-0.555915	-0.754494
N	-4.781387	-0.652398	-1.601547
C	-5.430159	0.318557	-2.477076
H	-4.867972	0.379415	-3.434478
H	-6.493265	0.070090	-2.738331
H	-5.418200	1.320957	-2.004116
C	-4.820828	-2.001838	-2.164944
H	-4.315681	-2.712906	-1.484296
H	-5.868517	-2.368430	-2.334877
H	-4.287954	-2.019563	-3.140214
C	0.896940	4.841288	0.145128
H	1.340816	5.688838	-0.411941
H	0.550521	5.206490	1.140100
H	1.676554	4.061204	0.305876
O	-0.172767	4.353568	-0.648867

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ TS anti-Markovnikov

-3132.50511916 A.U.

P	-4.271528	-0.451402	-0.171533
H	0.410912	-0.152573	-0.063724
C	-0.007663	0.862845	0.073301
C	0.217128	1.705657	-1.078227
C	1.014398	0.599073	2.341565
C	0.255239	1.380460	1.445972
C	1.401217	1.078599	3.603963
C	-0.145266	2.672268	1.874819
C	1.012841	2.377318	4.003972
H	2.007202	0.434254	4.256322
C	0.224487	3.164875	3.126937
H	-0.752346	3.301508	1.204723
H	-0.080743	4.166843	3.464150
C	-5.513713	0.637734	0.618597
C	-6.625379	0.105598	1.308090
C	-5.357695	2.036562	0.499725
C	-7.578722	0.973493	1.867273
H	-6.740956	-0.984983	1.412501
C	-6.317135	2.896677	1.057487
H	-4.477029	2.446460	-0.022050
C	-7.426990	2.366141	1.740583

H	-8.443908	0.558842	2.407732
H	-6.193802	3.987002	0.965918
H	-8.174848	3.042602	2.183091
C	-4.366005	-2.047911	0.732727
C	-4.980201	-3.191863	0.181713
C	-3.748721	-2.120464	2.002647
C	-4.969684	-4.403068	0.897553
H	-5.456332	-3.141260	-0.809955
C	-3.751971	-3.329125	2.715073
H	-3.249558	-1.231200	2.422602
C	-4.356827	-4.473716	2.160716
H	-5.444172	-5.296647	0.462926
H	-3.272496	-3.381275	3.705187
H	-4.349289	-5.424391	2.716340
C	-4.888906	-0.810153	-1.860788
C	-6.254442	-0.690615	-2.197121
C	-3.960488	-1.256131	-2.828517
C	-6.685423	-1.027240	-3.492155
H	-6.980349	-0.329886	-1.451371
C	-4.399433	-1.596689	-4.117694
H	-2.891534	-1.323838	-2.566629
C	-5.762117	-1.482975	-4.450129
H	-7.750497	-0.929925	-3.754264
H	-3.673862	-1.943024	-4.870249
H	-6.104778	-1.743435	-5.463742
Au	-2.087344	0.350859	-0.130016
H	-0.090648	2.763406	-1.058242
H	0.166688	1.230540	-2.070776
H	1.328011	-0.409126	2.032915
P	3.356235	-1.843491	-0.247340
C	2.212752	4.234938	-2.761756
C	2.210673	5.174964	-1.676505
C	2.295603	2.869386	-2.520256
C	2.312602	4.645204	-0.348425
C	2.350047	2.309294	-1.197631
H	2.287134	2.186927	-3.386573
C	2.393260	3.274348	-0.129565
H	2.335377	5.316377	0.520464
H	2.473502	2.920574	0.909784
C	4.013724	-2.139889	1.441792
C	4.360627	-3.438736	1.875456
C	4.124923	-1.048846	2.331871
C	4.799968	-3.642864	3.193622
H	4.294622	-4.290854	1.180338
C	4.561360	-1.261081	3.650834
H	3.866817	-0.033200	1.990450
C	4.896537	-2.556322	4.083343
H	5.073447	-4.655971	3.527470
H	4.650557	-0.405461	4.338754
H	5.244831	-2.720571	5.115146
C	4.279083	-2.951420	-1.375840
C	3.888445	-4.291006	-1.596299
C	5.429714	-2.436419	-2.012838
C	4.656691	-5.111528	-2.439240
H	2.977795	-4.687321	-1.118847
C	6.194707	-3.264295	-2.850594
H	5.716763	-1.383709	-1.854059
C	5.809913	-4.600868	-3.062625
H	4.351316	-6.155361	-2.612420
H	7.091499	-2.861761	-3.346713
H	6.408284	-5.246809	-3.724066
C	1.629547	-2.499115	-0.212324
C	0.973260	-2.841715	0.988175
C	0.901377	-2.485153	-1.426273
C	-0.399608	-3.150331	0.975132
H	1.532004	-2.858250	1.937146
C	-0.461885	-2.814534	-1.434055
H	1.405905	-2.202337	-2.364735
C	-1.119349	-3.137345	-0.231180
H	-0.916840	-3.399086	1.914120
H	-1.018143	-2.813621	-2.384406
H	-2.192196	-3.379722	-0.230435
Au	3.066653	0.393741	-0.829772
H	2.157596	4.586267	-3.800937

N	2.119176	6.525629	-1.903198
C	2.048037	7.042646	-3.266416
H	1.968044	8.144224	-3.236605
H	2.954519	6.782173	-3.856901
H	1.158886	6.651542	-3.808666
C	2.134991	7.462785	-0.784532
H	3.085807	7.406010	-0.209092
H	2.031525	8.493588	-1.168631
H	1.294532	7.275844	-0.080170
C	2.118403	2.213169	6.120443
H	1.608940	1.275692	6.441138
H	3.118213	1.954065	5.701055
H	2.258246	2.866303	7.002211
O	1.332690	2.952433	5.194512

[(PPh_3)Au(*para*-aniline-alkene)Au(PPh_3)]$^+$ Intermediate anti-Markovnikov

-3132.54444487 A.U.

P	-4.419372	0.010575	-0.454493
H	0.260936	0.346486	-0.509388
C	-0.199580	1.353480	-0.361215
C	0.417122	2.283456	-1.431036
C	0.338913	0.762682	2.044152
C	0.023191	1.744147	1.078325
C	0.560452	1.078574	3.397347
C	-0.091765	3.081110	1.540213
C	0.472794	2.421075	3.825080
H	0.806029	0.269396	4.100004
C	0.133879	3.418205	2.878806
H	-0.364193	3.879733	0.831390
H	0.048822	4.458275	3.228899
C	-5.708344	1.258774	-0.067655
C	-6.807426	0.972447	0.771042
C	-5.588892	2.534648	-0.662729
C	-7.785591	1.955435	1.000111
H	-6.895300	-0.015893	1.249563
C	-6.572522	3.509876	-0.433072
H	-4.716925	2.760834	-1.298807
C	-7.671282	3.220859	0.397036
H	-8.641286	1.731605	1.656285
H	-6.476862	4.503671	-0.897669
H	-8.438678	3.988968	0.581292
C	-4.536225	-1.218620	0.914436
C	-5.177828	-2.467148	0.775687
C	-3.935253	-0.872025	2.147326
C	-5.226662	-3.355726	1.866369
H	-5.639024	-2.749637	-0.183520
C	-3.995787	-1.758267	3.233427
H	-3.407726	0.091003	2.249584
C	-4.641692	-3.001818	3.095422
H	-5.727923	-4.329750	1.752993
H	-3.528171	-1.479657	4.190599
H	-4.685830	-3.698781	3.947017
C	-5.025967	-0.864695	-1.951265
C	-6.405006	-1.037261	-2.203816
C	-4.077532	-1.399709	-2.850992
C	-6.825507	-1.754788	-3.336198
H	-7.150746	-0.603635	-1.518580
C	-4.503693	-2.119262	-3.979923
H	-3.003015	-1.228816	-2.670805
C	-5.877409	-2.299862	-4.221548
H	-7.901568	-1.884773	-3.531158
H	-3.760124	-2.531639	-4.679870
H	-6.211825	-2.858843	-5.109535
Au	-2.228216	0.830417	-0.552115
H	0.030062	3.320287	-1.326942
H	0.078988	1.943096	-2.431008
H	0.393195	-0.290300	1.728825
P	2.884541	-1.822444	0.127610
C	3.990413	2.575141	-2.887494
C	4.726614	3.195875	-1.827160
C	2.664847	2.173906	-2.706060
C	4.049786	3.364260	-0.575371
C	1.955076	2.349682	-1.463161
H	2.118935	1.746126	-3.562965

C	2.724007	2.960389	-0.402928
H	4.562299	3.824519	0.279011
H	2.228904	3.152694	0.560961
C	3.782331	-1.865109	1.723999
C	4.588518	-2.964872	2.087211
C	3.599667	-0.789616	2.623347
C	5.202788	-2.988647	3.351705
H	4.740280	-3.799962	1.385209
C	4.209279	-0.828019	3.886814
H	2.970745	0.071001	2.341675
C	5.011280	-1.925595	4.252260
H	5.835580	-3.844612	3.633424
H	4.060100	0.009849	4.586010
H	5.494621	-1.949769	5.241472
C	3.675282	-3.047508	-0.973859
C	3.253856	-4.395279	-0.975939
C	4.749785	-2.636744	-1.792831
C	3.915386	-5.328122	-1.792569
H	2.407765	-4.710924	-0.344820
C	5.408074	-3.576555	-2.601646
H	5.059485	-1.578401	-1.797961
C	4.991552	-4.920917	-2.601670
H	3.586076	-6.378824	-1.798212
H	6.245688	-3.257786	-3.241286
H	5.505487	-5.654872	-3.241839
C	1.189765	-2.433766	0.486752
C	0.835174	-2.922631	1.762755
C	0.202614	-2.298950	-0.516959
C	-0.503744	-3.258712	2.030483
H	1.597459	-3.017371	2.551613
C	-1.130145	-2.636437	-0.238700
H	0.473245	-1.899072	-1.507746
C	-1.486326	-3.110722	1.036826
H	-0.784230	-3.627279	3.029321
H	-1.901596	-2.513241	-1.013262
H	-2.535766	-3.354780	1.257745
Au	2.677252	0.293640	-0.732628
H	4.454821	2.404390	-3.867070
N	6.025131	3.604442	-1.999737
C	6.670914	3.467288	-3.301222
H	7.704958	3.851252	-3.239399
H	6.723834	2.403928	-3.624424
H	6.139936	4.043033	-4.092144
C	6.740252	4.259633	-0.908875
H	6.800097	3.608172	-0.009448
H	7.773234	4.483150	-1.230581
H	6.259759	5.218684	-0.611509
C	1.018180	1.892452	6.092791
H	0.212488	1.133640	6.228162
H	1.969203	1.358976	5.855153
H	1.148412	2.449133	7.040191
O	0.685801	2.852132	5.103338

[(PPh_3)Au(*para*-aniline-alkene)] anti-Markovnikov

-1960.98069808 A.U.

P	2.908676	-0.257185	-0.031186
H	-1.812668	-0.936164	-1.262445
C	-1.522544	-0.561214	-0.254827
C	-2.178899	-1.509499	0.794822
C	-2.737895	1.502178	-1.142168
C	-1.994043	0.870035	-0.125594
C	-3.204595	2.825818	-1.021756
C	-1.739271	1.631481	1.046687
C	-2.939725	3.556449	0.154125
H	-3.782614	3.266359	-1.846686
C	-2.200205	2.942517	1.192197
H	-1.156231	1.172308	1.862905
H	-1.999815	3.525548	2.104529
C	3.643013	-0.853038	1.548337
C	4.716223	-0.197999	2.189596
C	3.103519	-2.031032	2.112296
C	5.252353	-0.727062	3.376702
H	5.129417	0.729602	1.762660
C	3.646464	-2.557400	3.295573

H	2.247402	-2.524256	1.622309
C	4.721889	-1.907140	3.928219
H	6.088300	-0.211100	3.875229
H	3.220765	-3.475060	3.731238
H	5.142611	-2.317296	4.860024
C	3.379425	1.521333	-0.136294
C	4.623928	1.939084	-0.657467
C	2.456518	2.484794	0.330867
C	4.946325	3.306545	-0.695594
H	5.338152	1.193685	-1.042653
C	2.786058	3.849591	0.291152
H	1.469493	2.165323	0.706452
C	4.030353	4.261918	-0.219227
H	5.917127	3.627375	-1.105762
H	2.058269	4.594223	0.649932
H	4.283429	5.333463	-0.255807
C	3.912707	-1.070641	-1.342106
C	5.168100	-1.665025	-1.091927
C	3.383442	-1.076928	-2.652627
C	5.890420	-2.249223	-2.147591
H	5.579630	-1.675729	-0.070153
C	4.112327	-1.656211	-3.703348
H	2.391309	-0.633329	-2.840173
C	5.366789	-2.242835	-3.452537
H	6.868725	-2.714344	-1.947054
H	3.694055	-1.658089	-4.722263
H	5.934588	-2.703415	-4.276493
Au	0.580501	-0.543822	-0.180231
H	-1.944179	-1.154451	1.821706
H	-1.725709	-2.519606	0.703931
H	-2.974387	0.936157	-2.058071
C	-5.632531	-2.655901	-0.464401
C	-6.518608	-1.689984	0.093036
C	-4.255177	-2.601299	-0.207223
C	-5.938537	-0.670948	0.902145
C	-3.680266	-1.603067	0.605728
H	-3.601636	-3.366551	-0.660607
C	-4.559037	-0.639356	1.145899
H	-6.565454	0.113002	1.349125
H	-4.148815	0.174370	1.765607
H	-6.015126	-3.463488	-1.103915
N	-7.892029	-1.740401	-0.141980
C	-8.427544	-2.721792	-1.064858
H	-9.528613	-2.621214	-1.113438
H	-8.027452	-2.607732	-2.102502
H	-8.203457	-3.762985	-0.737322
C	-8.743240	-0.669504	0.338699
H	-8.479715	0.325096	-0.098123
H	-9.795700	-0.887701	0.074920
H	-8.693002	-0.567276	1.446951
C	-4.107289	5.498394	-0.612256
H	-3.547207	5.596638	-1.572389
H	-5.068887	4.971851	-0.819890
H	-4.332386	6.511779	-0.226319
O	-3.346054	4.845913	0.387342

Using CH_2=CMePh as alkene:

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

-1520.24655048 A.U.

P	1.187372	0.135629	0.024695
H	-2.152673	-3.384497	-1.405906
C	-2.404087	-2.312360	-1.349603
C	-2.922595	-1.792372	-0.150418
C	-3.817004	0.338042	-1.214376
C	-3.508237	-0.421772	-0.055067
C	-4.296409	1.648709	-1.107947
C	-3.720467	0.177620	1.213476
C	-4.485848	2.234030	0.159055
H	-4.533706	2.217589	-2.019907
C	-4.200223	1.492364	1.318182
H	-3.491724	-0.375784	2.134882
H	-4.867436	3.263778	0.240082
H	-4.352166	1.938282	2.313044

C	0.715725	1.902424	-0.069683
C	1.676000	2.880570	-0.410345
C	-0.609384	2.285571	0.239759
C	1.307997	4.236496	-0.433763
H	2.706109	2.583502	-0.663098
C	-0.965924	3.642509	0.214717
H	-1.369388	1.527445	0.492323
C	-0.009335	4.618190	-0.121192
H	2.055463	4.998804	-0.702664
H	-2.001230	3.932790	0.450703
H	-0.293106	5.681828	-0.146198
C	2.637917	-0.096376	-1.061712
C	3.948191	-0.052155	-0.537770
C	2.430021	-0.271205	-2.448446
C	5.045929	-0.178005	-1.406463
H	4.110652	0.074338	0.544224
C	3.532763	-0.394522	-3.307572
H	1.405464	-0.312218	-2.854603
C	4.839821	-0.347593	-2.787050
H	6.068557	-0.146747	-0.999795
H	3.372048	-0.533490	-4.387781
H	5.703249	-0.450106	-3.462575
C	1.748778	-0.190597	1.734725
C	2.013486	0.862360	2.635762
C	1.947794	-1.533840	2.128397
C	2.481632	0.566017	3.928248
H	1.854298	1.908717	2.331604
C	2.420216	-1.818583	3.418335
H	1.735826	-2.354446	1.422624
C	2.686156	-0.768972	4.318656
H	2.687911	1.386044	4.633375
H	2.578578	-2.864094	3.724941
H	3.052278	-0.995050	5.332192
Au	-0.630641	-1.184960	-0.537988
H	-2.556616	-1.805405	-2.317026
H	-3.689890	-0.100785	-2.214758
C	-2.985607	-2.684960	1.070263
H	-2.485890	-2.231792	1.949826
H	-4.050008	-2.841290	1.347842
H	-2.520422	-3.669559	0.878278

[(PPh_3)Au(alkene)(*para*-aniline)]$^+$

-1886.24304009 A.U.

P	-0.055037	0.913010	-0.180609
H	1.418305	-3.839154	-1.277351
C	1.746213	-3.138405	-0.491378
C	2.604263	-2.073849	-0.843325
C	3.724550	-1.884045	1.428145
C	3.403415	-1.320350	0.168104
C	4.439468	-1.145152	2.383184
C	3.838277	0.000413	-0.107527
C	4.843025	0.173316	2.103188
H	4.691977	-1.606719	3.350562
C	4.538696	0.741504	0.853350
H	3.589325	0.471480	-1.068671
H	5.398094	0.754000	2.855973
H	4.843580	1.774085	0.623686
C	0.446534	1.527557	1.475549
C	0.071051	2.819164	1.915724
C	1.281376	0.729181	2.285954
C	0.528688	3.296739	3.154291
H	-0.580091	3.451075	1.291821
C	1.737169	1.214309	3.522467
H	1.591286	-0.272304	1.947633
C	1.360675	2.495806	3.959148
H	0.233486	4.301977	3.493242
H	2.393352	0.583084	4.140781
H	1.714758	2.874098	4.930870
C	-1.708239	1.665561	-0.477018
C	-2.034065	2.262782	-1.713814
C	-2.652997	1.674276	0.573828
C	-3.288909	2.870232	-1.891724
H	-1.302845	2.279295	-2.536212
C	-3.891097	2.309266	0.398063

H	-2.410447	1.201497	1.538458
C	-4.214608	2.905519	-0.834392
H	-3.533694	3.338883	-2.857539
H	-4.610352	2.338795	1.230674
H	-5.186956	3.404707	-0.967945
C	1.078006	1.738762	-1.377171
C	1.913373	2.811440	-1.001755
C	1.147187	1.225189	-2.692498
C	2.814242	3.355922	-1.933541
H	1.881511	3.205937	0.024850
C	2.038315	1.783216	-3.623743
H	0.513862	0.369431	-2.981500
C	2.879649	2.844870	-3.241952
H	3.472964	4.185200	-1.631958
H	2.085432	1.379238	-4.647018
H	3.589065	3.273441	-3.966750
Au	0.322501	-1.402111	-0.385209
H	1.721234	-3.532215	0.539095
H	3.433152	-2.920150	1.657030
C	-3.512288	-1.630246	-0.930631
C	-3.872861	-1.330650	0.422741
C	-2.431541	-2.461720	-1.216282
C	-3.025365	-1.833737	1.461677
C	-1.624105	-3.008895	-0.178746
H	-2.215980	-2.721194	-2.264735
C	-1.945450	-2.665837	1.164856
H	-3.239929	-1.609103	2.514401
H	-0.959193	-3.859862	-0.388234
H	-1.351472	-3.089299	1.990127
H	-4.103892	-1.229727	-1.763368
N	-5.001940	-0.602579	0.712085
C	-5.914351	-0.213476	-0.357255
H	-6.756156	0.359043	0.072089
H	-5.411201	0.441538	-1.101273
H	-6.332657	-1.098070	-0.888079
C	-5.378485	-0.360717	2.098397
H	-4.578179	0.179724	2.651136
H	-6.287955	0.266133	2.128063
H	-5.594521	-1.305433	2.647260
C	2.921670	-1.833356	-2.303531
H	2.896303	-0.760375	-2.571939
H	3.955549	-2.190822	-2.502700
H	2.224930	-2.376100	-2.970701

[(PPh_3)Au(alkene)(*ortho*-aniline)]$^+$

-1886.24727203 A.U.

P	-0.269129	1.071095	0.014700
H	0.763152	-3.330107	-2.316084
C	1.244387	-2.880402	-1.431467
C	2.110196	-1.775965	-1.611291
C	3.404556	-2.156738	0.547649
C	3.032265	-1.311093	-0.528052
C	4.217766	-1.681759	1.587602
C	3.515712	0.022225	-0.528642
C	4.672334	-0.350340	1.581284
H	4.506289	-2.360565	2.405288
C	4.316293	0.498135	0.518060
H	3.225211	0.712139	-1.333371
H	5.305334	0.022936	2.400911
H	4.659279	1.544033	0.504590
C	0.423497	1.375250	1.684345
C	0.201016	2.602305	2.354285
C	1.254680	0.398638	2.273550
C	0.793502	2.834724	3.605722
H	-0.438331	3.375366	1.899999
C	1.846786	0.639814	3.523586
H	1.452628	-0.551679	1.753692
C	1.614040	1.853252	4.193064
H	0.613781	3.788812	4.125180
H	2.496766	-0.128029	3.970071
H	2.074730	2.039028	5.175892
C	-1.944295	1.841510	0.001402
C	-2.489507	2.337342	-1.204055
C	-2.713497	1.904447	1.185408

C	-3.781835	2.888824	-1.221472
H	-1.903232	2.316743	-2.134775
C	-4.000268	2.468537	1.163596
H	-2.304282	1.520377	2.130386
C	-4.539073	2.959851	-0.038213
H	-4.193143	3.277807	-2.165820
H	-4.583648	2.525439	2.095895
H	-5.546680	3.403314	-0.052548
C	0.740383	2.092329	-1.146075
C	1.640880	3.081369	-0.697453
C	0.643811	1.814631	-2.528851
C	2.430190	3.783342	-1.625280
H	1.748282	3.290050	0.377278
C	1.420001	2.532492	-3.453106
H	-0.022424	1.008918	-2.880723
C	2.319955	3.515062	-3.001155
H	3.139205	4.546104	-1.267477
H	1.334754	2.311324	-4.528435
H	2.940503	4.068273	-3.722983
Au	0.026023	-1.176953	-0.629358
H	1.345653	-3.545428	-0.559456
H	3.071534	-3.205419	0.565044
C	-1.606265	-2.796646	0.446479
C	-2.770223	-1.944160	0.459508
C	-0.799321	-2.929173	1.612937
C	-3.032440	-1.219377	1.663503
C	-1.061835	-2.183645	2.763572
H	0.046737	-3.633876	1.588476
C	-2.193856	-1.338283	2.772802
H	-3.904406	-0.557920	1.724747
H	-0.416732	-2.266027	3.649847
H	-2.428199	-0.756591	3.678680
H	-1.477574	-3.533026	-0.359598
N	-3.577535	-1.829207	-0.647622
C	-3.132853	-2.395209	-1.909550
H	-3.869366	-2.169008	-2.700937
H	-2.140631	-1.970380	-2.216425
H	-3.021541	-3.499505	-1.856567
C	-4.676323	-0.866787	-0.657390
H	-4.315650	0.184383	-0.600157
H	-5.255923	-0.987283	-1.590564
H	-5.372173	-1.046224	0.188189
C	2.297467	-1.198123	-2.995837
H	2.358723	-0.094536	-2.995940
H	3.261765	-1.575963	-3.401197
H	1.484680	-1.504420	-3.681780

[(PPh_3)Au(*para*-aniline)+(PPh_3)Au(alkene)]$^+$ adduct

-3057.36962520 A.U.

P	-4.087940	-0.666735	0.050665
H	0.597909	-0.024522	0.835360
C	0.029210	0.922892	0.823861
C	0.156791	1.707170	-0.359471
C	-0.580148	3.843026	0.756900
C	-0.123697	3.140347	-0.396818
C	-0.859645	5.210220	0.710192
C	0.063174	3.893832	-1.590076
C	-0.655832	5.936444	-0.480568
H	-1.229126	5.721632	1.612475
C	-0.208115	5.266390	-1.633397
H	0.432068	3.400955	-2.499762
H	-0.866307	7.016495	-0.513483
H	-0.057648	5.820624	-2.572613
C	-5.244886	0.527272	-0.720119
C	-6.258525	0.098838	-1.606416
C	-5.128268	1.895366	-0.388004
C	-7.156640	1.036333	-2.143472
H	-6.337946	-0.963669	-1.886645
C	-6.031311	2.825296	-0.928050
H	-4.321944	2.230726	0.285280
C	-7.045912	2.396756	-1.803386
H	-7.945583	0.701816	-2.835001
H	-5.937061	3.891395	-0.669600
H	-7.750044	3.128435	-2.229386

C	-4.906669	-1.316384	1.556170
C	-6.297094	-1.566504	1.569810
C	-4.127241	-1.609331	2.697285
C	-6.896110	-2.117807	2.713892
H	-6.913602	-1.323528	0.690001
C	-4.733385	-2.162684	3.837733
H	-3.045856	-1.395390	2.691986
C	-6.115871	-2.419122	3.845775
H	-7.980410	-2.309050	2.723539
H	-4.123876	-2.386944	4.726901
H	-6.590555	-2.848553	4.741788
C	-3.991833	-2.076183	-1.122117
C	-3.476035	-1.819382	-2.413478
C	-4.331687	-3.392162	-0.748519
C	-3.309909	-2.873064	-3.324403
H	-3.200852	-0.791125	-2.700842
C	-4.149080	-4.446269	-1.662527
H	-4.734942	-3.597122	0.255491
C	-3.640554	-4.189630	-2.947537
H	-2.913445	-2.669086	-4.331194
H	-4.409818	-5.474226	-1.366608
H	-3.501215	-5.017584	-3.659854
Au	-1.966914	0.196646	0.433453
H	0.023167	1.438454	1.799127
H	-0.740571	3.299607	1.698473
P	3.288316	-2.009320	-0.018632
C	3.072491	4.557493	-0.814595
C	2.576636	5.187742	0.365717
C	3.366400	3.188662	-0.827423
C	2.446470	4.373800	1.531373
C	3.186802	2.355212	0.307273
H	3.745756	2.756218	-1.768855
C	2.743151	3.006963	1.488105
H	2.106151	4.809989	2.480223
H	2.611066	2.423474	2.414335
C	4.309987	-3.054493	1.087033
C	3.898951	-4.341623	1.501899
C	5.561379	-2.547613	1.501885
C	4.741596	-5.116059	2.316408
H	2.915827	-4.734405	1.196572
C	6.400642	-3.329887	2.312681
H	5.869971	-1.535174	1.192793
C	5.992355	-4.612910	2.719210
H	4.419047	-6.118212	2.639770
H	7.375317	-2.931397	2.634509
H	6.649624	-5.222302	3.359104
C	3.588934	-2.606948	-1.732412
C	3.944097	-3.945458	-2.006219
C	3.408985	-1.697377	-2.798984
C	4.109284	-4.368345	-3.335590
H	4.103149	-4.656994	-1.180953
C	3.567992	-2.128460	-4.126859
H	3.153071	-0.647365	-2.580095
C	3.918087	-3.463610	-4.396019
H	4.394232	-5.411409	-3.544421
H	3.430238	-1.414806	-4.954280
H	4.052613	-3.798930	-5.436384
C	1.544102	-2.507544	0.335455
C	1.089139	-2.463494	1.674728
C	0.633314	-2.816584	-0.697554
C	-0.253211	-2.744973	1.973283
H	1.792186	-2.212989	2.485735
C	-0.712430	-3.089450	-0.394123
H	0.977313	-2.853834	-1.743114
C	-1.156436	-3.058029	0.939614
H	-0.596385	-2.719067	3.019569
H	-1.418461	-3.332311	-1.201732
H	-2.208565	-3.283749	1.170087
Au	3.420987	0.320084	0.207601
H	3.230248	5.140234	-1.732078
N	2.219563	6.528703	0.374754
C	2.521272	7.361814	-0.779759
H	2.111983	8.376233	-0.617998
H	3.616854	7.452361	-0.967872

H	2.049516	6.951899	-1.697925
C	1.891030	7.178587	1.634665
H	2.751426	7.195668	2.344058
H	1.580995	8.221950	1.439646
H	1.043681	6.665429	2.136652
C	0.537207	1.000519	-1.640865
H	1.474774	1.430396	-2.046749
H	0.700253	-0.079016	-1.463557
H	-0.252212	1.119454	-2.412653

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3057.34845539 A.U.

P	-3.941777	-1.235281	0.018317
H	0.791193	-0.175441	0.789131
C	-0.004912	0.593848	0.841021
C	0.125047	1.586996	-0.276700
C	-1.437928	3.193240	0.951830
C	-0.830999	2.757942	-0.252801
C	-2.333499	4.273233	0.973490
C	-1.153405	3.468985	-1.433235
C	-2.640511	4.965378	-0.212595
H	-2.802010	4.571363	1.924864
C	-2.045953	4.554284	-1.417703
H	-0.700022	3.174728	-2.389604
H	-3.345609	5.811450	-0.197462
H	-2.283182	5.075380	-2.358881
C	-4.813652	-0.031529	-1.065335
C	-5.774290	-0.450138	-2.013743
C	-4.503235	1.342796	-0.940574
C	-6.427710	0.500484	-2.815888
H	-5.999464	-1.521778	-2.136703
C	-5.159028	2.286511	-1.747858
H	-3.733388	1.677739	-0.224938
C	-6.122984	1.867879	-2.682417
H	-7.175365	0.170475	-3.554125
H	-4.899240	3.351738	-1.646771
H	-6.634448	2.608381	-3.317373
C	-5.071616	-1.654703	1.400140
C	-6.473259	-1.701766	1.236885
C	-4.497491	-1.978661	2.649511
C	-7.289821	-2.078022	2.315841
H	-6.928761	-1.436793	0.270090
C	-5.319645	-2.360631	3.723079
H	-3.403383	-1.921887	2.776016
C	-6.715058	-2.410622	3.556680
H	-8.383117	-2.109428	2.187726
H	-4.868726	-2.612283	4.695686
H	-7.359842	-2.703783	4.399989
C	-3.795464	-2.769588	-0.983178
C	-3.140742	-2.684943	-2.234095
C	-4.191858	-4.027673	-0.484561
C	-2.895226	-3.848230	-2.978815
H	-2.815899	-1.703972	-2.617822
C	-3.930580	-5.191661	-1.230894
H	-4.702050	-4.100326	0.488826
C	-3.283055	-5.105178	-2.475356
H	-2.393947	-3.776287	-3.957035
H	-4.240508	-6.171994	-0.836440
H	-3.082364	-6.018010	-3.057498
Au	-1.848977	-0.388883	0.580223
H	0.018652	1.043085	1.853426
H	-1.218925	2.664994	1.889759
P	3.915085	-1.349396	-0.002172
C	1.729065	4.836203	-0.985442
C	1.312848	5.369151	0.284956
C	2.007275	3.488611	-1.112973
C	1.458480	4.520706	1.439323
C	1.893761	2.552030	-0.017987
H	2.256361	3.107585	-2.116862
C	1.730139	3.177057	1.275873
H	1.282960	4.916842	2.448018
H	1.723819	2.534950	2.172232
C	4.715804	-1.888119	1.558169
C	5.340404	-3.151110	1.659102

C	4.666029	-1.036479	2.683199
C	5.903297	-3.556558	2.879413
H	5.397241	-3.816295	0.783197
C	5.227994	-1.450383	3.903341
H	4.190594	-0.045278	2.596376
C	5.845811	-2.709123	4.001959
H	6.393770	-4.539642	2.954057
H	5.189126	-0.782337	4.777813
H	6.291417	-3.030469	4.956392
C	4.992265	-1.897116	-1.376864
C	4.942070	-3.212135	-1.892226
C	5.921659	-0.970198	-1.898472
C	5.825067	-3.594423	-2.915802
H	4.204213	-3.931992	-1.503370
C	6.804274	-1.361523	-2.918545
H	5.946136	0.059194	-1.503965
C	6.756835	-2.672331	-3.426674
H	5.783785	-4.618674	-3.318215
H	7.528467	-0.637356	-3.322929
H	7.446208	-2.975898	-4.230014
C	2.358113	-2.332510	-0.124760
C	1.705256	-2.784208	1.042579
C	1.708313	-2.446139	-1.375943
C	0.414177	-3.334262	0.957015
H	2.201366	-2.693804	2.021851
C	0.421928	-3.003440	-1.452196
H	2.209149	-2.091854	-2.291456
C	-0.233036	-3.440907	-0.286767
H	-0.093207	-3.675352	1.872543
H	-0.085569	-3.085966	-2.425294
H	-1.247172	-3.863249	-0.355081
Au	3.136821	0.843243	-0.038704
H	1.775752	5.482145	-1.872085
N	0.760671	6.608668	0.384655
C	0.524531	7.407193	-0.818566
H	0.019525	8.348617	-0.538832
H	1.476171	7.668616	-1.328373
H	-0.126266	6.858871	-1.534001
C	0.249265	7.087490	1.669521
H	1.061110	7.187745	2.421000
H	-0.210290	8.082064	1.531040
H	-0.525017	6.396121	2.067548
C	0.265092	0.917699	-1.648414
H	0.739440	1.558587	-2.414109
H	0.853946	-0.013295	-1.559416
H	-0.745677	0.637310	-2.016977

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ Intermediate Markovnikov
-3057.37164960 A.U.

P	4.786247	-0.710127	-0.167666
H	-0.192425	-0.545896	-1.085825
C	0.562143	0.260561	-0.921826
C	0.161466	1.113229	0.319075
C	1.457221	3.227033	-0.332620
C	1.274129	2.162682	0.580003
C	2.499166	4.154794	-0.171944
C	2.168033	2.069324	1.669707
C	3.388652	4.040007	0.912112
H	2.618779	4.971654	-0.901447
C	3.218178	2.990810	1.829824
H	2.084384	1.249522	2.395523
H	4.213398	4.759102	1.034671
H	3.913251	2.868121	2.674839
C	5.828570	0.541701	-1.017401
C	7.129528	0.268648	-1.487912
C	5.283904	1.839349	-1.156980
C	7.881895	1.292878	-2.091131
H	7.555502	-0.741831	-1.384737
C	6.046044	2.858061	-1.747761
H	4.265020	2.054260	-0.794856
C	7.344835	2.586343	-2.217844
H	8.896091	1.077145	-2.462371
H	5.617206	3.867923	-1.844659
H	7.939745	3.384743	-2.688754

C	5.631274	-2.319948	-0.396753
C	6.696175	-2.729265	0.435636
C	5.212707	-3.145088	-1.463559
C	7.340718	-3.954140	0.193847
H	7.017150	-2.089964	1.273736
C	5.865229	-4.365743	-1.703176
H	4.370071	-2.826227	-2.099450
C	6.928378	-4.770450	-0.875413
H	8.169492	-4.273690	0.845000
H	5.537893	-5.007627	-2.536013
H	7.435235	-5.730524	-1.060836
C	4.977147	-0.303725	1.621562
C	5.950489	0.601916	2.090585
C	4.066513	-0.884831	2.532982
C	6.009522	0.923834	3.458577
H	6.653545	1.070052	1.384293
C	4.130072	-0.561621	3.897161
H	3.294140	-1.579912	2.163528
C	5.099380	0.347949	4.361864
H	6.770129	1.634558	3.818315
H	3.415380	-1.015805	4.601551
H	5.144493	0.607530	5.431218
Au	2.527452	-0.440834	-0.704602
H	0.570998	0.886998	-1.841011
H	0.778216	3.331453	-1.193701
P	-4.335215	-1.331447	0.051074
C	-2.566723	3.785652	0.950297
C	-3.069097	4.091689	-0.362932
C	-1.656943	2.759629	1.159491
C	-2.586163	3.293210	-1.438749
C	-1.149203	1.932218	0.093585
H	-1.267431	2.601016	2.176187
C	-1.659820	2.252507	-1.215029
H	-2.912984	3.474442	-2.470255
H	-1.232402	1.739609	-2.090582
C	-4.285463	-2.443783	-1.403054
C	-5.458454	-3.028369	-1.925895
C	-3.026512	-2.742437	-1.972696
C	-5.366730	-3.913660	-3.014434
H	-6.440538	-2.792046	-1.487027
C	-2.944967	-3.630645	-3.055814
H	-2.111684	-2.276532	-1.569329
C	-4.114373	-4.215821	-3.577392
H	-6.281749	-4.368042	-3.425149
H	-1.964017	-3.861856	-3.499011
H	-4.048521	-4.907806	-4.431436
C	-6.082149	-0.835067	0.279217
C	-6.953400	-1.583522	1.100135
C	-6.563987	0.290742	-0.425343
C	-8.303384	-1.206929	1.206191
H	-6.577950	-2.455272	1.658923
C	-7.914891	0.656370	-0.317554
H	-5.875917	0.880593	-1.053597
C	-8.784731	-0.091697	0.497557
H	-8.982214	-1.788375	1.849199
H	-8.290631	1.532750	-0.868209
H	-9.842927	0.200058	0.585216
C	-3.889943	-2.369641	1.495023
C	-4.028569	-3.773854	1.450542
C	-3.431987	-1.739540	2.674183
C	-3.716841	-4.540002	2.586998
H	-4.372361	-4.268369	0.528357
C	-3.125803	-2.512366	3.805023
H	-3.308061	-0.644119	2.702044
C	-3.268197	-3.911822	3.762359
H	-3.821904	-5.635453	2.550997
H	-2.767636	-2.020422	4.722648
H	-3.021712	-4.516684	4.648917
Au	-2.879426	0.428205	-0.164381
H	-2.891131	4.376349	1.816987
N	-3.970297	5.107817	-0.561663
C	-4.393344	5.949873	0.553609
H	-5.130629	6.689509	0.192857
H	-4.879863	5.353330	1.356136

H	-3.542147	6.508639	1.003419
C	-4.421497	5.425155	-1.911848
H	-4.901701	4.547068	-2.397545
H	-5.169935	6.236766	-1.868474
H	-3.584982	5.764315	-2.564128
C	-0.022580	0.164135	1.528664
H	-0.811379	-0.585387	1.306765
H	0.911317	-0.399691	1.721693
H	-0.307754	0.692640	2.461009

[(PPh_3)Au(*para*-aniline-alkene)] Markovnikov

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P	2.602501	-0.267770	-0.061142
H	-1.892228	-2.527371	0.082191
C	-1.626770	-1.496373	-0.241962
C	-2.398113	-0.447467	0.622941
C	-2.087177	1.533953	-0.964987
C	-1.815681	0.947159	0.293054
C	-1.503797	2.754321	-1.341166
C	-0.946782	1.639474	1.164170
C	-0.626803	3.423433	-0.465055
H	-1.733706	3.186934	-2.328648
C	-0.349563	2.856758	0.789741
H	-0.695775	1.212747	2.144600
H	-0.157368	4.374003	-0.764227
H	0.348445	3.350829	1.484620
C	2.981488	0.775768	-1.528208
C	4.257967	0.845823	-2.123860
C	1.921044	1.560100	-2.037459
C	4.471418	1.701635	-3.219809
H	5.085084	0.231857	-1.733454
C	2.145404	2.420262	-3.122830
H	0.920340	1.502467	-1.578379
C	3.419437	2.491652	-3.717087
H	5.468116	1.751260	-3.686547
H	1.313949	3.032670	-3.506152
H	3.592215	3.161497	-4.574517
C	4.061036	-1.364769	0.146209
C	5.225740	-0.959843	0.834066
C	3.998383	-2.652532	-0.430438
C	6.320822	-1.835118	0.933724
H	5.271124	0.039627	1.295634
C	5.098544	-3.520543	-0.333595
H	3.076323	-2.970441	-0.945210
C	6.259778	-3.112951	0.348135
H	7.226797	-1.517885	1.474255
H	5.044852	-4.524287	-0.783869
H	7.118948	-3.797497	0.430412
C	2.691459	0.924324	1.344935
C	3.283847	2.198367	1.222390
C	2.083034	0.551874	2.564530
C	3.266899	3.089194	2.310226
H	3.742407	2.503312	0.268704
C	2.069001	1.444017	3.647859
H	1.592586	-0.431967	2.650076
C	2.657904	2.716156	3.521350
H	3.724222	4.085902	2.205811
H	1.582333	1.150459	4.591307
H	2.635575	3.420751	4.367757
Au	0.438680	-1.153286	-0.173427
H	-1.934983	-1.403289	-1.308039
H	-2.773624	1.017350	-1.654505
C	-6.105103	0.666942	0.597803
C	-6.779114	-0.398782	-0.067046
C	-4.719356	0.632365	0.791465
C	-5.974223	-1.478190	-0.526409
C	-3.917252	-0.439488	0.339154
H	-4.239152	1.483579	1.301873
C	-4.585621	-1.488371	-0.321044
H	-6.427408	-2.327525	-1.056100
H	-4.013166	-2.349117	-0.697415
H	-6.663404	1.538868	0.965954
N	-8.158026	-0.380532	-0.260928
C	-8.923825	0.790248	0.121673

H	-9.995359	0.617308	-0.094049
H	-8.834834	1.005793	1.211160
H	-8.609435	1.712043	-0.426251
C	-8.787851	-1.428800	-1.040564
H	-8.624487	-2.434796	-0.590280
H	-9.880328	-1.256488	-1.077089
H	-8.412706	-1.471251	-2.092367
C	-2.218067	-0.810975	2.118470
H	-2.691310	-1.794164	2.314583
H	-1.143050	-0.896753	2.384744
H	-2.696699	-0.064279	2.785488

[(PPh_3)Au(*ortho*-aniline)+(PPh_3)Au(alkene)]$^+$ adduct

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P	3.672963	-0.964685	0.068876
H	-1.001250	0.680438	-0.121026
C	-0.159467	1.314576	-0.459152
C	0.321687	2.271090	0.462063
C	1.872852	3.414051	-1.190939
C	1.174680	3.413157	0.046702
C	2.661437	4.505287	-1.574452
C	1.307167	4.547696	0.887478
C	2.768193	5.630625	-0.733774
H	3.202443	4.475623	-2.532987
C	2.087039	5.645904	0.495950
H	0.759140	4.595585	1.838533
H	3.385096	6.491242	-1.036065
H	2.161082	6.523054	1.157131
C	4.914276	-0.015790	-0.895398
C	5.920264	-0.660345	-1.647326
C	4.867229	1.395782	-0.840056
C	6.875173	0.108985	-2.335233
H	5.952694	-1.759992	-1.704161
C	5.824547	2.155528	-1.528890
H	4.074247	1.904301	-0.266674
C	6.829551	1.513359	-2.276341
H	7.657974	-0.394014	-2.924027
H	5.777705	3.254824	-1.484886
H	7.578176	2.110445	-2.820044
C	3.640611	-2.644908	-0.657881
C	4.018149	-3.791870	0.068904
C	3.135620	-2.773488	-1.972365
C	3.882907	-5.063591	-0.517415
H	4.408136	-3.696879	1.093942
C	3.013671	-4.043821	-2.554259
H	2.828288	-1.876221	-2.534824
C	3.381330	-5.191276	-1.824488
H	4.172045	-5.959600	0.053353
H	2.621832	-4.141316	-3.578537
H	3.276152	-6.188908	-2.278382
C	4.354840	-1.112784	1.761993
C	5.718801	-1.434155	1.947889
C	3.519319	-0.907971	2.880972
C	6.232100	-1.569179	3.247584
H	6.381022	-1.570700	1.078001
C	4.041054	-1.042677	4.178580
H	2.461493	-0.639566	2.731542
C	5.394409	-1.376770	4.362295
H	7.294609	-1.819456	3.391475
H	3.388286	-0.879585	5.050210
H	5.802557	-1.479171	5.379857
Au	1.629506	0.115219	-0.047726
H	-0.148033	1.531365	-1.539751
H	1.827119	2.531923	-1.847819
P	-3.212911	-1.483317	0.017357
C	-2.046983	4.848403	0.050633
C	-2.617835	3.587883	-0.253341
C	-2.100668	5.371537	1.354968
C	-3.207427	2.809541	0.798701
C	-2.752162	4.659128	2.373373
H	-1.651367	6.356252	1.561238
C	-3.299502	3.389894	2.080956
H	-2.824140	5.074989	3.390867
H	-3.760905	2.812932	2.899090

C	-1.572220	-2.070380	0.627836
C	-0.717578	-2.874611	-0.155891
C	-1.177956	-1.695730	1.932601
C	0.508998	-3.318567	0.368602
H	-1.012105	-3.158908	-1.178122
C	0.051541	-2.135552	2.449125
H	-1.840414	-1.057075	2.540834
C	0.894617	-2.949670	1.669013
H	1.168541	-3.952012	-0.242664
H	0.350437	-1.846405	3.469001
H	1.860788	-3.289925	2.072289
C	-3.117571	-1.718182	-1.806882
C	-3.518997	-2.917652	-2.432510
C	-2.588742	-0.662262	-2.585942
C	-3.381122	-3.062825	-3.824465
H	-3.946773	-3.737177	-1.833500
C	-2.449660	-0.817114	-3.974637
H	-2.308222	0.290188	-2.105318
C	-2.843763	-2.016998	-4.595811
H	-3.702552	-3.997883	-4.309391
H	-2.044710	0.010933	-4.577832
H	-2.743771	-2.132497	-5.686484
C	-4.421263	-2.716325	0.629147
C	-4.056057	-4.047467	0.928421
C	-5.764354	-2.302484	0.772502
C	-5.035345	-4.959310	1.357382
H	-3.006781	-4.369677	0.832592
C	-6.737934	-3.221164	1.197477
H	-6.040531	-1.256884	0.557069
C	-6.374422	-4.548633	1.489115
H	-4.750140	-5.996461	1.593637
H	-7.784046	-2.896414	1.309412
H	-7.138201	-5.265735	1.828448
Au	-3.458587	0.786279	0.530564
H	-1.565655	5.448102	-0.734718
N	-2.570308	3.063476	-1.579842
C	-1.671790	3.707944	-2.527599
H	-1.562785	3.056637	-3.420366
H	-2.038365	4.703406	-2.887912
H	-0.668522	3.853555	-2.081305
C	-3.866594	2.757175	-2.199179
H	-4.541633	2.276895	-1.466278
H	-4.366101	3.681163	-2.584420
H	-3.728264	2.055807	-3.048556
C	-0.074140	2.159838	1.907788
H	-0.781582	2.981600	2.159692
H	-0.598266	1.205156	2.095703
H	0.802963	2.250384	2.580338

[(PPh_3)Au(*ortho*-aniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3057.34339563 A.U.

P	3.910135	-1.041044	-0.103021
H	-0.716508	0.275234	-0.996642
C	0.081867	1.030223	-0.862133
C	-0.110241	1.808501	0.400128
C	1.564863	3.530728	-0.483409
C	0.841731	2.973691	0.600200
C	2.482417	4.573172	-0.290283
C	1.073404	3.515614	1.885083
C	2.702062	5.096547	0.997505
H	3.040041	4.973889	-1.151538
C	1.990337	4.562526	2.083765
H	0.532724	3.116634	2.754347
H	3.425270	5.912636	1.151173
H	2.149543	4.959317	3.098841
C	4.723710	-0.027595	1.203199
C	5.767170	-0.557870	1.995910
C	4.306356	1.308717	1.400259
C	6.386798	0.242361	2.968452
H	6.088206	-1.603374	1.865874
C	4.931283	2.104437	2.375942
H	3.485920	1.731855	0.796439
C	5.971319	1.574419	3.158154
H	7.198119	-0.176676	3.584005

H	4.590769	3.141833	2.517931
H	6.460416	2.198228	3.922811
C	5.169435	-1.326690	-1.406367
C	6.282736	-2.171379	-1.194541
C	5.030377	-0.644292	-2.634449
C	7.246678	-2.325359	-2.203035
H	6.390653	-2.721665	-0.246667
C	6.001329	-0.799346	-3.639063
H	4.156280	0.008090	-2.796341
C	7.108471	-1.638189	-3.423998
H	8.111508	-2.986325	-2.036176
H	5.889989	-0.264591	-4.595196
H	7.867451	-1.761390	-4.212409
C	3.591601	-2.679217	0.667194
C	3.183244	-2.746628	2.018280
C	3.581060	-3.850100	-0.123470
C	2.775122	-3.972636	2.570076
H	3.189207	-1.837524	2.640534
C	3.168672	-5.072514	0.433580
H	3.899662	-3.807788	-1.177357
C	2.763525	-5.136543	1.779320
H	2.465259	-4.018845	3.625855
H	3.165623	-5.981371	-0.188155
H	2.442186	-6.096055	2.213403
Au	1.903989	-0.022920	-0.699282
H	0.129218	1.662760	-1.768102
H	1.428396	3.123196	-1.494261
P	-3.749946	-1.241312	0.091764
C	-1.579048	5.068089	-0.565032
C	-1.718844	3.672484	-0.844121
C	-1.743065	5.572533	0.719387
C	-1.878289	2.737480	0.283176
C	-2.043177	4.717679	1.810674
H	-1.656050	6.658866	0.880696
C	-2.095951	3.355215	1.581046
H	-2.207331	5.130837	2.817081
H	-2.265265	2.693393	2.445358
C	-2.210704	-2.062990	-0.511791
C	-1.865794	-1.942861	-1.878461
C	-1.284506	-2.621124	0.395547
C	-0.610375	-2.381433	-2.327248
H	-2.579225	-1.496703	-2.590479
C	-0.024204	-3.048131	-0.058804
H	-1.543201	-2.716181	1.461697
C	0.315123	-2.925279	-1.417218
H	-0.345312	-2.281886	-3.391173
H	0.702569	-3.470623	0.651365
H	1.307624	-3.252707	-1.761404
C	-5.081488	-1.696448	-1.072778
C	-5.103100	-2.950317	-1.725101
C	-6.123872	-0.768404	-1.289146
C	-6.170350	-3.272032	-2.579927
H	-4.280701	-3.667509	-1.572524
C	-7.189383	-1.099505	-2.142374
H	-6.092170	0.213757	-0.789030
C	-7.213299	-2.350044	-2.786116
H	-6.186781	-4.247922	-3.089797
H	-8.001945	-0.375608	-2.309738
H	-8.047245	-2.606183	-3.458146
C	-4.126870	-2.017197	1.710049
C	-4.872362	-3.212184	1.803078
C	-3.605693	-1.418669	2.879454
C	-5.086985	-3.804080	3.058777
H	-5.294517	-3.676786	0.898278
C	-3.816079	-2.021804	4.130493
H	-3.037745	-0.476215	2.804648
C	-4.556929	-3.213848	4.220704
H	-5.675403	-4.732078	3.130042
H	-3.408684	-1.552697	5.039618
H	-4.729888	-3.681294	5.202665
Au	-3.087309	0.981170	0.187308
H	-1.389828	5.779814	-1.378745
N	-1.591702	3.255760	-2.152099
C	-1.025450	4.151875	-3.162138

H	-0.655281	3.538511	-4.007196
H	-1.776464	4.870447	-3.564447
H	-0.165944	4.714755	-2.752436
C	-2.292918	2.119102	-2.746335
H	-2.861466	1.561110	-1.972144
H	-3.008516	2.485250	-3.516663
H	-1.588015	1.408078	-3.224015
C	-0.226280	0.895307	1.634001
H	-0.774324	1.346297	2.481075
H	-0.716601	-0.060509	1.367136
H	0.796571	0.653029	1.992818

[(PPh_3)Au(*ortho*-aniline-alkene)Au(PPh_3)]$^+$ Intermediate Markovnikov

-3057.36983232 A.U.

P	4.196307	-0.857781	0.018070
C	0.366308	0.586539	-1.713449
C	-0.186775	1.518487	-0.593982
C	1.173221	3.657268	-0.931398
C	0.888405	2.518562	-0.150739
C	2.184885	4.557616	-0.550457
C	1.645952	2.300988	1.021854
C	2.919337	4.339830	0.628982
H	2.395403	5.438730	-1.177163
C	2.645684	3.205346	1.414065
H	1.471452	1.394311	1.625171
H	3.706726	5.047143	0.932465
H	3.220276	3.016426	2.333982
C	5.500790	0.426718	-0.167012
C	6.857664	0.152830	0.113680
C	5.111017	1.731570	-0.543979
C	7.812199	1.178634	0.022838
H	7.172942	-0.863766	0.396274
C	6.070468	2.754986	-0.623317
H	4.054605	1.949508	-0.769223
C	7.419930	2.480620	-0.341823
H	8.870110	0.959983	0.236872
H	5.754256	3.769772	-0.910841
H	8.172451	3.281818	-0.411685
C	4.955534	-2.459116	-0.451711
C	5.768782	-3.205614	0.431188
C	4.732167	-2.928357	-1.765513
C	6.359005	-4.403774	-0.004434
H	5.931949	-2.855962	1.463157
C	5.329793	-4.124540	-2.196239
H	4.083415	-2.351061	-2.445177
C	6.143469	-4.861923	-1.317245
H	6.991872	-4.983337	0.685882
H	5.155037	-4.484938	-3.222015
H	6.608645	-5.801403	-1.654688
C	3.906450	-0.958816	1.834407
C	4.182629	0.143082	2.670937
C	3.267337	-2.098485	2.373551
C	3.814336	0.107736	4.027389
H	4.688217	1.029131	2.256864
C	2.908720	-2.132481	3.730780
H	3.060955	-2.966917	1.727721
C	3.175506	-1.026178	4.559763
H	4.037939	0.970372	4.674867
H	2.419879	-3.028845	4.144086
H	2.894257	-1.053628	5.624122
Au	2.185468	-0.226210	-0.993090
H	0.642486	1.220762	-2.588246
H	-0.395649	0.863784	0.275575
H	0.592926	3.844388	-1.849996
P	-3.986067	-1.131951	0.213805
C	-2.654146	4.501927	-0.555485
C	-2.988227	4.582917	-1.909135
C	-1.929586	3.396546	-0.022472
C	-2.613232	3.565922	-2.808283
C	-1.483485	2.335241	-0.940136
H	-3.566754	5.449313	-2.266971
C	-1.860506	2.488947	-2.329587
H	-2.877918	3.625614	-3.873911
H	-1.465384	1.755741	-3.046306

C	-5.116669	-2.092202	-0.850663
C	-6.090883	-2.954404	-0.302654
C	-4.966357	-1.987092	-2.252091
C	-6.907628	-3.710976	-1.159783
H	-6.218721	-3.029467	0.788618
C	-5.780786	-2.754325	-3.099872
H	-4.212957	-1.301344	-2.674662
C	-6.751895	-3.614276	-2.554416
H	-7.672803	-4.378400	-0.733973
H	-5.663556	-2.672809	-4.191536
H	-7.396485	-4.207741	-3.221369
C	-4.759948	-0.928306	1.854965
C	-4.652049	-1.942512	2.832945
C	-5.492609	0.247648	2.128854
C	-5.287877	-1.779953	4.075154
H	-4.064674	-2.851395	2.625412
C	-6.126752	0.400617	3.372410
H	-5.557954	1.042094	1.367042
C	-6.025567	-0.612376	4.343880
H	-5.204661	-2.569067	4.838578
H	-6.699400	1.316484	3.585799
H	-6.520730	-0.488709	5.319678
C	-2.472591	-2.147545	0.463840
C	-2.208374	-3.284112	-0.325947
C	-1.463518	-1.627912	1.311212
C	-0.929154	-3.871935	-0.293188
H	-2.985231	-3.691655	-0.991399
C	-0.187970	-2.207689	1.326400
H	-1.667864	-0.746458	1.938728
C	0.083990	-3.323063	0.510382
H	-0.720235	-4.751222	-0.921789
H	0.604785	-1.781420	1.960095
H	1.094697	-3.758751	0.496279
Au	-3.121526	0.822867	-0.654701
H	-2.979728	5.305866	0.118743
N	-1.592405	3.389322	1.316708
C	-1.597856	2.184142	2.130809
H	-2.103331	2.396602	3.096856
H	-2.183181	1.389567	1.620224
H	-0.579142	1.797368	2.349108
C	-1.498370	4.639384	2.064261
H	-2.472418	4.964450	2.500643
H	-0.776979	4.500419	2.894353
H	-1.101434	5.446345	1.419144
C	-0.557274	-0.556230	-2.158821
H	-0.786767	-1.237340	-1.319467
H	-1.540863	-0.229021	-2.582871
H	-0.069649	-1.165902	-2.946922

[(PPh_3)Au(*ortho*-aniline-alkene)] Markovnikov

-1885.82287490 A.U.

P	2.290674	-0.134913	0.067633
C	-1.755831	-1.918620	-0.258074
C	-2.675546	-0.743277	0.179429
C	-2.302559	0.934176	-1.719913
C	-2.176096	0.602983	-0.354971
C	-1.781940	2.142587	-2.217777
C	-1.533039	1.523173	0.500643
C	-1.123670	3.040736	-1.356832
H	-1.888395	2.382987	-3.288264
C	-0.998987	2.724516	0.008911
H	-1.430221	1.273230	1.568248
H	-0.703982	3.980439	-1.749755
H	-0.474373	3.408573	0.694879
C	2.767438	0.571036	-1.562651
C	4.095064	0.603501	-2.037303
C	1.725289	1.123270	-2.342775
C	4.376981	1.190561	-3.284317
H	4.908709	0.170494	-1.434129
C	2.016951	1.718830	-3.579087
H	0.684931	1.093532	-1.979242
C	3.341810	1.751532	-4.053515
H	5.414136	1.210610	-3.655236
H	1.198589	2.153387	-4.174717

H	3.568127	2.211663	-5.028592
C	3.793268	-0.993377	0.683869
C	4.825946	-0.315988	1.368561
C	3.908605	-2.378540	0.432850
C	5.967766	-1.019549	1.788184
H	4.732170	0.761873	1.576944
C	5.055269	-3.075254	0.849100
H	3.087791	-2.905526	-0.081851
C	6.085020	-2.396981	1.526455
H	6.770260	-0.488868	2.324851
H	5.140707	-4.155478	0.651790
H	6.980351	-2.945927	1.858990
C	2.116094	1.350231	1.147292
C	2.582674	2.624630	0.764420
C	1.436376	1.195170	2.376073
C	2.370855	3.732427	1.604135
H	3.097531	2.754567	-0.200268
C	1.229921	2.303082	3.212412
H	1.048512	0.203212	2.661315
C	1.693444	3.574954	2.825998
H	2.731126	4.726780	1.296087
H	0.692161	2.176364	4.165288
H	1.520411	4.446316	3.477255
Au	0.242210	-1.270517	-0.060437
H	-1.881885	-2.084571	-1.354410
H	-2.583471	-0.685286	1.282847
H	-2.820102	0.234482	-2.395728
C	-6.446180	0.014025	-0.014285
C	-6.868448	-0.840080	-1.047443
C	-5.109868	-0.002825	0.442654
C	-5.954279	-1.730658	-1.629006
C	-4.164071	-0.880200	-0.171613
H	-7.916352	-0.813448	-1.387561
C	-4.617100	-1.739314	-1.189805
H	-6.272501	-2.410424	-2.435369
H	-3.896172	-2.413047	-1.678195
H	-7.169144	0.700068	0.453014
N	-4.662198	0.882936	1.466436
C	-4.450615	0.291699	2.780860
H	-5.403806	0.186375	3.363670
H	-4.009131	-0.719584	2.687472
H	-3.752676	0.919058	3.378739
C	-5.260897	2.203369	1.524574
H	-6.275287	2.228884	2.005871
H	-4.601957	2.876598	2.115219
H	-5.347158	2.622538	0.502640
C	-2.085657	-3.216160	0.496984
H	-1.915602	-3.099102	1.589170
H	-3.149283	-3.524319	0.365994
H	-1.447227	-4.056465	0.153757

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ TS anti-Markovnikov

-3057.34407815 A.U.

P	3.977339	-1.039417	0.192995
C	0.350340	1.430904	-0.819750
C	-0.227058	1.390112	0.524938
C	0.532543	3.280197	-2.572975
C	0.800004	2.801033	-1.268245
C	0.826809	4.605723	-2.937036
C	1.433126	3.693541	-0.363441
C	1.408455	5.486690	-2.010369
H	0.592815	4.952970	-3.955978
C	1.724263	5.014465	-0.720380
H	1.692558	3.345070	0.648728
H	1.642056	6.523885	-2.298212
H	2.204121	5.684092	0.011015
C	5.579401	-0.251436	-0.220289
C	6.695594	-1.015708	-0.627938
C	5.692470	1.150939	-0.092649
C	7.918773	-0.377297	-0.892926
H	6.605286	-2.106855	-0.749733
C	6.919150	1.780833	-0.357624
H	4.813615	1.747931	0.202367
C	8.032210	1.018063	-0.755436

H	8.787433	-0.973663	-1.212908
H	7.003614	2.874442	-0.261830
H	8.991686	1.514841	-0.968236
C	3.952384	-2.609381	-0.761774
C	3.863997	-3.870689	-0.137506
C	3.969126	-2.520605	-2.173219
C	3.800074	-5.036365	-0.923139
H	3.844135	-3.945270	0.960869
C	3.916859	-3.688055	-2.949813
H	4.025384	-1.534336	-2.662725
C	3.830231	-4.947985	-2.325704
H	3.728535	-6.019547	-0.432713
H	3.938019	-3.615113	-4.048295
H	3.783547	-5.862921	-2.936518
C	4.076284	-1.545330	1.955110
C	5.297553	-1.966218	2.526076
C	2.895758	-1.561181	2.731301
C	5.330026	-2.410223	3.858179
H	6.225098	-1.941093	1.932722
C	2.934539	-2.010785	4.061823
H	1.947957	-1.207885	2.291893
C	4.150507	-2.437009	4.625107
H	6.284386	-2.734527	4.301524
H	2.012302	-2.020226	4.663500
H	4.181707	-2.784438	5.669605
Au	2.119809	0.271117	-0.286089
H	0.206678	2.047549	1.290920
H	-0.528852	0.404477	0.912560
H	0.056447	2.622808	-3.314201
P	-3.713015	-1.591536	-0.034911
C	-1.833392	4.385169	2.118355
C	-1.719888	5.290986	1.010174
C	-2.016732	3.024599	1.906465
C	-1.882161	4.746939	-0.303419
C	-2.093617	2.437742	0.594748
H	-2.053874	2.360920	2.787149
C	-2.058146	3.383760	-0.489417
H	-1.829076	5.394780	-1.187819
H	-2.154886	3.018483	-1.522436
C	-4.891588	-1.925595	-1.397898
C	-5.616745	-3.134539	-1.474361
C	-5.032270	-0.952938	-2.412853
C	-6.471426	-3.367502	-2.564475
H	-5.522630	-3.890091	-0.678470
C	-5.884084	-1.195560	-3.503231
H	-4.476117	-0.003314	-2.339813
C	-6.603319	-2.401910	-3.579467
H	-7.041492	-4.308037	-2.619478
H	-5.993818	-0.434810	-4.291735
H	-7.276949	-2.587694	-4.430638
C	-4.308526	-2.517002	1.428673
C	-3.988732	-3.878827	1.626542
C	-5.132094	-1.842688	2.357102
C	-4.502825	-4.560969	2.742092
H	-3.331904	-4.401596	0.912856
C	-5.644455	-2.532283	3.468234
H	-5.363741	-0.775129	2.207470
C	-5.331665	-3.890478	3.660231
H	-4.253484	-5.622589	2.895889
H	-6.286640	-2.004995	4.190722
H	-5.731604	-4.428637	4.533864
C	-2.135251	-2.411592	-0.532004
C	-1.927009	-2.892390	-1.840402
C	-1.057784	-2.395034	0.387185
C	-0.649268	-3.337775	-2.228544
H	-2.757516	-2.903789	-2.563379
C	0.211983	-2.842969	-0.007164
H	-1.215440	-2.014289	1.410135
C	0.420855	-3.308841	-1.319699
H	-0.490656	-3.706236	-3.254044
H	1.050954	-2.826581	0.705601
H	1.419455	-3.649177	-1.628049
Au	-3.095284	0.623555	0.323244
H	-1.754120	4.754981	3.149604

N	-1.447397	6.621950	1.196089
C	-1.334798	7.173168	2.542588
H	-1.150842	8.260776	2.479301
H	-2.267833	7.019912	3.127990
H	-0.492980	6.715134	3.108653
C	-1.258019	7.498722	0.044528
H	-2.194535	7.620286	-0.544343
H	-0.941899	8.498471	0.393016
H	-0.471000	7.102018	-0.635163
C	-0.376847	0.578120	-1.862076
H	-1.344412	1.050314	-2.153065
H	0.221641	0.435296	-2.783465
H	-0.617366	-0.422295	-1.459267

[(PPh_3)Au(*para*-aniline-alkene)Au(PPh_3)]$^+$ Intermediate anti-Markovnikov

-3057.38530206 A.U.

P	5.068362	-0.075807	0.017154
C	0.792861	-1.001186	-0.804460
C	0.305776	-2.297705	-0.103327
C	0.039729	1.460336	-0.779347
C	0.364362	0.260865	-0.080879
C	-0.225603	2.663329	-0.105340
C	0.359299	0.342670	1.348963
C	-0.192553	2.721386	1.296936
H	-0.477625	3.561185	-0.691536
C	0.100522	1.546329	2.019044
H	0.622323	-0.547875	1.939115
H	-0.402195	3.664806	1.823912
H	0.134399	1.567981	3.120347
C	5.806191	-1.023454	1.405737
C	6.527193	-0.405305	2.449246
C	5.655556	-2.428700	1.389202
C	7.100752	-1.192568	3.463337
H	6.637902	0.690194	2.471683
C	6.237161	-3.208912	2.400874
H	5.076841	-2.905925	0.580666
C	6.960189	-2.591474	3.438635
H	7.661497	-0.708055	4.278031
H	6.121128	-4.303902	2.382923
H	7.411924	-3.203978	4.234682
C	5.006881	1.679765	0.571763
C	6.128570	2.529419	0.447395
C	3.809971	2.177918	1.136521
C	6.054089	3.859298	0.895981
H	7.058481	2.154113	-0.009161
C	3.742655	3.508103	1.580104
H	2.919150	1.532647	1.216069
C	4.863492	4.349755	1.462747
H	6.930852	4.518184	0.795706
H	2.800257	3.885832	2.007062
H	4.807967	5.394850	1.806069
C	6.331959	-0.106622	-1.313777
C	7.673688	-0.470782	-1.071408
C	5.929920	0.280171	-2.612049
C	8.606742	-0.439103	-2.122880
H	7.988753	-0.782201	-0.062900
C	6.868262	0.315177	-3.655285
H	4.877326	0.549877	-2.800752
C	8.207235	-0.044077	-3.411681
H	9.652715	-0.726254	-1.932273
H	6.552325	0.617766	-4.665922
H	8.941008	-0.021635	-4.232594
Au	2.906160	-0.762911	-0.540497
H	0.701864	-2.345550	0.930533
H	0.758667	-3.166190	-0.626871
H	0.013063	1.459552	-1.876674
P	-3.956593	1.143499	-0.074942
C	-3.195715	-3.649392	-1.050036
C	-3.854993	-3.775013	0.217393
C	-1.940513	-3.057221	-1.160395
C	-3.145879	-3.313565	1.366273
C	-1.211895	-2.552675	-0.024830
H	-1.463939	-3.015812	-2.150243
C	-1.876943	-2.718665	1.241897

H	-3.579308	-3.399285	2.370568
H	-1.337059	-2.436972	2.160787
C	-4.453575	1.854111	1.538193
C	-5.759560	2.348441	1.749195
C	-3.488246	1.939489	2.565083
C	-6.090637	2.932590	2.983521
H	-6.518223	2.272535	0.954399
C	-3.827177	2.528467	3.793919
H	-2.472876	1.548607	2.393087
C	-5.126666	3.024557	4.004308
H	-7.109655	3.315469	3.149424
H	-3.073171	2.594207	4.593825
H	-5.392362	3.480027	4.971121
C	-5.501672	0.507215	-0.837999
C	-6.297964	1.323890	-1.669352
C	-5.919368	-0.807405	-0.530522
C	-7.511501	0.828656	-2.178962
H	-5.967659	2.344248	-1.921568
C	-7.137477	-1.289311	-1.033491
H	-5.282854	-1.457672	0.091488
C	-7.935089	-0.472946	-1.857525
H	-8.129365	1.465583	-2.830923
H	-7.463624	-2.310555	-0.782934
H	-8.887787	-0.855153	-2.256204
C	-3.410555	2.544955	-1.117823
C	-3.521197	3.882987	-0.689517
C	-2.820551	2.245048	-2.365840
C	-3.039885	4.917999	-1.511281
H	-3.969078	4.117134	0.288712
C	-2.350171	3.282659	-3.183596
H	-2.708813	1.194502	-2.681515
C	-2.454676	4.620184	-2.754443
H	-3.120570	5.963209	-1.174525
H	-1.888504	3.048020	-4.155305
H	-2.075026	5.433237	-3.392700
Au	-2.388463	-0.516728	0.097509
H	-3.679149	-4.013184	-1.965659
N	-5.126736	-4.292863	0.311480
C	-5.786296	-4.834321	-0.871953
H	-6.802997	-5.172248	-0.600655
H	-5.886768	-4.065495	-1.669394
H	-5.238762	-5.705412	-1.297545
C	-5.766499	-4.420028	1.615644
H	-5.832168	-3.436131	2.130882
H	-6.795884	-4.799879	1.484337
H	-5.223797	-5.125160	2.285506
C	0.435542	-0.998491	-2.300175
H	0.729430	-1.958320	-2.771513
H	-0.659077	-0.848348	-2.471742
H	0.958523	-0.197521	-2.859752

[(PPh_3)Au(*para*-aniline-alkene)] anti-Markovnikov

-1885.82205649 A.U.

P	2.695905	-0.245311	0.046520
C	-1.709646	-0.424841	-0.457887
C	-2.505649	-1.175100	0.657061
C	-1.949330	1.949551	-1.435289
C	-1.768895	1.090731	-0.321532
C	-1.879473	3.348957	-1.308775
C	-1.557712	1.723280	0.938230
C	-1.649424	3.947194	-0.059323
H	-2.013150	3.978430	-2.203980
C	-1.496588	3.116497	1.069483
H	-1.403248	1.097049	1.831182
H	-1.598359	5.043237	0.039257
H	-1.319070	3.560488	2.062688
C	3.311393	-0.411556	1.771709
C	4.211423	0.504806	2.356243
C	2.853500	-1.519002	2.520952
C	4.657453	0.305591	3.674702
H	4.559387	1.377941	1.782098
C	3.307780	-1.716204	3.834770
H	2.129481	-2.218146	2.069991
C	4.210453	-0.804496	4.413101

H	5.357058	1.025620	4.128218
H	2.946528	-2.580448	4.414192
H	4.559626	-0.955492	5.446883
C	3.032784	1.506100	-0.424833
C	4.290701	1.915624	-0.920191
C	1.995864	2.456523	-0.275649
C	4.509805	3.263973	-1.251615
H	5.097609	1.177525	-1.055155
C	2.222390	3.801482	-0.609411
H	1.000026	2.150991	0.087293
C	3.477771	4.207744	-1.096181
H	5.491867	3.577118	-1.640449
H	1.397729	4.522906	-0.497762
H	3.651362	5.261914	-1.365246
C	3.873183	-1.233651	-0.963114
C	5.141983	-1.631833	-0.489962
C	3.467778	-1.593381	-2.268351
C	5.999432	-2.373953	-1.321407
H	5.457695	-1.365786	0.531427
C	4.331054	-2.328885	-3.095790
H	2.466338	-1.301291	-2.626301
C	5.597865	-2.720128	-2.623802
H	6.987774	-2.684659	-0.946884
H	4.008867	-2.606792	-4.111725
H	6.271450	-3.303430	-3.271446
Au	0.401104	-0.642896	-0.213554
H	-2.162159	-0.846899	1.659966
H	-2.252401	-2.254327	0.591195
H	-2.130431	1.518991	-2.430120
C	-6.195370	-1.787449	-0.280813
C	-6.852292	-0.620630	0.204724
C	-4.814170	-1.957995	-0.110803
C	-6.046250	0.340817	0.880007
C	-4.010757	-1.003311	0.546740
H	-4.342235	-2.873376	-0.506268
C	-4.667858	0.146103	1.037573
H	-6.494493	1.255655	1.291371
H	-4.083164	0.920156	1.558759
H	-6.761800	-2.574105	-0.798067
N	-8.221051	-0.430619	0.031898
C	-9.021442	-1.470883	-0.583648
H	-10.075396	-1.139287	-0.644699
H	-8.682746	-1.699763	-1.620954
H	-8.998747	-2.428644	-0.008905
C	-8.865240	0.738668	0.597845
H	-8.437132	1.685972	0.195428
H	-9.941987	0.726824	0.342937
H	-8.779449	0.782510	1.710860
C	-2.129313	-0.938885	-1.845353
H	-2.066492	-2.046057	-1.877399
H	-3.180519	-0.658564	-2.089859
H	-1.477488	-0.552207	-2.655347

[(PPh_3)Au(*para*-aniline-alkene)]$^+$ Markovnikov

-1885.82205649 A.U.

P	2.695905	-0.245311	0.046520
C	-1.709646	-0.424841	-0.457887
C	-2.505649	-1.175100	0.657061
C	-1.949330	1.949551	-1.435289
C	-1.768895	1.090731	-0.321532
C	-1.879473	3.348957	-1.308775
C	-1.557712	1.723280	0.938230
C	-1.649424	3.947194	-0.059323
H	-2.013150	3.978430	-2.203980
C	-1.496588	3.116497	1.069483
H	-1.403248	1.097049	1.831182
H	-1.598359	5.043237	0.039257
H	-1.319070	3.560488	2.062688
C	3.311393	-0.411556	1.771709
C	4.211423	0.504806	2.356243
C	2.853500	-1.519002	2.520952
C	4.657453	0.305591	3.674702
H	4.559387	1.377941	1.782098
C	3.307780	-1.716204	3.834770

H	2.129481	-2.218146	2.069991
C	4.210453	-0.804496	4.413101
H	5.357058	1.025620	4.128218
H	2.946528	-2.580448	4.414192
H	4.559626	-0.955492	5.446883
C	3.032784	1.506100	-0.424833
C	4.290701	1.915624	-0.920191
C	1.995864	2.456523	-0.275649
C	4.509805	3.263973	-1.251615
H	5.097609	1.177525	-1.055155
C	2.222390	3.801482	-0.609411
H	1.000026	2.150991	0.087293
C	3.477771	4.207744	-1.096181
H	5.491867	3.577118	-1.640449
H	1.397729	4.522906	-0.497762
H	3.651362	5.261914	-1.365246
C	3.873183	-1.233651	-0.963114
C	5.141983	-1.631833	-0.489962
C	3.467778	-1.593381	-2.268351
C	5.999432	-2.373953	-1.321407
H	5.457695	-1.365786	0.531427
C	4.331054	-2.328885	-3.095790
H	2.466338	-1.301291	-2.626301
C	5.597865	-2.720128	-2.623802
H	6.987774	-2.684659	-0.946884
H	4.008867	-2.606792	-4.111725
H	6.271450	-3.303430	-3.271446
Au	0.401104	-0.642896	-0.213554
H	-2.162159	-0.846899	1.659966
H	-2.252401	-2.254327	0.591195
H	-2.130431	1.518991	-2.430120
C	-6.195370	-1.787449	-0.280813
C	-6.852292	-0.620630	0.204724
C	-4.814170	-1.957995	-0.110803
C	-6.046250	0.340817	0.880007
C	-4.010757	-1.003311	0.546740
H	-4.342235	-2.873376	-0.506268
C	-4.667858	0.146103	1.037573
H	-6.494493	1.255655	1.291371
H	-4.083164	0.920156	1.558759
H	-6.761800	-2.574105	-0.798067
N	-8.221051	-0.430619	0.031898
C	-9.021442	-1.470883	-0.583648
H	-10.075396	-1.139287	-0.644699
H	-8.682746	-1.699763	-1.620954
H	-8.998747	-2.428644	-0.008905
C	-8.865240	0.738668	0.597845
H	-8.437132	1.685972	0.195428
H	-9.941987	0.726824	0.342937
H	-8.779449	0.782510	1.710860
C	-2.129313	-0.938885	-1.845353
H	-2.066492	-2.046057	-1.877399
H	-3.180519	-0.658564	-2.089859
H	-1.477488	-0.552207	-2.655347

Using CH_2=CHPh as alkene and N,N-diethylaniline:

[(PPh_3)Au(*N,N*-diethylaniline)]$^+$
-1616.07473154 A.U.

P	-1.458449	0.083594	0.019046
C	2.773245	-1.079773	-1.129244
C	3.431897	-0.461677	0.022921
C	2.529190	-2.504675	-1.130712
C	3.643139	-1.300604	1.168899
C	2.783651	-3.286907	-0.008733
H	2.144138	-2.960241	-2.056690
C	3.335521	-2.658992	1.136946
H	4.078214	-0.882894	2.085711
H	2.573683	-4.365873	-0.012927
H	3.536404	-3.261472	2.037231
C	-2.666067	-1.285627	0.119957
C	-4.018583	-1.087750	-0.234050

C	-2.235358	-2.537265	0.614381
C	-4.935598	-2.142454	-0.085381
H	-4.353542	-0.115010	-0.627438
C	-3.159354	-3.583230	0.762190
H	-1.175948	-2.691182	0.879573
C	-4.508553	-3.386177	0.412926
H	-5.989912	-1.990861	-0.364038
H	-2.824508	-4.559324	1.145948
H	-5.230330	-4.210250	0.524257
C	-2.159933	1.318791	-1.134463
C	-2.871171	2.442407	-0.661451
C	-2.019317	1.099158	-2.523611
C	-3.443720	3.338686	-1.580992
H	-2.976853	2.618713	0.420597
C	-2.597796	1.997245	-3.433730
H	-1.457611	0.223712	-2.890294
C	-3.309791	3.116714	-2.962899
H	-3.997753	4.216175	-1.213135
H	-2.490022	1.825219	-4.515859
H	-3.759526	3.822087	-3.678899
C	-1.416126	0.875162	1.671381
C	-2.463879	0.697898	2.599778
C	-0.319281	1.706561	1.991747
C	-2.411070	1.357375	3.840583
H	-3.316263	0.043742	2.357939
C	-0.275333	2.362660	3.230842
H	0.504623	1.831890	1.269812
C	-1.321702	2.188466	4.156356
H	-3.226943	1.216730	4.566389
H	0.582403	3.007321	3.478480
H	-1.284575	2.699170	5.131136
Au	0.658615	-0.593087	-0.600723
H	2.869824	-0.599027	-2.116241
N	3.807422	0.849311	0.002523
C	3.471252	1.728725	-1.125410
H	3.377628	2.758039	-0.721338
H	2.454916	1.465261	-1.498795
C	4.435424	1.494932	1.165867
H	5.140305	0.783993	1.642165
H	5.068376	2.320050	0.778971
C	4.506495	1.703559	-2.256302
H	4.206665	2.395064	-3.069614
H	5.501919	2.021940	-1.884934
H	4.619989	0.689337	-2.690083
C	3.415743	2.027621	2.180576
H	2.759002	2.792995	1.716883
H	2.770374	1.213315	2.568768
H	3.931984	2.501199	3.039989

[(PPh_3)Au(*para*- *N*,*N*-diethylaniline)]$^+$ (TS extraction proton by a second *N*,*N*-diethylaniline)

-2060.62122345 A.U.

P	-2.820963	-0.426706	0.007359
C	3.831376	2.087505	0.029653
C	2.661290	2.870429	-0.001402
C	5.064009	2.686795	0.338968
C	2.733341	4.251102	0.270765
C	5.137441	4.061608	0.619865
H	5.974878	2.068593	0.360952
C	3.968453	4.842210	0.583374
H	1.825942	4.872310	0.236631
H	6.104638	4.526603	0.865392
H	4.016454	5.921329	0.797004
C	-3.135687	1.351540	-0.355098
C	-3.513478	2.255574	0.658593
C	-2.807650	1.835701	-1.643464
C	-3.556585	3.635237	0.385158
H	-3.768283	1.883989	1.663440
C	-2.858026	3.212064	-1.910160
H	-2.507136	1.130319	-2.435620
C	-3.226188	4.115381	-0.893891
H	-3.855239	4.337804	1.178801
H	-2.608915	3.583523	-2.916580
H	-3.262374	5.195770	-1.103669
C	-3.620551	-0.754008	1.623109

C	-4.991949	-1.076791	1.715476
C	-2.846496	-0.621437	2.798189
C	-5.582304	-1.257188	2.977193
H	-5.597933	-1.196740	0.803791
C	-3.445817	-0.796087	4.056455
H	-1.771776	-0.384761	2.724058
C	-4.813052	-1.113539	4.146477
H	-6.650538	-1.514866	3.046951
H	-2.840261	-0.692815	4.970259
H	-5.280544	-1.257701	5.133021
C	-3.726780	-1.376207	-1.265168
C	-4.919307	-0.885502	-1.843565
C	-3.227501	-2.643254	-1.640219
C	-5.609572	-1.667104	-2.784826
H	-5.301990	0.109552	-1.565592
C	-3.925877	-3.419611	-2.579364
H	-2.288531	-3.015043	-1.197664
C	-5.115850	-2.932884	-3.150448
H	-6.537638	-1.284291	-3.237241
H	-3.535741	-4.406996	-2.871075
H	-5.659240	-3.541314	-3.890151
Au	-0.504362	-0.620468	-0.005315
H	3.784235	1.013681	-0.195568
N	1.390092	2.240347	-0.351891
C	1.033280	2.348369	-1.806087
H	0.256137	1.567752	-1.977834
H	0.537618	3.331762	-1.974971
C	0.229656	2.670966	0.480925
H	-0.004774	3.739069	0.275722
H	-0.642175	2.096483	0.103779
C	3.514543	-1.469781	1.255258
C	4.150847	-1.958041	0.063754
C	2.304393	-0.791024	1.195913
C	3.460783	-1.729012	-1.176629
C	1.608626	-0.522646	-0.033998
H	1.880527	-0.417904	2.142853
C	2.244132	-1.059695	-1.207885
H	3.894642	-2.077625	-2.123254
H	1.462749	0.843172	-0.159327
H	1.763753	-0.910751	-2.189283
H	3.979479	-1.632126	2.236611
N	5.358014	-2.602611	0.105705
C	6.109037	-2.768784	1.358360
H	7.186295	-2.807790	1.092609
H	5.991818	-1.856745	1.979821
C	5.980453	-3.169172	-1.099110
H	6.596828	-4.033845	-0.775717
H	5.193666	-3.598478	-1.752936
C	2.207325	2.171838	-2.762008
H	2.931895	3.006020	-2.682113
H	2.754202	1.227768	-2.572452
H	1.826601	2.146465	-3.802877
C	0.414928	2.412686	1.970990
H	1.281134	2.963080	2.388517
H	-0.496395	2.736096	2.512233
H	0.558364	1.331644	2.169034
C	5.709266	-4.024302	2.143582
H	4.639779	-3.992235	2.435672
H	5.866820	-4.939626	1.536746
H	6.318452	-4.117043	3.065772
C	6.842979	-2.157630	-1.864764
H	7.306895	-2.632825	-2.753118
H	6.238053	-1.294320	-2.210310
H	7.659011	-1.765371	-1.223312

[(PPh_3)Au(*ortho*- *N,N*-diethylaniline)]$^+$ (TS extraction proton by a second *N,N*-diethylaniline)

-2060.62422926 A.U.

P	-2.222321	-0.194719	-0.017951
C	0.864681	2.383683	0.650266
C	2.242930	2.121972	0.472400
C	0.205771	3.334612	-0.144858
C	2.927832	2.804174	-0.559106
C	0.894831	4.019124	-1.158610
H	-0.864153	3.518907	0.035308

C	2.256550	3.740922	-1.362725
H	3.991996	2.622064	-0.753921
H	0.377020	4.762288	-1.783851
H	2.816392	4.264627	-2.153119
C	-2.618474	1.250238	1.050766
C	-2.206592	1.203843	2.401999
C	-3.292690	2.389490	0.562798
C	-2.452300	2.293487	3.251414
H	-1.690127	0.308875	2.786336
C	-3.535918	3.478890	1.419397
H	-3.619958	2.431196	-0.487769
C	-3.111581	3.436023	2.758857
H	-2.127971	2.252013	4.302977
H	-4.060464	4.367315	1.034532
H	-3.299001	4.293371	3.423801
C	-3.452749	-1.479059	0.410062
C	-4.744205	-1.127243	0.861822
C	-3.106686	-2.838151	0.242540
C	-5.683327	-2.134552	1.137987
H	-5.012767	-0.068112	1.002999
C	-4.053324	-3.839096	0.516419
H	-2.092388	-3.108877	-0.094743
C	-5.339966	-3.488029	0.963606
H	-6.688783	-1.861013	1.493921
H	-3.781882	-4.898292	0.387659
H	-6.078552	-4.274466	1.184172
C	-2.605380	0.356093	-1.725186
C	-3.736574	-0.104089	-2.430341
C	-1.730360	1.289552	-2.326193
C	-3.988271	0.371404	-3.730218
H	-4.420375	-0.833507	-1.968643
C	-1.997100	1.770894	-3.616604
H	-0.839842	1.640908	-1.780645
C	-3.124790	1.309520	-4.322099
H	-4.868620	0.006270	-4.281591
H	-1.315275	2.502942	-4.077242
H	-3.329211	1.680969	-5.338343
Au	-0.006092	-0.834095	0.249836
H	0.279692	1.844711	1.399793
N	2.881338	1.075710	1.259578
C	2.760327	1.149156	2.763187
H	3.370198	0.294290	3.120353
H	3.259810	2.080126	3.103259
C	4.299211	0.745411	0.892870
H	4.469924	-0.283091	1.274187
H	4.328573	0.657483	-0.207941
C	2.008716	-1.417764	0.569063
C	2.941743	-1.772613	-0.502128
C	2.147331	-2.123082	1.819434
C	3.922339	-2.782251	-0.223425
C	3.107070	-3.101948	2.059602
H	1.461893	-1.852135	2.639607
C	3.992590	-3.428504	1.008910
H	4.645466	-3.076397	-0.993975
H	2.286912	-0.073704	0.914196
H	4.763017	-4.202117	1.157865
H	3.172564	-3.607771	3.034343
N	2.971458	-1.138263	-1.729779
C	1.963749	-0.187827	-2.214269
H	2.495589	0.646326	-2.722570
H	1.448401	0.284195	-1.354182
C	4.024762	-1.436001	-2.715506
H	4.189837	-2.531279	-2.786479
H	3.637005	-1.141261	-3.710955
C	5.339990	-0.696246	-2.437883
H	5.757733	-0.969095	-1.447410
H	6.099192	-0.943259	-3.207724
H	5.184609	0.402983	-2.457792
C	0.939064	-0.840620	-3.150477
H	0.374347	-1.632260	-2.615408
H	0.208725	-0.092443	-3.515316
H	1.425011	-1.303989	-4.033303
C	5.377370	1.696686	1.415814
H	5.505420	1.625532	2.513757

H	6.348885	1.424309	0.956450
H	5.169258	2.755736	1.164067
C	1.367013	1.040354	3.383876
H	0.765972	0.232255	2.920255
H	1.490775	0.793051	4.457580
H	0.790136	1.981760	3.328396

[(PPh_3)Au(*N*,*N*-diethylaniline)Cl]

-1480.95355107 A.U.

P	-1.098126		

[(PPh_3)Au(alkene)(*para*-*N*,*N*-diethylaniline)]$^+$

-1925.53443868 A.U.

P	0.288237	1.078435	0.057011
H	2.135204	-1.641531	-3.665409
C	2.141802	-1.948946	-2.606548
C	2.890463	-1.201304	-1.676148
C	2.957800	-2.898946	0.215144
C	3.272829	-1.620231	-0.310945
C	3.276213	-3.220217	1.542088
C	3.927012	-0.682966	0.526177
C	3.906245	-2.270675	2.370494
H	3.035240	-4.220603	1.934325
C	4.232398	-1.003023	1.856495
H	4.177819	0.312652	0.128456
H	4.149175	-2.523611	3.414118
H	4.728200	-0.256332	2.495497
C	0.076658	0.438323	1.763256
C	-0.424432	1.257852	2.801163
C	0.541883	-0.860630	2.061229
C	-0.460585	0.774046	4.119404
H	-0.784763	2.274777	2.581303
C	0.508976	-1.334976	3.382334
H	0.949713	-1.501305	1.263594
C	0.006956	-0.520335	4.412513
H	-0.854995	1.414408	4.923582
H	0.884419	-2.346124	3.602060
H	-0.021844	-0.894238	5.447819
C	-1.037726	2.328086	-0.187139
C	-0.765552	3.549019	-0.841391
C	-2.347448	2.055910	0.271163
C	-1.792721	4.488353	-1.036538
H	0.252904	3.782477	-1.186880
C	-3.360222	3.012836	0.094839
H	-2.573652	1.109722	0.787204
C	-3.089653	4.225737	-0.564470
H	-1.570360	5.438344	-1.546714
H	-4.370357	2.815269	0.485272
H	-3.889223	4.970260	-0.700878
C	1.868408	2.032774	0.112023
C	2.489405	2.383676	1.328688
C	2.506387	2.345494	-1.111189
C	3.737309	3.031811	1.318514
H	2.016084	2.130747	2.289065
C	3.746676	3.003555	-1.116043
H	2.037243	2.055988	-2.066651
C	4.368850	3.339895	0.101037
H	4.221237	3.292611	2.272602
H	4.234736	3.245350	-2.073040
H	5.348817	3.841794	0.098548
Au	0.639592	-0.657630	-1.513151
H	1.880274	-3.002886	-2.414602
H	3.369570	-0.269846	-2.026681
H	2.462460	-3.650608	-0.418509
C	-3.204260	-0.651305	-1.602623
C	-3.242160	-1.297021	-0.322948
C	-2.252585	-0.993235	-2.558303
C	-2.240570	-2.289053	-0.060499
C	-1.276924	-2.001964	-2.307736
H	-2.270802	-0.491051	-3.537916
C	-1.315915	-2.654557	-1.037765
H	-2.200737	-2.796349	0.911240
H	-0.714563	-2.442050	-3.145813

H	-0.610574	-3.473962	-0.824773
H	-3.937406	0.125950	-1.851634
N	-4.196420	-0.975402	0.614757
C	-5.318620	-0.080989	0.300521
H	-5.650706	0.379137	1.254887
H	-4.955073	0.760319	-0.321565
C	-4.238810	-1.638633	1.925246
H	-5.287131	-1.597215	2.285348
H	-4.013968	-2.720063	1.808250
C	-3.296073	-0.986308	2.941689
H	-3.348231	-1.501452	3.922359
H	-2.245167	-1.021622	2.592006
H	-3.560386	0.079511	3.099257
C	-6.483543	-0.799099	-0.391461
H	-7.315855	-0.093842	-0.591362
H	-6.158892	-1.236009	-1.357910
H	-6.875627	-1.622284	0.240369

[(PPh_3)Au(alkene)(*ortho*-*N*,*N*-diethylaniline)]$^+$

-1925.53513257 A.U.

P	0.260580	1.081837	-0.071209
H	0.074241	-3.436721	-2.185865
C	0.733144	-3.141206	-1.352965
C	1.723086	-2.157598	-1.572992
C	3.196140	-2.629090	0.446849
C	2.891584	-1.871119	-0.712398
C	4.266201	-2.262811	1.274928
C	3.703716	-0.753076	-1.025907
C	5.047250	-1.131644	0.967254
H	4.496228	-2.865350	2.167528
C	4.764744	-0.382225	-0.188624
H	3.481589	-0.158089	-1.925418
H	5.881167	-0.841435	1.624811
H	5.374846	0.498472	-0.441449
C	1.192250	1.386714	1.476892
C	1.354470	2.692162	2.000213
C	1.841048	0.300026	2.101255
C	2.147130	2.895996	3.141271
H	0.863043	3.551549	1.517563
C	2.639559	0.512558	3.236197
H	1.737556	-0.717539	1.693295
C	2.789416	1.807679	3.760979
H	2.266306	3.912656	3.547050
H	3.148366	-0.342411	3.707103
H	3.411179	1.972902	4.654687
C	-1.173581	2.239208	-0.073784
C	-1.729863	2.658616	-1.303048
C	-1.751093	2.686173	1.135828
C	-2.838007	3.521482	-1.320080
H	-1.287626	2.330360	-2.255955
C	-2.852454	3.559592	1.111855
H	-1.337584	2.358629	2.100426
C	-3.397919	3.980013	-0.113869
H	-3.257448	3.848349	-2.284223
H	-3.284404	3.914475	2.060614
H	-4.258311	4.666736	-0.129577
C	1.361215	1.674765	-1.434196
C	2.479591	2.499099	-1.191906
C	1.110536	1.214371	-2.747999
C	3.333406	2.854998	-2.250693
H	2.706384	2.845416	-0.172854
C	1.958508	1.583097	-3.804728
H	0.259835	0.540143	-2.943258
C	3.077045	2.399859	-3.555760
H	4.210618	3.489696	-2.050263
H	1.753182	1.220444	-4.823965
H	3.752053	2.677112	-4.380189
Au	-0.058202	-1.236721	-0.453667
H	0.833207	-3.881022	-0.541374
H	1.732952	-1.646244	-2.552406
H	2.594022	-3.514475	0.703366
C	-1.935327	-2.221238	0.731420
C	-2.806339	-1.063072	0.748829
C	-1.111909	-2.523971	1.861601

C	-2.757437	-0.244596	1.923800
C	-1.053600	-1.675587	2.966447
H	-0.523687	-3.454922	1.839244
C	-1.895514	-0.538987	2.979366
H	-3.410038	0.632146	2.005821
H	-0.396947	-1.899146	3.819072
H	-1.887481	0.130200	3.854533
H	-2.116648	-3.029200	0.008834
N	-3.606463	-0.753202	-0.321480
C	-3.607555	-1.588036	-1.524671
H	-3.927685	-0.943443	-2.368835
H	-2.554175	-1.877853	-1.752364
C	-4.508907	0.406430	-0.286809
H	-3.977428	1.262838	0.174536
H	-4.689423	0.708999	-1.338210
C	-4.507250	-2.830455	-1.450021
H	-4.416043	-3.430899	-2.378349
H	-4.241397	-3.480208	-0.591596
H	-5.571111	-2.542695	-1.333493
C	-5.840694	0.143326	0.427416
H	-5.678890	-0.171564	1.478716
H	-6.460356	1.063384	0.437179
H	-6.421154	-0.654147	-0.078223

[(PPh_3)Au(*para*-*N*,*N*-diethylaniline)+(PPh_3)Au(alkene)]$^+$ adduct

-3096.65329838 A.U.

P	4.093696	0.441261	0.043074
H	-0.490426	-0.502480	-1.166777
C	-0.232938	0.570641	-1.108377
C	-0.689953	1.258486	0.043297
C	-0.514715	3.633556	-0.786541
C	-0.622447	5.005101	-0.542186
C	-1.220621	3.177661	1.506841
C	-1.029827	5.471277	0.726265
H	-0.391507	5.724092	-1.343608
C	-1.319268	4.552751	1.749760
H	-1.470203	2.456601	2.300273
H	-1.114198	6.552286	0.914946
H	-1.634783	4.911254	2.740841
C	5.040660	1.641260	-0.969524
C	6.288897	1.311592	-1.540601
C	4.509598	2.941020	-1.128847
C	7.002695	2.284325	-2.262107
H	6.699305	0.295325	-1.429793
C	5.231827	3.907413	-1.846081
H	3.527450	3.191311	-0.693766
C	6.477774	3.580066	-2.412857
H	7.974723	2.026042	-2.710372
H	4.817180	4.919961	-1.969414
H	7.039858	4.338024	-2.980406
C	4.751559	-1.213940	-0.394716
C	5.434918	-2.030864	0.528555
C	4.479059	-1.695264	-1.696240
C	5.834244	-3.326616	0.152437
H	5.650293	-1.663075	1.543857
C	4.891092	-2.983498	-2.068466
H	3.933876	-1.061358	-2.415078
C	5.563769	-3.803665	-1.141791
H	6.361152	-3.965382	0.878101
H	4.678655	-3.353861	-3.083338
H	5.877707	-4.818592	-1.431171
C	4.580290	0.766958	1.779492
C	5.934742	1.010159	2.102219
C	3.602471	0.765696	2.797329
C	6.305328	1.228740	3.438660
H	6.697783	1.035787	1.307843
C	3.980745	0.986565	4.132451
H	2.545090	0.597317	2.539084
C	5.330505	1.214039	4.453986
H	7.360779	1.418391	3.688531
H	3.215794	0.988312	4.924536
H	5.624832	1.390277	5.500351
Au	1.814631	0.534416	-0.392061
H	-0.220953	1.093871	-2.081406

H	-0.948458	0.634562	0.916167
H	-0.200687	3.280059	-1.780193
P	-2.202231	-3.038834	0.021166
C	-4.392466	3.148489	1.026344
C	-4.145879	3.910979	-0.158142
C	-4.207770	1.761553	1.048511
C	-3.705256	3.187835	-1.307623
C	-3.754176	1.035492	-0.084098
H	-4.407397	1.230300	1.993728
C	-3.522541	1.803457	-1.258232
H	-3.514890	3.710242	-2.254604
H	-3.171491	1.300100	-2.174619
C	-2.881805	-4.345662	1.111636
C	-2.052523	-5.279052	1.772174
C	-4.284702	-4.418040	1.258866
C	-2.629043	-6.285656	2.564942
H	-0.957273	-5.214535	1.670071
C	-4.853605	-5.429722	2.050026
H	-4.925864	-3.674544	0.756816
C	-4.027215	-6.363125	2.701846
H	-1.982534	-7.012649	3.081099
H	-5.947411	-5.484580	2.164025
H	-4.475021	-7.152092	3.326224
C	-0.483358	-2.760031	0.644733
C	0.663659	-3.237500	-0.023422
C	-0.337178	-2.024025	1.843769
C	1.942661	-2.994411	0.510403
H	0.558939	-3.802653	-0.962670
C	0.939991	-1.788553	2.374907
H	-1.232307	-1.641802	2.362224
C	2.081580	-2.274828	1.709492
H	2.835881	-3.366700	-0.013233
H	1.045889	-1.227800	3.316973
H	3.083275	-2.086233	2.124184
C	-1.957989	-3.817371	-1.625491
C	-1.826687	-5.213604	-1.784724
C	-1.851080	-2.969211	-2.751149
C	-1.580961	-5.752607	-3.059380
H	-1.922512	-5.880751	-0.913597
C	-1.598268	-3.513544	-4.020841
H	-1.980822	-1.880588	-2.629371
C	-1.462326	-4.905420	-4.175851
H	-1.486386	-6.843061	-3.181045
H	-1.520837	-2.849226	-4.895787
H	-1.274050	-5.332645	-5.173303
Au	-3.259436	-0.949669	-0.024662
H	-4.716406	3.653540	1.947545
N	-4.312825	5.286090	-0.178825
C	-5.107026	5.981119	0.841078
H	-5.677445	6.786303	0.329309
H	-5.875251	5.286186	1.240093
C	-3.953315	6.077295	-1.357675
H	-3.696074	7.099703	-1.005519
H	-3.015063	5.666612	-1.783958
C	-0.799266	2.689358	0.240702
C	-4.283277	6.583525	1.984949
H	-4.937331	7.150934	2.678754
H	-3.767894	5.792856	2.564748
H	-3.510936	7.278806	1.596355
C	-5.054628	6.149414	-2.426520
H	-4.723808	6.768052	-3.286151
H	-5.315930	5.140129	-2.803922
H	-5.980617	6.605660	-2.019439

[(PPh_3)Au(*para*-*N*,*N*-diethylaniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3096.64103209 A.U.

P	3.782794	-1.367748	-0.071267
H	-0.849215	-0.225754	-1.476489
C	-0.024905	0.500561	-1.330290
C	-0.162025	1.295007	-0.089390
C	1.351070	3.222942	-0.772241
C	0.825547	2.365997	0.222684
C	2.300695	4.205254	-0.445788
C	1.276136	2.529788	1.554866

C	2.749995	4.345292	0.879364
H	2.701203	4.859636	-1.236042
C	2.236005	3.498718	1.880623
H	0.873872	1.867646	2.338704
H	3.498888	5.111276	1.134068
H	2.587314	3.596718	2.919832
C	5.090517	-0.076015	-0.241698
C	6.457762	-0.382468	-0.413065
C	4.682945	1.278747	-0.188227
C	7.404838	0.651769	-0.505684
H	6.792181	-1.427015	-0.493730
C	5.636955	2.305385	-0.268788
H	3.615676	1.541270	-0.099884
C	6.999170	1.995547	-0.425330
H	8.468308	0.402453	-0.645535
H	5.301062	3.352601	-0.220770
H	7.745645	2.801995	-0.497592
C	4.439836	-2.946819	-0.721014
C	5.524265	-3.623346	-0.112788
C	3.828222	-3.499090	-1.868546
C	5.994585	-4.829051	-0.657509
H	5.993350	-3.215380	0.796580
C	4.303743	-4.706205	-2.408738
H	2.974503	-2.976758	-2.331419
C	5.387116	-5.369514	-1.806213
H	6.839012	-5.351267	-0.181224
H	3.824981	-5.130395	-3.305022
H	5.758690	-6.315251	-2.230784
C	3.557106	-1.603503	1.749054
C	3.261133	-0.457179	2.522387
C	3.503698	-2.877936	2.352579
C	2.919508	-0.587470	3.876949
H	3.285404	0.542924	2.062028
C	3.161320	-3.001877	3.711656
H	3.717011	-3.783898	1.765673
C	2.865766	-1.860408	4.475950
H	2.693338	0.312867	4.469898
H	3.122967	-4.001458	4.172105
H	2.595941	-1.961473	5.538700
Au	1.754109	-0.563034	-0.890573
H	0.118401	1.098145	-2.252596
H	-0.404646	0.690642	0.801225
H	1.018621	3.109563	-1.813817
P	-3.638443	-1.669196	0.064409
C	-1.620461	4.527378	1.098809
C	-1.430264	5.214700	-0.150268
C	-1.870734	3.167318	1.124892
C	-1.634758	4.452654	-1.355390
C	-1.959489	2.359252	-0.064481
H	-1.941878	2.672779	2.108113
C	-1.888324	3.093853	-1.298698
H	-1.573278	4.941923	-2.336610
H	-1.978890	2.539287	-2.247687
C	-4.426403	-2.353414	-1.441632
C	-5.163210	-3.557114	-1.409917
C	-4.241292	-1.671850	-2.665448
C	-5.704464	-4.075322	-2.598346
H	-5.321576	-4.085368	-0.456508
C	-4.779407	-2.199668	-3.850507
H	-3.678650	-0.723322	-2.683913
C	-5.511222	-3.400634	-3.817573
H	-6.284414	-5.010997	-2.570576
H	-4.634825	-1.665493	-4.802493
H	-5.939939	-3.809179	-4.746037
C	-4.595032	-2.287540	1.496095
C	-4.322499	-3.539550	2.090918
C	-5.652629	-1.487806	1.982383
C	-5.115913	-3.989378	3.159935
H	-3.487329	-4.157011	1.723040
C	-6.443634	-1.946805	3.048102
H	-5.847600	-0.503153	1.526048
C	-6.176354	-3.196831	3.635965
H	-4.903490	-4.964839	3.624861
H	-7.268133	-1.322644	3.426274

H	-6.794283	-3.553088	4.475023
C	-1.982589	-2.480021	0.168561
C	-1.470721	-3.285389	-0.868462
C	-1.170419	-2.175798	1.287402
C	-0.158456	-3.786487	-0.781007
H	-2.093061	-3.518582	-1.746522
C	0.133611	-2.682761	1.372636
H	-1.564074	-1.532636	2.091986
C	0.641300	-3.489363	0.334626
H	0.242524	-4.410370	-1.594842
H	0.767757	-2.437016	2.238272
H	1.668578	-3.879642	0.392731
Au	-3.079043	0.584773	0.014138
H	-1.516387	5.065320	2.049984
N	-1.048591	6.524271	-0.192096
C	-0.852630	7.315702	1.031505
H	-1.020126	8.379689	0.763865
H	-1.649343	7.065527	1.761335
C	-0.709125	7.196995	-1.454687
H	0.061471	7.961131	-1.220796
H	-0.211624	6.470917	-2.130344
C	-1.917978	7.851573	-2.134128
H	-2.689366	7.098541	-2.394315
H	-2.389541	8.601917	-1.466892
H	-1.608046	8.368044	-3.065369
C	0.539991	7.126005	1.646408
H	0.715358	6.064880	1.915782
H	1.333536	7.419937	0.928918
H	0.651430	7.748255	2.557661

[(PPh_3)Au(*para*-*N*,*N*-diethylaniline)--(PPh_3)Au(alkene)]$^+$ Intermediate Markovnikov
-3096.67024907 A.U.

P	4.314717	-0.061796	-0.095772
H	-0.531121	-0.145735	-1.223569
C	0.104266	0.762685	-1.095188
C	-0.430803	1.633284	0.071625
C	0.314004	3.961275	-0.700230
C	0.411540	2.902033	0.224852
C	1.165161	5.076788	-0.608974
C	1.373471	2.991610	1.254652
C	2.122892	5.154156	0.418480
H	1.078569	5.892481	-1.344269
C	2.220140	4.108491	1.353971
H	1.478784	2.159205	1.970632
H	2.787284	6.029236	0.493622
H	2.963042	4.161699	2.165619
C	5.320838	1.371933	-0.668504
C	6.716245	1.295020	-0.865779
C	4.652303	2.603229	-0.865506
C	7.434338	2.441607	-1.245002
H	7.247041	0.339508	-0.735248
C	5.379857	3.748537	-1.227989
H	3.559712	2.669630	-0.732223
C	6.770374	3.669809	-1.419663
H	8.521977	2.374402	-1.404425
H	4.847644	4.702553	-1.367015
H	7.339517	4.565797	-1.713448
C	5.198200	-1.591188	-0.589309
C	6.364071	-2.048911	0.067338
C	4.674007	-2.328493	-1.675218
C	6.996181	-3.227494	-0.363329
H	6.770077	-1.492012	0.926812
C	5.311872	-3.504883	-2.102773
H	3.755445	-1.976367	-2.173454
C	6.472248	-3.955224	-1.447624
H	7.902966	-3.580760	0.152200
H	4.900124	-4.073733	-2.951180
H	6.969966	-4.879286	-1.781149
C	4.416539	0.012580	1.746988
C	4.378209	1.272335	2.384450
C	4.369859	-1.160488	2.533458
C	4.287722	1.355444	3.783566
H	4.417470	2.192765	1.782335
C	4.283151	-1.071872	3.933527

H	4.412327	-2.151677	2.056052
C	4.236653	0.185289	4.562389
H	4.263166	2.343896	4.269090
H	4.257357	-1.993466	4.536329
H	4.170395	0.252578	5.659513
Au	2.076949	0.193692	-0.720527
H	0.060919	1.331815	-2.051124
H	-0.298242	1.059742	1.015451
H	-0.432156	3.911890	-1.509884
P	-2.680988	-2.400793	0.120357
C	-3.836545	3.128192	1.115435
C	-4.483186	3.401078	-0.137356
C	-2.621460	2.453165	1.170884
C	-3.824047	2.927235	-1.320081
C	-1.939896	1.975969	-0.006538
H	-2.129886	2.314473	2.147879
C	-2.604869	2.254121	-1.254305
H	-4.280259	3.075476	-2.307175
H	-2.113983	1.941533	-2.189409
C	-3.229142	-3.200385	-1.431809
C	-3.817790	-4.482786	-1.433486
C	-3.002784	-2.522067	-2.651583
C	-4.172512	-5.082743	-2.654284
H	-4.003827	-5.011182	-0.485279
C	-3.351789	-3.132895	-3.865945
H	-2.551033	-1.515976	-2.646477
C	-3.937905	-4.412612	-3.867898
H	-4.636261	-6.081388	-2.655087
H	-3.171520	-2.604754	-4.815117
H	-4.218134	-4.887333	-4.821140
C	-3.493388	-3.266093	1.507089
C	-2.928859	-4.438894	2.055661
C	-4.721011	-2.769939	1.997070
C	-3.601299	-5.114716	3.087498
H	-1.964055	-4.815773	1.680325
C	-5.387371	-3.453746	3.026573
H	-5.145370	-1.844218	1.574208
C	-4.828635	-4.624992	3.570727
H	-3.162145	-6.027710	3.518831
H	-6.343960	-3.067187	3.410969
H	-5.350240	-5.156555	4.381902
C	-0.875840	-2.725932	0.264495
C	-0.157547	-3.413012	-0.735003
C	-0.195414	-2.184514	1.380704
C	1.235989	-3.559619	-0.611790
H	-0.680369	-3.827120	-1.610878
C	1.192320	-2.340084	1.498314
H	-0.753581	-1.626538	2.150662
C	1.908447	-3.027544	0.499491
H	1.802421	-4.085315	-1.395847
H	1.726073	-1.903006	2.356233
H	3.001251	-3.130454	0.572363
Au	-2.802392	-0.110843	0.091290
H	-4.285706	3.466964	2.057810
N	-5.676801	4.072037	-0.197520
C	-6.390990	4.498388	1.013573
H	-7.472067	4.530664	0.763119
H	-6.294696	3.713172	1.792543
C	-6.301865	4.428607	-1.478286
H	-6.889989	5.355186	-1.311785
H	-5.514474	4.711058	-2.207633
C	-7.203239	3.321160	-2.039616
H	-7.667794	3.641407	-2.994534
H	-6.627750	2.391758	-2.228653
H	-8.018419	3.075402	-1.328185
C	-5.927170	5.860620	1.545019
H	-4.851256	5.842607	1.813957
H	-6.071197	6.654119	0.783078
H	-6.505658	6.144975	2.447693

[(PPh_3)Au(*para*-*N*,*N*-diethylaniline -alkene)] Markovnikov

-1925.11818411 A.U.

P	2.971103	-0.290699	0.005452
H	-1.550993	-2.499763	0.422183

C	-1.258053	-1.525149	-0.027214
C	-2.032618	-0.366479	0.656843
C	-1.739816	1.533012	-1.037375
C	-1.451495	0.986643	0.231556
C	-1.126778	2.723732	-1.464998
C	-0.545416	1.678266	1.064894
C	-0.212663	3.393582	-0.628748
H	-1.363543	3.133004	-2.460829
C	0.077011	2.864802	0.641833
H	-0.299275	1.257866	2.053487
H	0.276093	4.320225	-0.969297
H	0.801303	3.365262	1.304227
C	3.296698	0.561570	-1.592886
C	4.546084	0.533560	-2.246255
C	2.224606	1.295873	-2.151134
C	4.721771	1.240582	-3.449754
H	5.381879	-0.040935	-1.816464
C	2.411983	2.008347	-3.345156
H	1.244196	1.316241	-1.647072
C	3.658843	1.980505	-3.997890
H	5.697431	1.212924	-3.960636
H	1.572447	2.583317	-3.766869
H	3.801543	2.534125	-4.939628
C	4.437912	-1.358597	0.295227
C	5.625316	-0.873601	0.885637
C	4.358189	-2.707563	-0.115112
C	6.725144	-1.731979	1.054851
H	5.685079	0.175566	1.216904
C	5.462940	-3.559296	0.050699
H	3.420061	-3.084473	-0.555803
C	6.646359	-3.072677	0.635561
H	7.649037	-1.351764	1.519037
H	5.395852	-4.610893	-0.269883
H	7.509491	-3.743447	0.771978
C	3.113656	1.064493	1.248788
C	3.684003	2.317290	0.941369
C	2.574619	0.838847	2.534887
C	3.714621	3.333212	1.912982
H	4.085774	2.506422	-0.066345
C	2.608476	1.855501	3.501974
H	2.103127	-0.131035	2.764448
C	3.175364	3.106030	3.191345
H	4.153657	4.312422	1.664414
H	2.177339	1.676002	4.499488
H	3.189864	3.907464	3.946863
Au	0.805886	-1.181398	0.035394
H	-1.532422	-1.570614	-1.107226
H	-1.849022	-0.452342	1.752549
H	-2.457638	1.010971	-1.690648
C	-5.743032	0.650311	0.884807
C	-6.427739	-0.344498	0.124611
C	-4.353488	0.613385	1.040005
C	-5.622168	-1.365829	-0.452424
C	-3.552744	-0.394947	0.457954
H	-3.865561	1.414201	1.621141
C	-4.227661	-1.379279	-0.287683
H	-6.082892	-2.178386	-1.031531
H	-3.656817	-2.196388	-0.753922
H	-6.298150	1.477777	1.348475
N	-7.811618	-0.314283	-0.043436
C	-8.644231	0.670051	0.638395
H	-9.648059	0.217772	0.796620
H	-8.243635	0.851073	1.659387
C	-8.492546	-1.254790	-0.926160
H	-9.404025	-0.754687	-1.321658
H	-7.858389	-1.450524	-1.818099
C	-8.879220	-2.576424	-0.242666
H	-9.401453	-3.255349	-0.949604
H	-7.980818	-3.099894	0.143332
H	-9.555019	-2.391234	0.618531
C	-8.784860	1.997500	-0.124736
H	-7.794144	2.472210	-0.278132
H	-9.235253	1.830762	-1.125725
H	-9.431676	2.711133	0.428255

[(PPh_3)Au(*ortho*-*N*,*N*-diethylaniline)+(PPh_3)Au(alkene)]$^+$ adduct

-3096.68109008 A.U.

P	2.227317	-1.500513	0.479355
H	-0.693351	0.755970	-2.957413
C	0.397786	0.904446	-2.911613
C	0.916610	1.931430	-2.123752
C	3.323789	1.982243	-2.941620
C	2.298821	2.434829	-2.072386
C	4.629437	2.467109	-2.803981
C	2.617101	3.378484	-1.064917
C	4.934670	3.409049	-1.798739
H	5.419419	2.115093	-3.485170
C	3.926804	3.861434	-0.929409
H	1.833645	3.711743	-0.368451
H	5.963670	3.788701	-1.698595
H	4.155212	4.589241	-0.135744
C	3.951909	-0.918521	0.681330
C	4.967187	-1.829076	1.055169
C	4.252632	0.452401	0.523914
C	6.274725	-1.364707	1.270635
H	4.735719	-2.899398	1.174814
C	5.562265	0.906970	0.747418
H	3.470716	1.169759	0.227677
C	6.572593	0.002521	1.119362
H	7.065370	-2.074990	1.558358
H	5.787649	1.976236	0.618364
H	7.599556	0.362321	1.288552
C	2.349005	-3.211779	-0.176776
C	1.649939	-4.291900	0.399300
C	3.113678	-3.410803	-1.349959
C	1.710344	-5.562315	-0.202964
H	1.061645	-4.148574	1.318777
C	3.183247	-4.684653	-1.933803
H	3.657066	-2.565814	-1.802984
C	2.474989	-5.761398	-1.365339
H	1.161506	-6.403529	0.248102
H	3.787777	-4.837462	-2.841281
H	2.523471	-6.758806	-1.829064
C	1.512827	-1.613084	2.163151
C	2.316973	-1.444927	3.311931
C	0.125230	-1.839451	2.306187
C	1.733972	-1.507800	4.588446
H	3.395038	-1.247587	3.212945
C	-0.446468	-1.918085	3.584774
H	-0.520454	-1.949005	1.422554
C	0.355455	-1.747294	4.726990
H	2.363571	-1.364671	5.480154
H	-1.526350	-2.103321	3.678446
H	-0.097302	-1.795001	5.729529
Au	1.053624	-0.150752	-0.991971
H	0.989616	0.409227	-3.699298
H	0.202514	2.483498	-1.487330
H	3.095555	1.246386	-3.727978
P	-2.785219	-0.765501	-0.319049
C	0.487395	4.665720	1.755436
C	-0.425876	3.689887	1.299074
C	1.743743	4.305783	2.273299
C	-0.078379	2.304794	1.347594
C	2.086708	2.946257	2.359275
H	2.438636	5.083935	2.626949
C	1.181587	1.970330	1.904810
H	3.057322	2.638061	2.780666
H	1.464935	0.912105	2.003018
C	-2.030217	-1.648340	-1.745993
C	-2.410614	-1.345052	-3.070228
C	-0.942428	-2.526925	-1.521743
C	-1.702082	-1.899867	-4.151956
H	-3.259450	-0.669224	-3.259203
C	-0.248132	-3.090670	-2.605112
H	-0.646128	-2.802752	-0.498373
C	-0.618322	-2.765574	-3.922914
H	-2.006213	-1.655573	-5.181826
H	0.587496	-3.778594	-2.410380

H	-0.068694	-3.200012	-4.772363
C	-4.341093	-0.048313	-0.978216
C	-5.497480	-0.843089	-1.139848
C	-4.358710	1.309303	-1.365857
C	-6.661303	-0.277925	-1.685774
H	-5.491166	-1.900825	-0.831791
C	-5.525192	1.866455	-1.916436
H	-3.460248	1.930574	-1.226508
C	-6.676357	1.074789	-2.074839
H	-7.564211	-0.896755	-1.805460
H	-5.535780	2.926410	-2.214723
H	-7.592769	1.514290	-2.498812
C	-3.322004	-2.050054	0.877172
C	-3.420869	-3.421158	0.558761
C	-3.696355	-1.597423	2.163662
C	-3.882659	-4.331695	1.526147
H	-3.141483	-3.780043	-0.444205
C	-4.173705	-2.509737	3.118093
H	-3.607281	-0.526774	2.413505
C	-4.261230	-3.878654	2.802309
H	-3.955763	-5.401706	1.276248
H	-4.471518	-2.151286	4.115838
H	-4.628227	-4.594641	3.554110
Au	-1.320647	0.835569	0.602149
H	0.173571	5.719771	1.706383
N	-1.705622	4.169533	0.825792
C	-1.843287	4.207956	-0.628070
H	-1.726422	3.175024	-1.073981
H	-2.889906	4.508340	-0.853602
C	-2.879977	3.610872	1.503821
H	-3.763577	4.190839	1.157576
H	-3.074089	2.542519	1.187468
C	-2.777557	3.667162	3.026302
H	-1.964164	3.011487	3.398737
H	-2.566412	4.701275	3.367798
H	-3.728840	3.331374	3.486939
C	-0.882165	5.177219	-1.317246
H	-1.045507	5.174022	-2.414668
H	-1.033777	6.208666	-0.939397
H	0.177399	4.909428	-1.133271-

[(PPh_3)Au(*ortho*- *N*,*N*-diethylaniline)--(PPh_3)Au(alkene)]$^+$ TS Markovnikov

-3096.63605427 A.U.

P	3.918057	-0.990459	-0.208530
H	-0.756260	0.263679	-1.171528
C	0.037587	1.008961	-0.968533
C	-0.069522	1.610658	0.380696
C	1.517225	3.539029	-0.120930
C	0.963696	2.614525	0.794243
C	2.517252	4.436962	0.280041
C	1.443172	2.618271	2.123486
C	2.989421	4.425526	1.606371
H	2.939317	5.145900	-0.449354
C	2.453032	3.507910	2.526559
H	1.023360	1.899323	2.845299
H	3.774972	5.129929	1.921747
H	2.820569	3.487339	3.564431
C	5.249561	0.284196	-0.246134
C	6.585496	0.001188	-0.602571
C	4.887100	1.607552	0.102485
C	7.549801	1.023801	-0.583422
H	6.881138	-1.011020	-0.914890
C	5.859203	2.619223	0.132600
H	3.839021	1.862244	0.331791
C	7.192652	2.330226	-0.206865
H	8.588428	0.794880	-0.868923
H	5.559369	3.641160	0.410746
H	7.952760	3.126889	-0.191476
C	4.478536	-2.464138	-1.136820
C	5.599342	-3.234301	-0.743121
C	3.736583	-2.846897	-2.276679
C	5.972965	-4.363585	-1.489827
H	6.173302	-2.961727	0.156628
C	4.114898	-3.978370	-3.018813

H	2.854907	-2.254169	-2.571617
C	5.233147	-4.735408	-2.627765
H	6.845681	-4.958969	-1.179184
H	3.533290	-4.269609	-3.907307
H	5.529436	-5.622240	-3.209534
C	3.762452	-1.507658	1.561524
C	3.437129	-0.502267	2.502753
C	3.792456	-2.856278	1.974489
C	3.154201	-0.844460	3.833478
H	3.385060	0.553911	2.194736
C	3.505543	-3.193095	3.310401
H	4.024639	-3.656669	1.256338
C	3.184459	-2.191499	4.241791
H	2.905055	-0.052016	4.556794
H	3.530970	-4.249424	3.620463
H	2.958315	-2.458984	5.285706
Au	1.867035	-0.044082	-0.787677
H	0.099241	1.739575	-1.800385
H	-0.238974	0.858086	1.170834
H	1.168862	3.540477	-1.164231
P	-3.482144	-1.477667	0.169559
C	-1.505611	4.981168	0.268644
C	-1.772619	3.677747	-0.260113
C	-1.410268	5.210221	1.636512
C	-1.840497	2.549051	0.677449
C	-1.558479	4.155858	2.573781
H	-1.225622	6.236740	1.991504
C	-1.763252	2.876595	2.089384
H	-1.492805	4.352320	3.654144
H	-1.808655	2.041964	2.809048
C	-1.807668	-2.254091	0.093462
C	-1.328074	-2.925860	-1.048852
C	-0.952897	-2.064117	1.206326
C	-0.003355	-3.401918	-1.074496
H	-1.982732	-3.076294	-1.921215
C	0.362992	-2.545530	1.177413
H	-1.321286	-1.527076	2.096392
C	0.839606	-3.213841	0.032435
H	0.373006	-3.920338	-1.970118
H	1.029456	-2.385963	2.038688
H	1.876584	-3.580043	0.001394
C	-4.317981	-1.920512	-1.400866
C	-5.287731	-2.942696	-1.472749
C	-3.959627	-1.208442	-2.568883
C	-5.889512	-3.248863	-2.706276
H	-5.580093	-3.496047	-0.566605
C	-4.555676	-1.527462	-3.798570
H	-3.208391	-0.404248	-2.511840
C	-5.524234	-2.546548	-3.867830
H	-6.650657	-4.042901	-2.757336
H	-4.269556	-0.973014	-4.705994
H	-5.998965	-2.790215	-4.831032
C	-4.375499	-2.326578	1.517661
C	-4.131773	-3.686467	1.813173
C	-5.345955	-1.604049	2.245441
C	-4.867326	-4.319454	2.828501
H	-3.364424	-4.244411	1.252844
C	-6.079695	-2.245677	3.256901
H	-5.515520	-0.538219	2.019837
C	-5.841442	-3.601382	3.547199
H	-4.678034	-5.378877	3.061716
H	-6.836079	-1.682794	3.825524
H	-6.414681	-4.100970	4.343812
Au	-2.966081	0.760730	0.444112
H	-1.415213	5.843036	-0.405178
N	-1.850854	3.511077	-1.626672
C	-1.334428	4.541406	-2.544389
H	-0.873351	4.003193	-3.401490
H	-0.499332	5.064662	-2.038482
C	-2.670219	2.462110	-2.263394
H	-2.340620	2.388705	-3.319683
H	-2.427697	1.486160	-1.798921
C	-4.181182	2.711295	-2.174693
H	-4.499587	2.793504	-1.114582

H	-4.486225	3.636714	-2.699787
H	-4.729222	1.857081	-2.623369
C	-2.366081	5.552251	-3.064317
H	-1.859677	6.335243	-3.665139
H	-3.120287	5.069442	-3.717129
H	-2.904312	6.047497	-2.230918

[(PPh_3)Au(*ortho*- *N,N*-diethylaniline-alkene)Au(PPh_3)]$^+$ Intermediate Markovnikov

-3096.66968724 A.U.

P	4.056811	-0.916037	0.050082
H	-0.523648	-0.269712	-1.779691
C	0.256914	0.521991	-1.675486
C	-0.211889	1.612098	-0.685210
C	1.178766	3.605814	-1.468562
C	0.859119	2.679468	-0.456981
C	2.192883	4.560571	-1.271714
C	1.569156	2.730623	0.760680
C	2.892658	4.607271	-0.052445
H	2.434404	5.275804	-2.073648
C	2.576411	3.687222	0.965005
H	1.337475	1.995872	1.548784
H	3.681144	5.359196	0.106772
H	3.117882	3.718610	1.923832
C	5.380517	0.277975	-0.416072
C	6.751168	-0.058293	-0.422183
C	4.980653	1.593481	-0.750257
C	7.709950	0.916498	-0.746293
H	7.076493	-1.083401	-0.188610
C	5.946157	2.565974	-1.056713
H	3.911173	1.860297	-0.773144
C	7.311131	2.229620	-1.056476
H	8.777579	0.646568	-0.757084
H	5.619565	3.587668	-1.305777
H	8.067812	2.989413	-1.307669
C	4.705783	-2.608753	-0.218573
C	5.693319	-3.187840	0.612724
C	4.195194	-3.343493	-1.312188
C	6.165638	-4.482972	0.344367
H	6.083716	-2.630844	1.479328
C	4.674459	-4.637689	-1.577518
H	3.418002	-2.891505	-1.950733
C	5.658886	-5.207364	-0.750673
H	6.934228	-4.929991	0.994167
H	4.276136	-5.204017	-2.433848
H	6.032333	-6.222472	-0.957939
C	3.882535	-0.729541	1.880510
C	3.908176	0.568036	2.439605
C	3.561368	-1.829963	2.706156
C	3.607255	0.759381	3.797852
H	4.162193	1.434047	1.809299
C	3.265457	-1.633301	4.066467
H	3.544693	-2.849411	2.290984
C	3.281455	-0.338716	4.615009
H	3.635474	1.775356	4.222794
H	3.023996	-2.500646	4.700899
H	3.050778	-0.186806	5.681028
Au	2.026159	-0.325432	-0.948248
H	0.440089	0.950148	-2.686531
H	-0.343116	1.099624	0.287501
H	0.628823	3.579183	-2.423565
P	-3.561899	-1.431711	0.119246
C	-3.075525	4.215558	-0.658145
C	-3.585076	4.093882	-1.963893
C	-2.096146	3.333359	-0.141225
C	-3.136091	3.074230	-2.808792
C	-1.548770	2.313697	-1.025915
H	-4.356614	4.799878	-2.308917
C	-2.121448	2.195635	-2.342541
H	-3.526855	2.963175	-3.830715
H	-1.624113	1.524269	-3.061597
C	-4.518007	-2.652412	-0.845151
C	-5.029833	-3.804514	-0.206603
C	-4.700220	-2.468138	-2.232447
C	-5.716220	-4.768286	-0.961584

H	-4.897434	-3.945083	0.878210
C	-5.387585	-3.438800	-2.980591
H	-4.306744	-1.562523	-2.722948
C	-5.894062	-4.586885	-2.346324
H	-6.118657	-5.665075	-0.465557
H	-5.532269	-3.293939	-4.062297
H	-6.436781	-5.344118	-2.933351
C	-4.395118	-1.230047	1.733965
C	-3.995041	-1.957910	2.875503
C	-5.483253	-0.332380	1.810147
C	-4.680973	-1.777576	4.089307
H	-3.146293	-2.657413	2.820347
C	-6.167570	-0.165182	3.023187
H	-5.783904	0.244267	0.919963
C	-5.763752	-0.883374	4.164361
H	-4.366415	-2.341137	4.981420
H	-7.013737	0.536628	3.081623
H	-6.296060	-0.743824	5.118115
C	-1.903228	-2.158691	0.421463
C	-1.430248	-3.226704	-0.368151
C	-1.038874	-1.524991	1.345993
C	-0.098440	-3.657649	-0.229179
H	-2.096230	-3.716523	-1.095543
C	0.285987	-1.960744	1.478682
H	-1.405271	-0.684976	1.957291
C	0.758160	-3.026101	0.686247
H	0.273236	-4.486725	-0.850615
H	0.964581	-1.460626	2.186039
H	1.805632	-3.353119	0.770504
Au	-3.075451	0.548564	-0.926772
H	-3.470494	5.010965	-0.010237
N	-1.601190	3.472851	1.159349
C	-1.753240	2.344748	2.090536
H	-1.447049	1.413269	1.577278
H	-1.026362	2.485680	2.918857
C	-1.594572	4.806180	1.779496
H	-2.626612	5.207359	1.937680
H	-1.174800	4.668281	2.797779
C	-3.181618	2.179380	2.626155
H	-3.267565	1.275151	3.264260
H	-3.502237	3.055895	3.225451
H	-3.893556	2.057036	1.782749
C	-0.729105	5.805424	1.007408
H	-1.119031	5.989452	-0.014126
H	-0.702226	6.778774	1.537915
H	0.305893	5.421992	0.906867

[(PPh_3)Au(*ortho*- *N*,*N*-diethylaniline-alkene)] Markovnikov

-1925.11756015 A.U.

P	2.506451	-0.153920	0.133536
H	-1.615880	-3.079260	0.140907
C	-1.398363	-2.121386	-0.381533
C	-2.410948	-1.029239	0.050781
C	-2.148610	0.600542	-1.899882
C	-2.007306	0.332949	-0.523260
C	-1.710843	1.822001	-2.443893
C	-1.419760	1.321079	0.294742
C	-1.118562	2.795550	-1.617803
H	-1.834647	2.015766	-3.521771
C	-0.970399	2.537681	-0.241232
H	-1.301985	1.121151	1.371397
H	-0.767487	3.748042	-2.045368
H	-0.495875	3.281117	0.419075
C	2.973977	0.569009	-1.493397
C	4.307057	0.680181	-1.939292
C	1.917289	1.051598	-2.300086
C	4.580063	1.276121	-3.184297
H	5.132233	0.301608	-1.315503
C	2.199189	1.656608	-3.533829
H	0.872739	0.960656	-1.959779
C	3.529821	1.767883	-3.979727
H	5.622037	1.357390	-3.532633
H	1.368365	2.036795	-4.149015
H	3.748921	2.235607	-4.952836

C	4.054430	-0.883031	0.802721
C	5.021436	-0.115701	1.488266
C	4.275226	-2.261222	0.587500
C	6.204102	-0.723538	1.943030
H	4.845280	0.956940	1.668992
C	5.462314	-2.861915	1.038596
H	3.504483	-2.858505	0.072279
C	6.427163	-2.094030	1.715699
H	6.955652	-0.123369	2.480187
H	5.630249	-3.937080	0.868540
H	7.354625	-2.567550	2.075015
C	2.176382	1.331373	1.176385
C	2.608767	2.622995	0.809884
C	1.411663	1.158954	2.351360
C	2.280052	3.729280	1.613052
H	3.186208	2.766350	-0.116801
C	1.087739	2.265685	3.151546
H	1.045506	0.154115	2.619348
C	1.518237	3.553617	2.781694
H	2.614306	4.736351	1.317276
H	0.482827	2.124408	4.061088
H	1.253120	4.423430	3.403399
Au	0.549774	-1.424739	-0.061205
H	-1.485469	-2.317011	-1.475189
H	-2.324594	-0.935117	1.153637
H	-2.617520	-0.158298	-2.546907
C	-6.228605	-0.597316	-0.257072
C	-6.581734	-1.666379	-1.097054
C	-4.895439	-0.414586	0.173847
C	-5.598674	-2.579972	-1.506007
C	-3.881667	-1.313552	-0.281909
H	-7.628775	-1.790286	-1.417876
C	-4.265258	-2.395693	-1.096609
H	-5.862191	-3.430383	-2.154937
H	-3.494682	-3.100805	-1.442003
H	-7.002592	0.108462	0.081598
N	-4.532398	0.665177	1.034669
C	-4.313357	0.304118	2.439816
H	-3.680001	-0.607915	2.468715
H	-3.711002	1.114200	2.912169
C	-5.181893	1.959565	0.825378
H	-6.284860	1.936086	1.031478
H	-4.756762	2.650824	1.586676
C	-5.593901	0.048180	3.253565
H	-5.347435	-0.271947	4.287909
H	-6.225787	0.958033	3.325108
H	-6.200192	-0.752750	2.780788
C	-4.925692	2.527917	-0.572410
H	-5.302650	1.842938	-1.359225
H	-5.440927	3.503474	-0.693482
H	-3.840726	2.671539	-0.744195

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)]$^+$ TS anti-Markovnikov

-3096.63717109 A.U.

P	-4.284764	-0.328124	-0.173793
H	0.403732	-0.360363	0.128667
C	0.039982	0.651217	0.392318
C	0.352182	1.632772	-0.612714
C	0.899236	0.003064	2.650367
C	0.248748	0.959212	1.837130
C	1.209935	0.286037	3.990180
C	-0.108772	2.201860	2.412939
C	0.862396	1.530189	4.546819
H	1.730373	-0.470656	4.598848
C	0.195902	2.484146	3.752619
H	-0.627414	2.954306	1.797624
H	1.102496	1.755029	5.597718
H	-0.088454	3.456643	4.184841
C	-5.476824	0.712507	0.747364
C	-6.611406	0.154894	1.376226
C	-5.256510	2.107156	0.790424
C	-7.523006	0.994807	2.038662
H	-6.777442	-0.933852	1.353911
C	-6.174504	2.939396	1.450242

H	-4.359748	2.534703	0.311870
C	-7.306822	2.384060	2.074614
H	-8.406080	0.559983	2.532296
H	-6.001729	4.026302	1.484423
H	-8.022029	3.037785	2.597841
C	-4.500454	-2.030906	0.481952
C	-5.153196	-3.044590	-0.250187
C	-3.939819	-2.323154	1.746629
C	-5.236344	-4.345284	0.279650
H	-5.587084	-2.823223	-1.237799
C	-4.038357	-3.619614	2.273894
H	-3.412981	-1.535589	2.310555
C	-4.679971	-4.634163	1.537782
H	-5.740364	-5.136676	-0.296656
H	-3.604031	-3.842478	3.261112
H	-4.746263	-5.653904	1.948021
C	-4.876714	-0.394708	-1.907136
C	-6.237838	-0.209879	-2.233154
C	-3.941308	-0.695552	-2.922185
C	-6.656911	-0.337198	-3.568574
H	-6.968206	0.035862	-1.445984
C	-4.368416	-0.826411	-4.253097
H	-2.877131	-0.816664	-2.660335
C	-5.726285	-0.648489	-4.576514
H	-7.718038	-0.189994	-3.823280
H	-3.637854	-1.059531	-5.043391
H	-6.060077	-0.745344	-5.621427
Au	-2.058618	0.310193	0.039747
H	0.119157	2.696867	-0.450139
H	0.347481	1.308180	-1.664637
H	1.176661	-0.966920	2.211244
P	3.243364	-2.166633	-0.212438
C	2.515087	4.273144	-1.828829
C	2.480483	5.053480	-0.623116
C	2.573597	2.885736	-1.784814
C	2.521545	4.331487	0.615499
C	2.566251	2.140401	-0.557210
H	2.589180	2.337407	-2.741516
C	2.574241	2.942309	0.637548
H	2.532968	4.869881	1.572786
H	2.612770	2.441977	1.617297
C	3.782221	-2.781346	1.430594
C	4.023919	-4.154939	1.655916
C	3.911151	-1.860527	2.493724
C	4.379322	-4.601005	2.939127
H	3.941618	-4.875377	0.826533
C	4.263382	-2.314555	3.776234
H	3.735053	-0.787627	2.313805
C	4.495508	-3.683176	4.000099
H	4.572024	-5.671449	3.111433
H	4.366991	-1.591881	4.600745
H	4.777961	-4.037037	5.004021
C	4.157353	-3.140536	-1.465599
C	3.693475	-4.390047	-1.933219
C	5.378586	-2.616355	-1.944061
C	4.457180	-5.113277	-2.864912
H	2.730855	-4.791938	-1.578188
C	6.138685	-3.347670	-2.871266
H	5.725547	-1.630879	-1.591439
C	5.679373	-4.595547	-3.330998
H	4.094289	-6.086669	-3.230572
H	7.090593	-2.937370	-3.242709
H	6.274023	-5.164877	-4.062437
C	1.477665	-2.688257	-0.370731
C	0.733869	-3.181148	0.721636
C	0.822302	-2.419251	-1.596386
C	-0.652129	-3.387189	0.593192
H	1.235568	-3.397515	1.677726
C	-0.556131	-2.646642	-1.723070
H	1.397389	-2.019665	-2.447809
C	-1.299711	-3.121589	-0.625029
H	-1.235688	-3.755321	1.450386
H	-1.055946	-2.447939	-2.683920
H	-2.383287	-3.289154	-0.715120

Au	3.139729	0.151684	-0.444924
H	2.489709	4.768351	-2.809077
N	2.414949	6.424941	-0.656439
C	2.486503	7.177637	-1.914666
H	2.946549	8.161889	-1.685526
H	3.196262	6.675575	-2.604051
C	2.285475	7.225685	0.567135
H	1.735203	8.152673	0.299277
H	1.630528	6.690931	1.286111
C	1.119019	7.375659	-2.582199
H	0.655385	6.401977	-2.841945
H	0.422010	7.913981	-1.906976
H	1.220448	7.970603	-3.512956
C	3.633644	7.576306	1.210644
H	4.187966	6.661062	1.501649
H	4.272914	8.149034	0.507498
H	3.484013	8.196432	2.118203

[(PPh_3)Au(*para*- *N*,*N*-diethylaniline -alkene)Au(PPh_3)]$^+$ Intermediate anti-Markovnikov

-3096.68796070 A.U.

P	-4.519480	0.199137	-0.370599
H	0.164488	0.942241	-0.243922
C	-0.414744	1.678937	0.357441
C	0.078407	3.094696	-0.036982
C	-0.086189	-0.052725	2.180267
C	-0.296847	1.303678	1.813014
C	-0.041795	-0.455972	3.523898
C	-0.444310	2.237791	2.870094
C	-0.184697	0.488858	4.556824
H	0.104828	-1.521586	3.764280
C	-0.385379	1.839434	4.216060
H	-0.623431	3.299318	2.637306
H	-0.149788	0.177652	5.612396
H	-0.506730	2.593963	5.009980
C	-5.826745	0.944365	0.681117
C	-6.801104	0.161693	1.337889
C	-5.850889	2.351326	0.805918
C	-7.800574	0.787702	2.102621
H	-6.773117	-0.936909	1.260390
C	-6.854921	2.969733	1.568223
H	-5.073725	2.957002	0.310845
C	-7.830335	2.189175	2.215742
H	-8.558630	0.175579	2.615981
H	-6.871143	4.066574	1.664543
H	-8.613328	2.675695	2.818260
C	-4.412888	-1.551859	0.199846
C	-4.944973	-2.635846	-0.527876
C	-3.726112	-1.793118	1.413523
C	-4.799217	-3.948748	-0.040926
H	-5.469802	-2.460970	-1.479983
C	-3.594062	-3.102661	1.899348
H	-3.278261	-0.953793	1.971704
C	-4.129443	-4.184052	1.172936
H	-5.215159	-4.791340	-0.615283
H	-3.060663	-3.279570	2.846380
H	-4.020448	-5.212395	1.551742
C	-5.234519	0.135082	-2.061294
C	-6.604465	-0.136695	-2.274581
C	-4.381945	0.346323	-3.167374
C	-7.107365	-0.218673	-3.583510
H	-7.279103	-0.276691	-1.414901
C	-4.890480	0.262127	-4.474752
H	-3.321913	0.593627	-2.992790
C	-6.251314	-0.024373	-4.683489
H	-8.175980	-0.429353	-3.746074
H	-4.223484	0.431996	-5.334499
H	-6.650411	-0.085053	-5.708115
Au	-2.399502	1.151447	-0.126091
H	-0.302984	3.855133	0.677147
H	-0.340825	3.379699	-1.022561
H	-0.007436	-0.805191	1.381799
P	2.601560	-1.712273	-0.167695
C	3.654048	3.220605	-1.501308
C	4.495259	2.839681	-0.409944

C	2.268180	3.345290	-1.349491
C	3.819658	2.572002	0.851321
C	1.592027	3.131955	-0.123121
H	1.674394	3.627274	-2.234969
C	2.404887	2.796968	0.982644
H	4.411056	2.493761	1.777157
H	1.957867	2.700753	1.984375
C	2.671660	-2.936456	1.189853
C	2.775562	-4.315501	0.899352
C	2.582327	-2.498004	2.528099
C	2.778191	-5.248489	1.948595
H	2.859963	-4.658615	-0.144092
C	2.585239	-3.438534	3.571768
H	2.498292	-1.422022	2.749484
C	2.681420	-4.811494	3.283244
H	2.861109	-6.323039	1.723175
H	2.515321	-3.093652	4.615122
H	2.688267	-5.546715	4.103082
C	3.753304	-2.313513	-1.463249
C	3.300431	-3.127390	-2.524108
C	5.123914	-1.988672	-1.356896
C	4.220295	-3.617653	-3.467480
H	2.230507	-3.371506	-2.618191
C	6.036088	-2.485637	-2.300606
H	5.472162	-1.341452	-0.536124
C	5.585456	-3.300097	-3.356354
H	3.865762	-4.250569	-4.295862
H	7.104425	-2.232770	-2.214742
H	6.301885	-3.685105	-4.098698
C	0.926361	-1.817246	-0.904820
C	-0.057056	-2.696901	-0.406552
C	0.615338	-0.934471	-1.964946
C	-1.345116	-2.692609	-0.969383
H	0.174179	-3.375975	0.428543
C	-0.670449	-0.942010	-2.523663
H	1.376618	-0.230121	-2.339164
C	-1.651851	-1.818799	-2.024416
H	-2.117929	-3.366330	-0.571232
H	-0.912957	-0.246962	-3.342053
H	-2.667358	-1.811570	-2.448480
Au	3.090432	0.434966	0.478681
H	4.093246	3.449373	-2.480897
N	5.855640	2.728971	-0.531276
C	6.523831	2.864909	-1.832652
H	7.435034	2.230672	-1.803782
H	5.881855	2.419530	-2.621633
C	6.717672	2.405495	0.611167
H	7.711488	2.859440	0.414492
H	6.339174	2.919786	1.518849
C	6.897209	4.312615	-2.174273
H	5.997329	4.958489	-2.229196
H	7.572285	4.739630	-1.404341
H	7.419336	4.361574	-3.151638
C	6.864284	0.898218	0.860162
H	5.883438	0.427816	1.085816
H	7.288785	0.390794	-0.030795
H	7.539761	0.706755	1.718378

[(PPh_3)Au(*para*- *N,N*-diethylaniline -alkene)] anti-Markovnikov

-1925.11488118 A.U.

P	3.063643	-0.241667	0.002894
H	-1.641253	-0.909138	-1.291124
C	-1.326753	-0.541555	-0.289251
C	-2.134263	-1.311618	0.784900
C	-1.487461	1.709145	-1.465560
C	-1.439592	0.963344	-0.259760
C	-1.460840	3.112158	-1.465321
C	-1.399186	1.701712	0.952942
C	-1.403276	3.824432	-0.252512
H	-1.489079	3.657052	-2.423148
C	-1.378694	3.105337	0.957576
H	-1.346810	1.159129	1.909845
H	-1.387607	4.926051	-0.249657
H	-1.337454	3.644538	1.918259

C	3.766798	-0.431524	1.692267
C	4.666238	0.497110	2.257931
C	3.384760	-1.575371	2.429085
C	5.188486	0.273289	3.544046
H	4.954176	1.399039	1.695098
C	3.915079	-1.796870	3.710123
H	2.660442	-2.284557	1.994582
C	4.818071	-0.873442	4.268812
H	5.887536	1.002717	3.983132
H	3.613412	-2.690063	4.279663
H	5.227350	-1.044188	5.277167
C	3.307797	1.534719	-0.434762
C	4.536069	2.008715	-0.947753
C	2.233706	2.435895	-0.247336
C	4.690313	3.371300	-1.255862
H	5.370490	1.309038	-1.116520
C	2.395179	3.795587	-0.559262
H	1.257192	2.081718	0.124273
C	3.621731	4.265878	-1.061027
H	5.649515	3.734200	-1.658280
H	1.540908	4.476487	-0.420295
H	3.743759	5.331654	-1.312146
C	4.234585	-1.147545	-1.089146
C	5.535865	-1.512488	-0.682494
C	3.791122	-1.471470	-2.391329
C	6.387596	-2.185413	-1.576418
H	5.882247	-1.273694	0.335627
C	4.648483	-2.137655	-3.281226
H	2.765989	-1.204899	-2.698553
C	5.947920	-2.495167	-2.875501
H	7.401618	-2.470208	-1.253511
H	4.296800	-2.387455	-4.294687
H	6.617186	-3.023755	-3.572678
Au	0.778195	-0.724050	-0.163670
H	-1.814619	-1.015747	1.806585
H	-1.889617	-2.391328	0.693301
H	-1.524192	1.162811	-2.422732
C	-5.724439	-1.581128	-0.574455
C	-6.443345	-0.609123	0.181308
C	-4.359854	-1.807558	-0.352937
C	-5.706104	0.096606	1.175077
C	-3.628726	-1.105057	0.627891
H	-3.845247	-2.569059	-0.964142
C	-4.342054	-0.152116	1.382834
H	-6.192270	0.867789	1.788767
H	-3.813393	0.429934	2.155069
H	-6.235945	-2.183675	-1.338028
N	-7.798798	-0.364537	-0.040458
C	-8.512196	-0.973546	-1.156815
H	-9.315183	-0.272103	-1.474571
H	-7.831734	-1.051013	-2.032557
C	-8.557856	0.546995	0.807576
H	-9.618162	0.210629	0.808363
H	-8.218440	0.439520	1.860750
C	-9.121680	-2.346564	-0.829251
H	-8.334939	-3.067709	-0.526919
H	-9.843991	-2.267671	0.010252
H	-9.659627	-2.765159	-1.706200
C	-8.477216	2.017676	0.365829
H	-7.426844	2.373823	0.367851
H	-8.870931	2.142104	-0.664871
H	-9.069355	2.671758	1.040404

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov (where alkene = H_2C=C(Ph(*p*Me))(Me))

-3096.64068991 A.U.

P	3.914039	-1.204320	-0.052101
H	-0.682649	-0.022487	-0.803134
C	0.041239	0.820287	-0.798656
C	-0.262410	1.774197	0.323395
C	0.948924	3.656869	-0.910030
C	0.465100	3.096917	0.298737
C	1.521232	4.934170	-0.952456
C	0.619160	3.880509	1.466218
C	1.635620	5.726902	0.211925

H	1.883949	5.330490	-1.915786
C	1.194453	5.161001	1.425093
H	0.264237	3.499364	2.434285
H	1.294493	5.736775	2.360107
C	5.303272	-0.104096	0.426651
C	6.273436	-0.494527	1.376212
C	5.399592	1.157660	-0.201237
C	7.339744	0.368361	1.681232
H	6.188984	-1.467836	1.885818
C	6.469566	2.013498	0.107122
H	4.626272	1.468354	-0.923297
C	7.440364	1.619433	1.045993
H	8.094744	0.062674	2.422430
H	6.541160	2.997016	-0.382953
H	8.276156	2.293918	1.289700
C	4.556676	-2.291861	-1.384076
C	5.888642	-2.761838	-1.377283
C	3.676471	-2.691412	-2.414427
C	6.327907	-3.635649	-2.385244
H	6.585025	-2.439401	-0.587137
C	4.121692	-3.567624	-3.418710
H	2.644528	-2.303582	-2.428234
C	5.445323	-4.042074	-3.403437
H	7.367710	-3.998233	-2.378653
H	3.433828	-3.873835	-4.222406
H	5.794798	-4.724856	-4.193682
C	3.668283	-2.303161	1.404877
C	3.174385	-1.703862	2.587108
C	3.866440	-3.697703	1.358418
C	2.890319	-2.493315	3.711495
H	3.004286	-0.614933	2.617521
C	3.564695	-4.486808	2.484100
H	4.251297	-4.171448	0.441774
C	3.078577	-3.888455	3.659249
H	2.511381	-2.020447	4.631058
H	3.715326	-5.576796	2.440649
H	2.846180	-4.509400	4.538459
Au	1.913617	-0.096161	-0.517564
H	0.014220	1.287073	-1.802938
H	0.865238	3.082997	-1.843392
P	-3.597213	-1.747318	0.017642
C	-2.426818	4.686064	1.006436
C	-2.102096	5.269133	-0.268965
C	-2.443728	3.312577	1.151418
C	-2.101813	4.397484	-1.415204
C	-2.143924	2.401232	0.068488
H	-2.615578	2.903492	2.160554
C	-2.116761	3.029835	-1.235352
H	-2.007663	4.808054	-2.429030
H	-1.993629	2.389810	-2.124629
C	-4.544098	-2.323372	-1.444452
C	-5.004518	-3.655832	-1.534107
C	-4.778248	-1.425228	-2.508458
C	-5.688857	-4.082885	-2.682807
H	-4.837187	-4.359060	-0.703381
C	-5.460671	-1.860640	-3.657692
H	-4.428997	-0.382256	-2.429944
C	-5.915538	-3.187729	-3.745323
H	-6.050977	-5.120765	-2.748064
H	-5.643923	-1.156708	-4.484344
H	-6.455647	-3.526497	-4.643264
C	-4.383704	-2.496759	1.492140
C	-4.091322	-3.815029	1.909230
C	-5.337965	-1.729967	2.196748
C	-4.759132	-4.360438	3.018237
H	-3.332753	-4.409746	1.375740
C	-6.004548	-2.283884	3.302039
H	-5.551530	-0.696695	1.876564
C	-5.716351	-3.598061	3.712481
H	-4.529146	-5.387205	3.343227
H	-6.748499	-1.684057	3.848982
H	-6.236746	-4.029195	4.582002
C	-1.931586	-2.525781	-0.131582
C	-1.424667	-2.891739	-1.396304

C	-1.097169	-2.604129	1.008214
C	-0.099044	-3.344193	-1.514675
H	-2.066493	-2.824791	-2.288766
C	0.223517	-3.061902	0.883153
H	-1.485056	-2.310657	1.997018
C	0.722630	-3.433121	-0.378914
H	0.291880	-3.632073	-2.503214
H	0.874522	-3.121696	1.768316
H	1.759419	-3.788289	-0.471488
Au	-3.120261	0.523907	0.099444
H	-2.601207	5.324858	1.882347
N	-1.761038	6.580875	-0.378901
C	-1.660487	7.420531	0.815547
H	-1.257336	8.408948	0.532712
H	-2.651464	7.576716	1.293836
H	-0.970225	6.963510	1.556183
C	-1.379951	7.140033	-1.676040
H	-2.218841	7.097093	-2.403054
H	-1.096878	8.199577	-1.546834
H	-0.509850	6.593977	-2.100123
C	-0.285003	1.083834	1.692361
H	-0.698979	0.062269	1.596052
H	0.757629	0.990939	2.065350
H	-0.870974	1.626357	2.457194
C	2.211577	7.121757	0.145606
H	3.267331	7.108737	-0.200183
H	1.650490	7.753092	-0.577217
H	2.186318	7.628142	1.130959

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov (where alkene = H_2C=C(Ph(*p*OMe))(Me))

-3171.79769685 A.U.

P	3.753555	-1.638636	-0.037382
H	-0.707963	-0.040041	-0.719957
C	0.079096	0.744105	-0.719840
C	-0.158531	1.723326	0.400479
C	1.227435	3.484760	-0.821888
C	0.668740	2.983527	0.376414
C	1.895408	4.718238	-0.885287
C	0.849428	3.778616	1.538224
C	2.011363	5.511487	0.277698
H	2.310147	5.052346	-1.846617
C	1.510268	5.009157	1.499780
H	0.448182	3.437890	2.503090
H	1.647364	5.613683	2.409074
C	5.269303	-0.706309	0.413839
C	6.203995	-1.202860	1.348922
C	5.496604	0.536400	-0.218140
C	7.364830	-0.464817	1.636130
H	6.018150	-2.160498	1.861151
C	6.661096	1.266170	0.070736
H	4.750183	0.932001	-0.926795
C	7.595677	0.766252	0.995978
H	8.091750	-0.852386	2.367053
H	6.835862	2.234993	-0.422713
H	8.505463	1.342890	1.225469
C	4.244078	-2.774264	-1.395618
C	5.513176	-3.394523	-1.416938
C	3.311733	-3.049670	-2.420406
C	5.836521	-4.293549	-2.446533
H	6.252630	-3.168957	-0.632240
C	3.640639	-3.951815	-3.446455
H	2.331022	-2.546585	-2.412980
C	4.900676	-4.575937	-3.458966
H	6.827662	-4.773282	-2.461101
H	2.912116	-4.161123	-4.245432
H	5.159388	-5.279110	-4.266071
C	3.423710	-2.720324	1.415381
C	3.003263	-2.087101	2.608460
C	3.488764	-4.127185	1.357280
C	2.659957	-2.855484	3.730893
H	2.935591	-0.987432	2.649114
C	3.127786	-4.893509	2.481204
H	3.814006	-4.628524	0.432148
C	2.714974	-4.261583	3.666649

H	2.338656	-2.356402	4.658512
H	3.172996	-5.992476	2.427807
H	2.435060	-4.864886	4.544308
Au	1.870934	-0.321631	-0.454350
H	0.077013	1.210583	-1.724792
H	1.134870	2.899295	-1.747257
P	-3.767459	-1.543107	-0.016759
C	-2.112134	4.763929	1.090815
C	-1.717344	5.326645	-0.174005
C	-2.230541	3.394475	1.224811
C	-1.787980	4.469817	-1.329870
C	-1.979471	2.471216	0.138758
H	-2.447549	2.991645	2.227726
C	-1.906030	3.105830	-1.161324
H	-1.665359	4.882729	-2.339830
H	-1.828593	2.464944	-2.055221
C	-4.730297	-1.991121	-1.512681
C	-5.402777	-3.229206	-1.609636
C	-4.752024	-1.091550	-2.601159
C	-6.084274	-3.563077	-2.791045
H	-5.404026	-3.929797	-0.759965
C	-5.431013	-1.434698	-3.782674
H	-4.239009	-0.119186	-2.514986
C	-6.096542	-2.669495	-3.878249
H	-6.612661	-4.526604	-2.862080
H	-5.447125	-0.729905	-4.628547
H	-6.634527	-2.934937	-4.801772
C	-4.642612	-2.260752	1.422329
C	-4.467933	-3.608875	1.808500
C	-5.539408	-1.433744	2.134232
C	-5.195439	-4.123031	2.894816
H	-3.755168	-4.252004	1.268154
C	-6.265526	-1.956185	3.217059
H	-5.661174	-0.378617	1.838017
C	-6.094573	-3.299737	3.597064
H	-5.057458	-5.173287	3.195980
H	-6.964002	-1.309308	3.770293
H	-6.661266	-3.706684	4.449128
C	-2.175082	-2.462725	-0.162033
C	-1.703851	-2.907725	-1.414683
C	-1.349600	-2.580382	0.981072
C	-0.420492	-3.473648	-1.517471
H	-2.338535	-2.813954	-2.309748
C	-0.072107	-3.149458	0.871376
H	-1.712163	-2.227146	1.960089
C	0.392941	-3.596285	-0.379232
H	-0.056407	-3.823733	-2.496179
H	0.573250	-3.236003	1.758344
H	1.397023	-4.037878	-0.461633
Au	-3.099980	0.676014	0.132912
H	-2.255663	5.410010	1.967085
N	-1.247480	6.598955	-0.266200
C	-1.103622	7.427332	0.931936
H	-0.541452	8.342410	0.675590
H	-2.090201	7.725794	1.348580
H	-0.530158	6.884419	1.711444
C	-0.814970	7.135798	-1.556619
H	-1.665650	7.248252	-2.263234
H	-0.362633	8.131239	-1.401855
H	-0.051444	6.473490	-2.016954
C	-0.228622	1.035874	1.769579
H	-0.734953	0.055919	1.679833
H	0.806338	0.849131	2.128689
H	-0.753441	1.627558	2.542356
O	2.573343	6.752491	0.324187
C	3.175561	7.274498	-0.854207
H	4.005433	6.626842	-1.217493
H	2.436366	7.403590	-1.678217
H	3.585496	8.265436	-0.582476

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov (where alkene = H_2C=CH(Ph(*p*CF_3)))

-3354.86277862 A.U.

P	-2.644255	2.811417	-0.016360
H	1.229123	0.047999	-1.388093

C	0.180447	-0.309657	-1.367478
C	-0.105257	-1.198969	-0.210103
C	-2.219782	-2.202442	-1.204288
C	-1.472616	-1.786643	-0.075048
C	-3.448621	-2.854763	-1.056811
C	-2.030221	-2.002573	1.205374
C	-3.957317	-3.113615	0.231167
H	-4.013237	-3.177576	-1.944886
C	-3.261035	-2.655541	1.364488
H	-1.472495	-1.669683	2.094888
H	-3.675442	-2.830765	2.367721
C	-4.355417	2.154376	-0.226681
C	-5.491732	2.984621	-0.336482
C	-4.515862	0.748244	-0.267328
C	-6.769843	2.413690	-0.462496
H	-5.388748	4.079653	-0.342576
C	-5.796896	0.184579	-0.379409
H	-3.635358	0.086071	-0.229119
C	-6.926282	1.016560	-0.475228
H	-7.649702	3.069522	-0.554436
H	-5.907698	-0.909561	-0.404256
H	-7.930187	0.574521	-0.572400
C	-2.613056	4.557923	-0.558387
C	-3.335391	5.574102	0.112249
C	-1.824605	4.888971	-1.683005
C	-3.275062	6.899090	-0.348491
H	-3.933268	5.334020	1.005723
C	-1.769082	6.216998	-2.139326
H	-1.252048	4.097956	-2.195042
C	-2.494654	7.221038	-1.474574
H	-3.838672	7.686093	0.176497
H	-1.155166	6.468151	-3.018230
H	-2.449708	8.261600	-1.832229
C	-2.341498	2.825358	1.808540
C	-2.544782	1.617066	2.515350
C	-1.764541	3.927169	2.475417
C	-2.178580	1.517906	3.866196
H	-2.984920	0.745141	2.006021
C	-1.400191	3.821614	3.830357
H	-1.585307	4.872483	1.941388
C	-1.602333	2.618823	4.527932
H	-2.346663	0.573837	4.408243
H	-0.951917	4.688550	4.340338
H	-1.314971	2.539207	5.587874
Au	-1.078654	1.325284	-0.904209
H	-0.078751	-0.740532	-2.355363
H	0.262243	-0.796743	0.750647
H	-1.824764	-2.017054	-2.212496
P	4.308592	0.027378	0.074423
C	-0.211007	-4.660780	0.969892
C	-0.773809	-5.107007	-0.277400
C	0.645045	-3.576477	0.992342
C	-0.199995	-4.577995	-1.489830
C	1.042237	-2.858616	-0.199357
H	0.976539	-3.197038	1.973537
C	0.667689	-3.503205	-1.435825
H	-0.495858	-4.982281	-2.466954
H	1.009083	-3.057489	-2.385020
C	5.328178	0.394212	-1.401732
C	6.520679	1.144406	-1.311191
C	4.868507	-0.052261	-2.661210
C	7.242812	1.448468	-2.477461
H	6.889463	1.484699	-0.330643
C	5.591660	0.262635	-3.823062
H	3.944772	-0.651596	-2.725364
C	6.779050	1.011785	-3.731635
H	8.175904	2.028639	-2.404773
H	5.232219	-0.087307	-4.803278
H	7.350137	1.250395	-4.642480
C	5.417351	0.113583	1.526076
C	5.676137	1.333230	2.189730
C	6.048143	-1.074924	1.955505
C	6.571459	1.359941	3.272344
H	5.172568	2.257289	1.863744

C	6.945275	-1.038578	3.035270
H	5.828764	-2.026573	1.443579
C	7.206940	0.177405	3.693150
H	6.772851	2.310138	3.791289
H	7.437216	-1.965240	3.369436
H	7.906522	0.202574	4.543273
C	3.137630	1.447052	0.240149
C	3.021745	2.449560	-0.743609
C	2.245420	1.436546	1.339760
C	2.019552	3.431054	-0.626550
H	3.706056	2.460872	-1.606276
C	1.251197	2.417779	1.452816
H	2.326502	0.646139	2.104575
C	1.135670	3.415959	0.464851
H	1.925422	4.208873	-1.400198
H	0.548583	2.399752	2.299828
H	0.345766	4.178310	0.542683
Au	2.841138	-1.767584	-0.084312
H	-0.510006	-5.131426	1.915556
N	-1.840741	-5.950259	-0.307234
C	-2.452391	-6.418667	0.937598
H	-3.385245	-6.958710	0.702885
H	-1.775968	-7.101521	1.495753
H	-2.716371	-5.561637	1.591945
C	-2.433659	-6.351662	-1.582809
H	-1.728093	-6.958379	-2.190107
H	-3.337463	-6.954529	-1.390542
H	-2.737951	-5.461344	-2.172591
C	-5.234426	-3.907385	0.364953
F	-5.115389	-5.123973	-0.253723
F	-5.566223	-4.145890	1.653329
F	-6.289189	-3.283890	-0.226872

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov (where alkene = H_2C=CH(Ph(*p*Cl)))

-3477.56799923 A.U.

P	3.355408	-2.045163	-0.015755
H	-1.017775	-0.106877	-1.230693
C	-0.075611	0.476826	-1.223500
C	-0.002516	1.445629	-0.093882
C	1.885055	2.817572	-1.109684
C	1.209927	2.311465	0.025933
C	2.984264	3.678608	-0.982107
C	1.693197	2.681302	1.300863
C	3.416458	4.051606	0.302425
H	3.507967	4.063094	-1.869522
C	2.791694	3.538344	1.452559
H	1.189047	2.291189	2.199366
H	3.165269	3.812813	2.449543
C	4.644812	-0.948772	0.698074
C	5.592721	-1.445961	1.622616
C	4.675366	0.415198	0.327542
C	6.572158	-0.589468	2.151042
H	5.552719	-2.499402	1.943318
C	5.656345	1.267226	0.863135
H	3.917615	0.817393	-0.365517
C	6.606298	0.764948	1.769826
H	7.309460	-0.980414	2.869646
H	5.669403	2.330889	0.579519
H	7.372941	1.434540	2.190472
C	4.145367	-3.128472	-1.268858
C	5.520966	-3.442361	-1.251651
C	3.308651	-3.686204	-2.262781
C	6.049922	-4.315620	-2.217092
H	6.183958	-2.996963	-0.493936
C	3.842052	-4.567573	-3.217538
H	2.239196	-3.416967	-2.288028
C	5.212799	-4.882319	-3.195326
H	7.125107	-4.553268	-2.205818
H	3.187092	-5.000849	-3.989530
H	5.632865	-5.565843	-3.949712
C	2.874083	-3.162154	1.365861
C	2.519330	-2.575950	2.603224
C	2.723285	-4.552127	1.182792
C	2.020739	-3.375371	3.643508

H	2.633820	-1.489436	2.748694
C	2.211494	-5.345810	2.225630
H	3.005829	-5.017885	0.225327
C	1.858500	-4.761373	3.454163
H	1.753435	-2.914198	4.607248
H	2.095238	-6.430675	2.076477
H	1.461432	-5.386746	4.268800
Au	1.515876	-0.832145	-0.764846
H	0.075476	0.929106	-2.224629
H	-0.272749	0.997020	0.878540
H	1.546345	2.531520	-2.115464
P	-4.137151	-0.709001	0.096715
C	-0.664421	4.834461	0.989238
C	-0.183800	5.350414	-0.265606
C	-1.280450	3.598620	1.036252
C	-0.622962	4.686318	-1.466838
C	-1.489700	2.776503	-0.136655
H	-1.547406	3.187643	2.024374
C	-1.247697	3.456017	-1.388146
H	-0.399867	5.114434	-2.453078
H	-1.472379	2.922828	-2.326898
C	-5.318113	-1.090743	-1.251911
C	-6.199176	-2.190947	-1.161676
C	-5.306991	-0.289564	-2.414445
C	-7.057724	-2.486432	-2.232490
H	-6.221202	-2.812021	-0.252297
C	-6.166472	-0.593516	-3.484016
H	-4.626581	0.576216	-2.474389
C	-7.041153	-1.690597	-3.393371
H	-7.747575	-3.341574	-2.158849
H	-6.157989	0.034718	-4.388273
H	-7.719200	-1.924171	-4.229106
C	-4.986652	-1.088708	1.673852
C	-5.000906	-2.391311	2.220580
C	-5.671783	-0.040982	2.328199
C	-5.705563	-2.640665	3.410360
H	-4.451084	-3.206032	1.723014
C	-6.377586	-0.299323	3.514579
H	-5.644618	0.977445	1.906420
C	-6.395058	-1.597911	4.055524
H	-5.714941	-3.656005	3.836689
H	-6.911681	0.518711	4.022536
H	-6.945173	-1.797483	4.988427
C	-2.779894	-1.950173	-0.062142
C	-2.570968	-2.659343	-1.262916
C	-1.848233	-2.075021	0.996495
C	-1.442864	-3.489788	-1.399227
H	-3.287427	-2.563378	-2.093935
C	-0.732821	-2.914359	0.858722
H	-1.997378	-1.510351	1.931433
C	-0.527004	-3.620732	-0.342436
H	-1.285032	-4.039908	-2.340037
H	-0.009925	-3.014208	1.682226
H	0.354710	-4.271769	-0.443679
Au	-3.009016	1.319146	-0.021430
H	-0.485682	5.386289	1.921548
N	0.697125	6.386319	-0.310983
C	1.240408	6.955421	0.923997
H	2.080426	7.627463	0.675353
H	0.475904	7.539080	1.481415
H	1.634212	6.154118	1.583437
C	1.204207	6.870350	-1.594822
H	0.383976	7.245349	-2.242771
H	1.907161	7.703348	-1.418762
H	1.747082	6.064926	-2.136120
Cl	4.760497	5.167549	0.473427

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov (where alkene = $H_2C=C(Ph)_2$)

-3248.96651583 A.U.

P	-4.018398	-0.587750	-0.231843
H	0.459809	0.954211	-2.071817
C	0.095401	0.717107	-1.053438
C	0.286825	1.817201	-0.063928
C	0.531645	0.391039	2.062917

C	-0.119443	1.418616	1.347861
C	0.056793	-0.062991	3.302256
C	-1.307546	1.949799	1.911769
C	-1.111622	0.491854	3.856412
H	0.603326	-0.861496	3.829555
C	-1.800026	1.489921	3.143689
H	-1.886381	2.700104	1.355188
H	-1.494782	0.134621	4.825032
H	-2.745485	1.903097	3.529660
C	-3.787504	-2.049574	0.858045
C	-4.382466	-3.301301	0.604304
C	-2.894518	-1.899280	1.944214
C	-4.084864	-4.396089	1.438683
H	-5.075377	-3.425050	-0.242863
C	-2.614875	-2.989263	2.779935
H	-2.412604	-0.927401	2.130976
C	-3.206408	-4.242625	2.526188
H	-4.547725	-5.374805	1.237321
H	-1.920210	-2.858738	3.624620
H	-2.980169	-5.102618	3.175766
C	-5.310398	-1.065251	-1.436129
C	-6.680517	-1.062174	-1.095152
C	-4.900708	-1.492852	-2.718110
C	-7.632538	-1.492596	-2.033838
H	-7.000787	-0.717626	-0.098750
C	-5.857967	-1.928324	-3.649961
H	-3.829571	-1.472426	-2.980145
C	-7.222330	-1.928055	-3.307943
H	-8.701835	-1.485915	-1.770695
H	-5.538805	-2.260071	-4.650319
H	-7.972647	-2.262494	-4.041438
C	-4.731460	0.699603	0.873091
C	-5.398452	0.371163	2.073162
C	-4.541487	2.056567	0.526245
C	-5.864492	1.392505	2.919104
H	-5.536063	-0.683480	2.359030
C	-5.011461	3.072202	1.373782
H	-3.999291	2.315535	-0.398138
C	-5.668333	2.741697	2.573834
H	-6.380152	1.131219	3.856489
H	-4.853020	4.127199	1.100773
H	-6.028424	3.539114	3.242709
Au	-1.924223	0.111271	-0.956602
H	0.586407	-0.214254	-0.713555
H	1.439445	-0.060407	1.625568
P	3.226661	-2.169544	-0.129402
C	3.008051	4.205071	-1.248063
C	3.202152	4.928288	-0.020519
C	2.620226	2.879182	-1.221741
C	3.089722	4.195286	1.212108
C	2.401638	2.143703	-0.001233
H	2.408178	2.379753	-2.181924
C	2.696213	2.867043	1.207167
H	3.271374	4.693974	2.173405
H	2.559974	2.356532	2.174895
C	3.382134	-2.959987	1.521997
C	3.493635	-4.363601	1.636918
C	3.335188	-2.163310	2.686771
C	3.546865	-4.960594	2.906340
H	3.542155	-4.991795	0.733627
C	3.386039	-2.766975	3.955422
H	3.268421	-1.066709	2.599515
C	3.489735	-4.164485	4.065938
H	3.636763	-6.054777	2.991586
H	3.353954	-2.139745	4.860062
H	3.534743	-4.636916	5.059723
C	4.456605	-2.969375	-1.223120
C	4.187560	-4.183985	-1.892926
C	5.720785	-2.353899	-1.356489
C	5.186323	-4.781631	-2.679642
H	3.194164	-4.653591	-1.812497
C	6.715269	-2.960254	-2.141064
H	5.917509	-1.395203	-0.848429
C	6.449341	-4.173903	-2.800966

H	4.975304	-5.726709	-3.204060
H	7.700186	-2.478845	-2.243827
H	7.228407	-4.645174	-3.420362
C	1.566518	-2.679828	-0.748143
C	0.556944	-3.116125	0.135825
C	1.257641	-2.463340	-2.112297
C	-0.742928	-3.351212	-0.344942
H	0.778744	-3.269627	1.203212
C	-0.044540	-2.689952	-2.582526
H	2.037209	-2.103501	-2.803297
C	-1.047444	-3.132267	-1.698697
H	-1.524266	-3.697870	0.345256
H	-0.280143	-2.511088	-3.643009
H	-2.072765	-3.302529	-2.061878
Au	3.091240	0.150683	-0.065746
H	3.119241	4.709557	-2.216207
N	3.450037	6.270066	-0.026809
C	3.424423	7.019167	-1.284161
H	3.589774	8.090684	-1.073355
H	4.223950	6.681442	-1.977976
H	2.442644	6.911573	-1.794083
C	3.609025	7.002030	1.228395
H	4.434033	6.581545	1.841258
H	3.856515	8.055792	1.008247
H	2.676794	6.983726	1.836063
C	-0.107290	3.208702	-0.485441
C	-0.006860	4.301326	0.411600
C	-0.538748	3.481800	-1.806712
C	-0.283867	5.613593	-0.002751
C	-0.820424	4.792025	-2.221462
C	-0.682818	5.868734	-1.326051
H	0.302857	4.119208	1.449540
H	-0.668830	2.653643	-2.517282
H	-0.189702	6.441859	0.717648
H	-1.158316	4.973324	-3.254113
H	-0.903286	6.896930	-1.654031

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov (where alkene = H_2C=CH(Ph(*p*Me)))

-3057.35146849 A.U.

P	3.458771	-1.801824	-0.020087
H	-0.949600	-0.043419	-1.494890
C	-0.019902	0.552394	-1.395618
C	-0.025679	1.438353	-0.199462
C	1.821201	3.001494	-0.999453
C	1.146695	2.332438	0.045824
C	2.901760	3.858044	-0.731564
C	1.606141	2.547986	1.366578
C	3.354709	4.077915	0.586087
H	3.413759	4.358901	-1.569673
C	2.691057	3.393094	1.631260
H	1.098443	2.033085	2.198453
H	3.033722	3.529346	2.670257
C	4.950846	-0.728666	-0.192859
C	6.261257	-1.245484	-0.283431
C	4.750709	0.672187	-0.230235
C	7.356961	-0.371635	-0.387393
H	6.435221	-2.331460	-0.291880
C	5.851776	1.538312	-0.323418
H	3.732328	1.093972	-0.206206
C	7.156245	1.019964	-0.399844
H	8.375068	-0.784313	-0.463895
H	5.678269	2.624632	-0.352768
H	8.018310	1.700256	-0.482972
C	3.892780	-3.486741	-0.584627
C	4.822843	-4.305946	0.099378
C	3.262229	-3.972481	-1.752059
C	5.118582	-5.589647	-0.387116
H	5.307320	-3.946932	1.021286
C	3.564527	-5.257138	-2.234942
H	2.531587	-3.335217	-2.277358
C	4.491994	-6.065104	-1.554178
H	5.841875	-6.223732	0.149027
H	3.071843	-5.628555	-3.146947
H	4.726849	-7.072469	-1.932075

C	3.144090	-1.914503	1.798332
C	2.999885	-0.697746	2.505244
C	2.871991	-3.132912	2.456068
C	2.595739	-0.704107	3.848527
H	3.188390	0.262252	1.999107
C	2.468473	-3.132474	3.804143
H	2.958155	-4.089933	1.919883
C	2.326592	-1.921485	4.502661
H	2.488820	0.249894	4.388774
H	2.259028	-4.089239	4.307542
H	2.007613	-1.925364	5.556559
Au	1.583396	-0.742138	-0.917889
H	0.186319	1.073067	-2.352483
H	-0.331098	0.912612	0.722559
H	1.502458	2.842465	-2.039279
P	-3.983998	-0.884404	0.063288
C	-0.831152	4.804253	0.946454
C	-0.424235	5.393063	-0.299944
C	-1.372251	3.532690	0.967914
C	-0.810956	4.719859	-1.512528
C	-1.565558	2.738394	-0.223458
H	-1.587471	3.076122	1.948510
C	-1.356157	3.450105	-1.459351
H	-0.615238	5.178945	-2.490596
H	-1.548539	2.922487	-2.408390
C	-4.909641	-1.514104	-1.386850
C	-5.869040	-2.542803	-1.270039
C	-4.603999	-0.974232	-2.656495
C	-6.513179	-3.028396	-2.420473
H	-6.119033	-2.959544	-0.281728
C	-5.245967	-1.470568	-3.802653
H	-3.863228	-0.161446	-2.740524
C	-6.201233	-2.496668	-3.684920
H	-7.266276	-3.826388	-2.327467
H	-5.006389	-1.047672	-4.790688
H	-6.710831	-2.879309	-4.583042
C	-4.994048	-1.232658	1.547410
C	-4.961270	-2.493990	2.182917
C	-5.844602	-0.216045	2.034298
C	-5.786645	-2.735516	3.293785
H	-4.285152	-3.280991	1.812072
C	-6.669317	-0.466702	3.143237
H	-5.851323	0.771609	1.544169
C	-6.641449	-1.725155	3.771666
H	-5.760958	-3.718098	3.790393
H	-7.332352	0.326356	3.522500
H	-7.285570	-1.918024	4.643848
C	-2.488291	-1.959134	0.205717
C	-2.112124	-2.864666	-0.806492
C	-1.635037	-1.754526	1.316915
C	-0.889510	-3.555165	-0.707439
H	-2.767311	-3.027078	-1.676520
C	-0.421088	-2.448346	1.412779
H	-1.922742	-1.040608	2.106564
C	-0.043879	-3.346290	0.394444
H	-0.593386	-4.255785	-1.503514
H	0.245275	-2.280106	2.272282
H	0.916822	-3.879326	0.459993
Au	-3.021400	1.220822	-0.116816
H	-0.658051	5.330489	1.894131
N	0.343804	6.518912	-0.328513
C	0.870712	7.080151	0.916124
H	1.547717	7.920017	0.679062
H	0.059023	7.470587	1.566704
H	1.446077	6.315907	1.483222
C	0.810533	7.061362	-1.603073
H	-0.038328	7.330404	-2.266065
H	1.396153	7.979300	-1.417689
H	1.459769	6.332118	-2.137249
C	4.510031	5.004408	0.885788
H	4.980143	5.393102	-0.039431
H	4.180056	5.878670	1.488411
H	5.295685	4.490769	1.479464

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov (where alkene = H_2C=CH(Ph(*p*NO_2)))

-3222.44151482 A.U.

P	3.078388	-2.364664	-0.009749
H	-1.156596	-0.177769	-1.391263
C	-0.162099	0.309850	-1.382494
C	0.018182	1.225151	-0.226169
C	2.037107	2.432647	-1.193191
C	1.312792	1.952518	-0.073913
C	3.214644	3.170373	-1.029387
C	1.812535	2.230715	1.221399
C	3.644425	3.470849	0.272487
H	3.800845	3.528277	-1.887416
C	2.963529	3.002163	1.407544
H	1.268733	1.844875	2.097527
H	3.345615	3.249892	2.407660
C	4.687430	-1.498259	-0.259870
C	5.924470	-2.175686	-0.313097
C	4.660680	-0.088619	-0.386312
C	7.116341	-1.447059	-0.468951
H	5.966252	-3.273256	-0.251802
C	5.855601	0.635062	-0.530722
H	3.697441	0.445997	-0.388926
C	7.086081	-0.044650	-0.569560
H	8.076985	-1.983394	-0.516073
H	5.823752	1.732225	-0.628052
H	8.023397	0.520209	-0.691531
C	3.279680	-4.122186	-0.473074
C	4.101695	-5.010989	0.260356
C	2.575611	-4.593653	-1.603616
C	4.221316	-6.350420	-0.143742
H	4.636285	-4.660331	1.157424
C	2.700738	-5.935113	-2.003107
H	1.926950	-3.901598	-2.165799
C	3.523581	-6.812512	-1.275361
H	4.861719	-7.038787	0.429514
H	2.151692	-6.296484	-2.886491
H	3.619967	-7.863955	-1.588199
C	2.779364	-2.331406	1.814322
C	2.876804	-1.085309	2.475677
C	2.297972	-3.454344	2.520667
C	2.499870	-0.969172	3.822362
H	3.242789	-0.198962	1.933922
C	1.924029	-3.331910	3.871528
H	2.205360	-4.430528	2.021080
C	2.019959	-2.091138	4.524384
H	2.586118	0.004626	4.330085
H	1.553349	-4.215582	4.414092
H	1.726173	-1.998517	5.581522
Au	1.311510	-1.141964	-0.921244
H	0.032687	0.766444	-2.373455
H	-0.313973	0.785793	0.730669
H	1.676181	2.214640	-2.207575
P	-4.225612	-0.423909	0.064535
C	-0.219400	4.695026	0.971080
C	0.273976	5.225588	-0.271919
C	-0.953685	3.524148	0.982437
C	-0.221638	4.631526	-1.489421
C	-1.275562	2.780648	-0.215283
H	-1.234861	3.098251	1.960205
C	-0.960002	3.463439	-1.446292
H	0.030751	5.070801	-2.463585
H	-1.238890	2.984387	-2.399700
C	-5.206078	-0.918406	-1.400766
C	-6.301333	-1.802653	-1.294971
C	-4.811708	-0.429499	-2.666521
C	-6.991364	-2.197923	-2.453255
H	-6.620712	-2.175898	-0.309168
C	-5.501789	-0.835460	-3.820370
H	-3.965273	0.273706	-2.741680
C	-6.591267	-1.719129	-3.714053
H	-7.849838	-2.882379	-2.369338
H	-5.193890	-0.452368	-4.805691
H	-7.137102	-2.030128	-4.618508
C	-5.302739	-0.608872	1.529892

C	-5.431821	-1.843574	2.203940
C	-6.040387	0.515455	1.961989
C	-6.305321	-1.949788	3.299392
H	-4.843714	-2.716136	1.877381
C	-6.914307	0.399465	3.055083
H	-5.921347	1.480672	1.442412
C	-7.047330	-0.831905	3.722739
H	-6.405983	-2.911384	3.826552
H	-7.489108	1.276171	3.391717
H	-7.729145	-0.919462	4.583086
C	-2.899573	-1.700449	0.235940
C	-2.649970	-2.662146	-0.763271
C	-2.029151	-1.602659	1.348648
C	-1.535952	-3.514841	-0.650938
H	-3.317862	-2.740365	-1.635124
C	-0.925016	-2.459273	1.459574
H	-2.217291	-0.843579	2.126162
C	-0.672811	-3.413212	0.453029
H	-1.336620	-4.257703	-1.438686
H	-0.242976	-2.374237	2.319623
H	0.204206	-4.074291	0.527571
Au	-2.958742	1.515513	-0.112182
H	0.046445	5.173213	1.922822
N	1.214355	6.209635	-0.299169
C	1.795087	6.731508	0.942032
H	2.429290	7.604159	0.705653
H	1.006424	7.070690	1.643602
H	2.431851	5.970819	1.446709
C	1.799002	6.631857	-1.572822
H	1.041109	7.102407	-2.234537
H	2.594463	7.373237	-1.381459
H	2.250703	5.768875	-2.109195
N	4.835851	4.321155	0.453972
O	4.901188	4.985352	1.495395
O	5.677907	4.327740	-0.450749

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov (where alkene = (Me)HC=CH(Ph(*p*OMe)))

-3171.79359997 A.U.

P	3.226633	-2.108132	-0.000182
H	-1.164238	-0.273656	-0.917059
C	-0.277248	0.303937	-1.246911
C	0.008042	1.351247	-0.207920
C	1.823693	2.770664	-1.353766
C	1.298216	2.115419	-0.211947
C	3.046390	3.447132	-1.308269
C	2.043700	2.208235	0.984010
C	3.791130	3.500865	-0.107969
H	3.463666	3.933541	-2.202838
C	3.276415	2.877515	1.050718
H	1.662677	1.707784	1.888749
H	3.832103	2.889322	1.998506
C	4.786315	-1.244441	-0.464706
C	6.040839	-1.891522	-0.469177
C	4.708180	0.134257	-0.770794
C	7.204400	-1.161319	-0.763979
H	6.114292	-2.968473	-0.253990
C	5.877685	0.861990	-1.049595
H	3.730274	0.642258	-0.792235
C	7.126232	0.215115	-1.045893
H	8.179625	-1.672783	-0.773648
H	5.804292	1.937462	-1.274869
H	8.042467	0.781984	-1.274636
C	3.427300	-3.894315	-0.348745
C	4.248260	-4.735207	0.438611
C	2.722870	-4.434877	-1.448095
C	4.367478	-6.097664	0.119222
H	4.781279	-4.328482	1.312790
C	2.848539	-5.798344	-1.763570
H	2.070432	-3.779897	-2.049292
C	3.670595	-6.629261	-0.981828
H	5.006387	-6.749385	0.735489
H	2.298562	-6.214458	-2.622007
H	3.765539	-7.698502	-1.227727
C	3.138640	-1.953223	1.837279

C	3.531002	-0.739274	2.444272
C	2.533533	-2.958080	2.624403
C	3.321943	-0.538332	3.818399
H	3.993576	0.055756	1.838935
C	2.329619	-2.751677	3.999788
H	2.223155	-3.909861	2.165984
C	2.719842	-1.541208	4.599995
H	3.637260	0.408970	4.284050
H	1.864915	-3.545345	4.605776
H	2.560929	-1.382626	5.678025
Au	1.343986	-1.007030	-0.820911
H	-0.159043	0.916152	0.795200
H	1.265950	2.747707	-2.298266
P	-4.191042	-0.588451	0.121438
C	-0.302381	4.561300	1.299613
C	0.045144	5.270971	0.097621
C	-0.977553	3.359667	1.219373
C	-0.566584	4.832389	-1.127778
C	-1.366775	2.746646	-0.035926
H	-1.133263	2.789167	2.150662
C	-1.246018	3.628445	-1.177930
H	-0.458870	5.425564	-2.045609
H	-1.650631	3.303460	-2.148301
C	-5.060695	-1.029934	-1.430080
C	-6.226288	-1.824511	-1.440380
C	-4.507135	-0.570060	-2.647569
C	-6.830737	-2.158404	-2.664906
H	-6.666304	-2.176849	-0.494185
C	-5.110738	-0.917084	-3.866355
H	-3.601936	0.060371	-2.634390
C	-6.274065	-1.709231	-3.875625
H	-7.744392	-2.773043	-2.671506
H	-4.677138	-0.559011	-4.813115
H	-6.752502	-1.972421	-4.831945
C	-5.347859	-0.888666	1.502854
C	-5.514320	-2.176438	2.059337
C	-6.106391	0.198214	1.990238
C	-6.445687	-2.372236	3.092673
H	-4.911586	-3.020630	1.687622
C	-7.038679	-0.007014	3.020475
H	-5.956145	1.203674	1.563305
C	-7.208507	-1.290624	3.570730
H	-6.575832	-3.375156	3.528527
H	-7.630010	0.840519	3.400437
H	-7.936001	-1.448564	4.382291
C	-2.835950	-1.835139	0.299447
C	-2.537077	-2.772151	-0.710355
C	-1.980251	-1.718973	1.421642
C	-1.385926	-3.574569	-0.603429
H	-3.190609	-2.863952	-1.591541
C	-0.838097	-2.525236	1.525587
H	-2.201092	-0.974398	2.204359
C	-0.533142	-3.448343	0.505739
H	-1.146978	-4.293707	-1.402082
H	-0.161933	-2.414525	2.387266
H	0.378668	-4.062266	0.568471
Au	-2.995142	1.406484	0.053440
H	0.024213	4.931091	2.280387
N	0.945728	6.292350	0.114722
C	1.633232	6.646847	1.356593
H	2.360200	7.452840	1.152822
H	0.923234	7.015629	2.127325
H	2.185014	5.773111	1.768884
C	1.365796	6.923964	-1.136012
H	0.519267	7.436904	-1.640383
H	2.140848	7.680615	-0.920757
H	1.795706	6.173232	-1.834664
O	4.991953	4.143997	-0.178756
C	5.839252	4.130095	0.966086
H	5.370034	4.643012	1.836517
H	6.111420	3.090210	1.258709
H	6.756749	4.677564	0.680043
C	-0.459055	0.666223	-2.717083
H	0.438150	1.114976	-3.187421

H	-0.706952	-0.243708	-3.300473
H	-1.306450	1.379566	-2.848482

[(PPh_3)Au(alkene)-- (aniline)]$^+$ TS Markovnikov (where alkene = H_2C=C(Ph)(tBu))

-3175.19931253 A.U.

P	-4.248861	-0.359577	0.198911
H	0.476816	-0.025144	0.414887
C	-0.015733	0.964344	0.432896
C	0.509111	1.855117	-0.651032
C	-0.756220	3.747933	0.506817
C	0.149794	3.324877	-0.499382
C	-1.092404	5.100434	0.678010
C	0.695227	4.339085	-1.325768
C	-0.532026	6.086024	-0.151007
H	-1.806585	5.381867	1.468376
C	0.364097	5.691929	-1.158882
H	1.413851	4.075157	-2.109695
H	-0.794650	7.147282	-0.017747
H	0.814130	6.444093	-1.826342
C	-5.560585	0.870061	0.551144
C	-6.817042	0.485152	1.068469
C	-5.301834	2.228264	0.260254
C	-7.810402	1.455716	1.282179
H	-7.015768	-0.571414	1.309684
C	-6.301598	3.191570	0.472275
H	-4.311866	2.527516	-0.123105
C	-7.555096	2.806328	0.981936
H	-8.789083	1.155425	1.688066
H	-6.098064	4.249569	0.244764
H	-8.335934	3.563937	1.152801
C	-4.565747	-1.770821	1.333383
C	-5.231241	-2.942634	0.915204
C	-4.072399	-1.674848	2.654283
C	-5.391744	-4.013578	1.812961
H	-5.610956	-3.024212	-0.115444
C	-4.240766	-2.744779	3.546745
H	-3.541883	-0.761642	2.971580
C	-4.894856	-3.918069	3.124799
H	-5.906615	-4.929345	1.482781
H	-3.852692	-2.667599	4.574491
H	-5.016876	-4.761320	3.822387
C	-4.600982	-1.020404	-1.479471
C	-5.828766	-0.805563	-2.139021
C	-3.589619	-1.785849	-2.104541
C	-6.042273	-1.359038	-3.414455
H	-6.616234	-0.203307	-1.659536
C	-3.812517	-2.341087	-3.373424
H	-2.627171	-1.944188	-1.591207
C	-5.038888	-2.126952	-4.030937
H	-7.000268	-1.186543	-3.929444
H	-3.021668	-2.936604	-3.856142
H	-5.210946	-2.556344	-5.030360
Au	-2.061421	0.422140	0.344960
H	0.138228	1.389824	1.442735
H	-1.231266	3.003935	1.160860
P	3.107998	-2.303648	0.115971
C	3.973599	4.056137	-0.654391
C	3.732312	4.640100	0.634184
C	3.413287	2.835772	-1.000429
C	2.991336	3.852754	1.578834
C	2.568686	2.068431	-0.116571
H	3.647045	2.446411	-2.000062
C	2.446568	2.638529	1.203889
H	2.815638	4.220807	2.597991
H	1.835599	2.106798	1.950123
C	4.046416	-2.994661	1.526344
C	3.609979	-4.146517	2.218148
C	5.258650	-2.367629	1.890442
C	4.392355	-4.670760	3.261090
H	2.656291	-4.626510	1.946582
C	6.036941	-2.900914	2.930397
H	5.584632	-1.457715	1.359706
C	5.605226	-4.051993	3.614646
H	4.051306	-5.567531	3.801636

H	6.981838	-2.411348	3.212993
H	6.214532	-4.465703	4.433389
C	3.667770	-3.196061	-1.385542
C	4.131879	-4.527771	-1.316581
C	3.574623	-2.545709	-2.636374
C	4.493717	-5.202524	-2.494257
H	4.217931	-5.035238	-0.342820
C	3.932247	-3.229075	-3.810297
H	3.221640	-1.502937	-2.686396
C	4.391741	-4.556594	-3.740012
H	4.860764	-6.239186	-2.437920
H	3.859652	-2.719064	-4.783525
H	4.679022	-5.088912	-4.660280
C	1.354113	-2.814239	0.365760
C	0.692960	-2.366788	1.534240
C	0.628079	-3.501118	-0.628350
C	-0.679051	-2.605200	1.700843
H	1.252833	-1.814325	2.306701
C	-0.748187	-3.736317	-0.452848
H	1.134026	-3.845350	-1.543696
C	-1.403870	-3.288736	0.706509
H	-1.196188	-2.248177	2.604184
H	-1.311600	-4.274708	-1.231121
H	-2.481997	-3.463354	0.840421
Au	3.052313	0.014119	-0.054976
H	4.608660	4.570888	-1.387867
N	4.185778	5.888686	0.947696
C	4.888298	6.693026	-0.050671
H	5.130714	7.680931	0.379840
H	5.841276	6.215241	-0.366263
H	4.262230	6.855181	-0.954937
C	3.920011	6.462929	2.266229
H	4.365897	5.847159	3.076884
H	4.366314	7.471736	2.322273
H	2.828660	6.556223	2.456659
C	0.350293	1.246886	-2.114215
C	0.247285	-0.295672	-2.100555
H	-0.649930	-0.661436	-1.563225
H	0.197460	-0.675107	-3.141207
H	1.133049	-0.757501	-1.616747
C	-0.982980	1.800088	-2.700487
H	-1.215645	1.274201	-3.649524
H	-1.828774	1.625884	-2.001080
H	-0.927046	2.886070	-2.907385
C	1.476801	1.573428	-3.119128
H	1.192116	1.185615	-4.118910
H	1.669838	2.654411	-3.237663
H	2.420282	1.070645	-2.824665

[(PPh_3)Au(*para*-aniline)--(PPh_3)Au(alkene)+benzene]$^+$

-2135.55942022 A.U.

P	2.901073	0.297087	0.058005
C	-4.179999	-0.173641	-1.016118
C	-3.270003	-0.763120	-0.112218
C	-5.486586	0.130411	-0.606055
C	-3.705287	-1.074632	1.194241
C	-5.913196	-0.161714	0.700979
H	-6.177515	0.601171	-1.322490
C	-5.017207	-0.776384	1.591609
H	-3.030765	-1.557176	1.911638
H	-6.942446	0.068213	1.016567
H	-5.339635	-1.030064	2.613449
C	2.645118	-1.485450	-0.331455
C	2.652948	-2.461309	0.687189
C	2.242326	-1.842554	-1.640556
C	2.253736	-3.779546	0.399529
H	2.964616	-2.189846	1.708180
C	1.851940	-3.161608	-1.921342
H	2.235522	-1.083917	-2.440453
C	1.848871	-4.130240	-0.899642
H	2.260633	-4.536625	1.199018
H	1.545199	-3.435073	-2.943072
H	1.536685	-5.162281	-1.120558
C	3.794407	0.332526	1.658077

C	5.158415	-0.027235	1.736716
C	3.091444	0.690146	2.829373
C	5.807565	-0.033922	2.981259
H	5.717737	-0.293289	0.826077
C	3.747080	0.678253	4.072527
H	2.031245	0.985945	2.763102
C	5.103310	0.316314	4.148761
H	6.871786	-0.310310	3.040103
H	3.197532	0.961436	4.983643
H	5.618044	0.313203	5.122247
C	4.044611	0.940277	-1.217222
C	5.011156	0.116297	-1.836917
C	3.972678	2.312814	-1.544138
C	5.904999	0.669449	-2.768810
H	5.057910	-0.958693	-1.600297
C	4.872734	2.858728	-2.473921
H	3.207908	2.950061	-1.069842
C	5.838711	2.038772	-3.084893
H	6.656814	0.026420	-3.252387
H	4.815631	3.928819	-2.726695
H	6.540613	2.468048	-3.816788
Au	0.755665	1.201555	0.063888
H	-3.872850	0.081708	-2.037867
N	-1.877582	-0.914017	-0.478211
C	-1.581249	-1.096569	-1.914756
H	-0.484728	-1.188852	-2.026509
H	-2.072653	-2.006335	-2.311974
H	-1.909636	-0.206376	-2.483449
C	-1.054828	-1.782089	0.393665
H	-1.464837	-2.808408	0.450677
H	-0.031417	-1.820530	-0.018697
H	-0.992479	-1.340652	1.406901
C	-3.263107	2.549670	1.240195
C	-3.815877	3.132639	0.054908
C	-2.046992	1.878294	1.203887
C	-3.028497	3.063117	-1.140834
C	-1.283031	1.710419	-0.002647
H	-1.684025	1.411918	2.134536
C	-1.820844	2.374214	-1.159261
H	-3.386362	3.525500	-2.070350
H	-1.414435	0.364761	-0.245855
H	-1.271680	2.315181	-2.113857
H	-3.811363	2.595896	2.189852
N	-5.061528	3.706190	0.057532
C	-5.883579	3.663661	1.261881
H	-6.862448	4.132475	1.055206
H	-6.063011	2.614464	1.590478
H	-5.414078	4.217263	2.104361
C	-5.615177	4.270943	-1.168377
H	-5.732915	3.500801	-1.964491
H	-6.612250	4.697680	-0.957824
H	-4.977171	5.088109	-1.569754
C	-3.582992	-4.484109	0.819822
C	-2.405254	-5.197556	1.110402
C	-3.859978	-4.088429	-0.501772
C	-1.498447	-5.509014	0.079121
C	-2.961226	-4.414742	-1.533708
C	-1.776620	-5.118169	-1.243171
H	-2.192742	-5.513292	2.144034
H	-4.777216	-3.521539	-0.724544
H	-0.575919	-6.065311	0.308061
H	-3.192534	-4.132648	-2.573668
H	-1.073445	-5.370229	-2.052703
H	-4.289637	-4.231468	1.625562

[(PPh_3)Au(alkene)-- (aniline)+benzene]$^+$

-3250.16478305 A.U.

P	4.306793	-0.911268	-0.127151
H	-0.464414	-0.207780	-1.335825
C	0.293441	0.594350	-1.237423
C	0.159730	1.373625	0.005984
C	1.447000	3.434409	-0.741535
C	1.059356	2.529186	0.273446
C	2.317906	4.499361	-0.457860

C	1.566293	2.726479	1.580457
C	2.822413	4.676905	0.843133
H	2.613008	5.190889	-1.262830
C	2.446833	3.781017	1.862514
H	1.274251	2.023122	2.377248
H	3.511070	5.507738	1.063188
H	2.844463	3.906587	2.881947
C	5.484543	0.483250	-0.392655
C	6.864971	0.292171	-0.616791
C	4.960506	1.797877	-0.353950
C	7.711222	1.402624	-0.778275
H	7.286817	-0.721533	-0.683562
C	5.815276	2.901599	-0.501012
H	3.878470	1.967797	-0.225060
C	7.191535	2.707548	-0.712065
H	8.785737	1.243961	-0.959798
H	5.390012	3.916270	-0.462079
H	7.859860	3.573780	-0.837629
C	5.062042	-2.446782	-0.773497
C	6.215324	-3.027295	-0.193652
C	4.454201	-3.065208	-1.888680
C	6.755303	-4.205264	-0.734761
H	6.683710	-2.566860	0.690787
C	5.000431	-4.243099	-2.426117
H	3.547011	-2.617793	-2.327488
C	6.150711	-4.811868	-1.851537
H	7.652567	-4.653813	-0.280510
H	4.524253	-4.719159	-3.297366
H	6.577555	-5.735540	-2.272707
C	4.187343	-1.112247	1.706288
C	3.875075	0.034360	2.472602
C	4.223383	-2.375920	2.333717
C	3.604049	-0.085710	3.844075
H	3.831642	1.026359	1.996642
C	3.951314	-2.489197	3.709327
H	4.454559	-3.281330	1.752748
C	3.638115	-1.347756	4.466862
H	3.364608	0.814796	4.431545
H	3.982676	-3.480118	4.188626
H	3.423788	-1.440336	5.542948
Au	2.180062	-0.306505	-0.865693
H	0.348862	1.192420	-2.168450
H	-0.009965	0.758715	0.905341
H	1.066124	3.297163	-1.763643
P	-3.046412	-1.822461	0.210302
C	-1.545383	4.530930	1.239370
C	-1.519466	5.212237	-0.023955
C	-1.648669	3.149418	1.291324
C	-1.691214	4.418108	-1.210804
C	-1.736645	2.325732	0.118184
H	-1.612137	2.662358	2.280107
C	-1.791503	3.038532	-1.125222
H	-1.708581	4.894219	-2.200304
H	-1.864299	2.459573	-2.061423
C	-3.771735	-2.447274	-1.352855
C	-4.809134	-3.400733	-1.378601
C	-3.306423	-1.881004	-2.562357
C	-5.376998	-3.783154	-2.607462
H	-5.187351	-3.834658	-0.440092
C	-3.866525	-2.277474	-3.785585
H	-2.515183	-1.113292	-2.540597
C	-4.907640	-3.225619	-3.809506
H	-6.194356	-4.520852	-2.623077
H	-3.500234	-1.834371	-4.724800
H	-5.357114	-3.525997	-4.768817
C	-3.939876	-2.634110	1.582106
C	-3.711319	-3.993135	1.894628
C	-4.883138	-1.885365	2.316859
C	-4.439644	-4.600440	2.930008
H	-2.961783	-4.570776	1.329746
C	-5.608777	-2.500662	3.351005
H	-5.041733	-0.824290	2.067845
C	-5.389629	-3.856135	3.655405
H	-4.263703	-5.659554	3.175059

H	-6.345195	-1.917124	3.925335
H	-5.957706	-4.335804	4.467903
C	-1.327093	-2.505938	0.270854
C	-0.790407	-3.333298	-0.735847
C	-0.506115	-2.093623	1.347764
C	0.556960	-3.735902	-0.667302
H	-1.418020	-3.658070	-1.580155
C	0.832291	-2.504616	1.417166
H	-0.919225	-1.431414	2.126992
C	1.367281	-3.323749	0.402945
H	0.976319	-4.373088	-1.461486
H	1.471815	-2.170671	2.248733
H	2.422876	-3.632434	0.441623
Au	-2.707826	0.465310	0.242801
H	-1.453968	5.093889	2.177287
N	-1.315027	6.562300	-0.097849
C	-1.052790	7.336577	1.114043
H	-0.858962	8.389138	0.840681
H	-1.920602	7.319275	1.808924
H	-0.162040	6.950569	1.655683
C	-1.272470	7.234535	-1.394252
H	-2.220905	7.097520	-1.956952
H	-1.125587	8.318456	-1.240258
H	-0.435780	6.859067	-2.024561
C	-5.336164	1.091990	-1.996740
C	-6.037862	-0.077084	-1.650162
C	-5.229278	2.150268	-1.075216
C	-6.627063	-0.190727	-0.379356
C	-5.824905	2.039213	0.195452
C	-6.523776	0.868751	0.542124
H	-6.113945	-0.907420	-2.368788
H	-4.664158	3.057902	-1.337924
H	-7.166811	-1.110473	-0.103856
H	-5.734850	2.865308	0.917883
H	-6.996672	0.784560	1.533873
H	-4.863169	1.173358	-2.988154

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

-1713.06179991 A.U.

P	-0.544964	-1.153375	0.010672
H	0.469093	3.685526	0.889018
C	1.178547	3.052729	0.329822
C	2.082429	2.236878	1.023824
C	3.597906	1.514053	-0.880743
C	3.271209	1.541442	0.499223
C	4.707769	0.791098	-1.331135
C	4.089168	0.827579	1.410040
C	5.515153	0.086050	-0.414531
H	4.950271	0.772591	-2.404705
C	5.205644	0.107737	0.956645
H	3.841001	0.837041	2.483764
H	6.388558	-0.479883	-0.774281
H	5.835508	-0.437794	1.675997
C	0.801698	-2.285998	-0.494575
C	0.515445	-3.458873	-1.231131
C	2.132853	-1.992095	-0.124825
C	1.557720	-4.332927	-1.581393
H	-0.517201	-3.680553	-1.544472
C	3.167779	-2.871931	-0.479156
H	2.368178	-1.068556	0.427893
C	2.882000	-4.041892	-1.205181
H	1.334123	-5.244510	-2.156999
H	4.202352	-2.629443	-0.192184
H	3.695639	-4.728266	-1.486980
C	-1.819405	-1.260067	-1.303060
C	-3.182719	-1.437428	-0.989528
C	-1.421708	-1.048558	-2.643885
C	-4.144805	-1.393408	-2.014636
H	-3.494236	-1.611874	0.052399
C	-2.387576	-1.015378	-3.661302
H	-0.355818	-0.914090	-2.890527
C	-3.750411	-1.180834	-3.346784
H	-5.209015	-1.530734	-1.768363
H	-2.076373	-0.857608	-4.705603

H	-4.506877	-1.148208	-4.146052
C	-1.318528	-1.813598	1.533198
C	-1.420781	-3.205975	1.746303
C	-1.868655	-0.912622	2.472771
C	-2.079317	-3.688486	2.889008
H	-0.979193	-3.914587	1.028328
C	-2.530732	-1.403831	3.610129
H	-1.774888	0.174381	2.314349
C	-2.637591	-2.790632	3.817592
H	-2.154322	-4.774048	3.056588
H	-2.958460	-0.700183	4.340990
H	-3.152238	-3.174574	4.712064
Au	0.201149	1.042649	0.253349
H	1.351032	3.342041	-0.720582
H	1.970185	2.187566	2.123601
H	2.966684	2.047508	-1.607932
C	-2.669399	3.033297	1.058999
C	-2.667222	2.013106	0.087709
C	-2.213329	4.321058	0.722178
C	-2.197199	2.278112	-1.218739
C	-1.751083	4.588497	-0.581233
C	-1.737222	3.567917	-1.549373
H	-3.064884	1.014906	0.326701
H	-2.230566	5.125046	1.474822
H	-2.224684	1.481759	-1.978402
H	-1.406529	5.601007	-0.844118
H	-1.384083	3.779396	-2.570840
H	-3.045355	2.827376	2.073497

-1403.59323160 A.U.

P	0.903515	0.001766	-0.044688
C	-4.456774	-0.690503	-1.068751
C	-4.464457	0.724094	-1.055175
C	-3.982476	-1.409395	0.035883
C	-3.997144	1.427196	0.062516
C	-3.511979	-0.714550	1.187180
H	-3.992193	-2.509647	0.035209
C	-3.519616	0.716680	1.199999
H	-4.018688	2.527104	0.081124
H	-3.295873	1.261796	2.132045
C	2.006966	0.012901	1.411774
C	3.184513	0.791192	1.418502
C	1.694957	-0.818815	2.511086
C	4.047004	0.731153	2.526788
H	3.426086	1.442335	0.564008
C	2.564545	-0.874541	3.610804
H	0.772216	-1.422743	2.504192
C	3.739548	-0.099190	3.619082
H	4.964507	1.339573	2.535712
H	2.322547	-1.521923	4.467740
H	4.417512	-0.140006	4.485721
C	1.327905	1.466577	-1.053216
C	2.174835	1.351578	-2.176583
C	0.842940	2.732091	-0.651845
C	2.536076	2.506588	-2.891878
H	2.550493	0.366097	-2.493509
C	1.213201	3.879153	-1.370101
H	0.178565	2.817361	0.224190
C	2.059119	3.766532	-2.489882
H	3.194914	2.418896	-3.769560
H	0.837549	4.865776	-1.057774
H	2.344541	4.667593	-3.054710
C	1.332639	-1.472561	-1.036871
C	2.543385	-2.163455	-0.818300
C	0.455141	-1.877607	-2.068322
C	2.872636	-3.258534	-1.636092
H	3.225199	-1.849072	-0.012844
C	0.796077	-2.967782	-2.882901
H	-0.493093	-1.338196	-2.231378
C	2.003530	-3.658966	-2.665999
H	3.815087	-3.801371	-1.465310
H	0.114785	-3.284454	-3.687690
H	2.265476	-4.518395	-3.302512
Au	-1.316198	-0.009090	0.559170

H	-4.837334	-1.229780	-1.949903
H	-4.849993	1.276097	-1.926209
H	-3.290807	-1.274470	2.111146

benzene

-232.082637612 A.U.

C	-0.290786	1.376435	-0.000019
C	1.046685	0.939999	-0.000080
C	-1.337522	0.436397	0.000149
C	1.337497	-0.436320	-0.000084
C	-1.046627	-0.940043	-0.000114
H	-2.384961	0.778260	-0.000092
C	0.290726	-1.376485	0.000188
H	2.384898	-0.778385	0.000254
H	0.518730	-2.454469	-0.000016
H	-0.518345	2.454544	0.000242
H	1.866377	1.676411	-0.000154
H	-1.866541	-1.676261	-0.000477