

Supporting Information

Two Metals Are Better Than One in the Gold Catalyzed Oxidative Heteroarylation of Alkenes

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General synthetic considerations. Unless otherwise stated, all manipulations were conducted under ambient air. Air-sensitive manipulations were conducted using standard Schlenk techniques under N₂ atmosphere. The starting materials (*E*)-*t*BuCHD=CHD, (*Z*)-*t*BuCHD=CHD,¹ (IPr)AuOH,² DIMes·2HBr,³ Ph₃PAuMe,⁴ [Mes-imid-Bn]AuCl (**5**),⁵ [(PhCH₂)(Ph)₂P]AuCl (**1**),⁶ and PhICl₂⁷ were prepared according to literature methods (IPr = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene, DIMes = 1,1'-di(mesityl)-3,3'-methylenediimidazol-2,2'-diylidene, Mes-imid-Bn = 1-mesityl-3-benzylimidazol-2-ylidene). All other reagents were purchased from commercial vendors and used as received. Tetrahydrofuran and dichloromethane were dried by passage through a packed column of activated neutral alumina under argon pressure.⁸ All other solvents were used as received without further drying. ¹H, ¹H{²H}, ²H, ¹¹B{¹H}, ¹³C{¹H}, and ¹⁹F, and ³¹P{¹H} NMR spectra were recorded at room temperature with Brüker AV-300, AVB-400, AVQ-400, DRX-500, and AV-600 spectrometers. ¹H, ¹H{²H}, ²H, and ¹³C{¹H} NMR spectra were referenced to the residual chloroform peaks. ¹¹B{¹H} NMR spectra were referenced to external BF₃·OEt₂ (δ = 0). ¹⁹F NMR spectra were referenced to external CFCl₃ (δ = 0). ³¹P{¹H} NMR spectra were referenced to external phosphoric acid (δ = 0). Combustion analysis data were obtained at the Micro-Mass Facility at the University of California, Berkeley.

Preparation of *neo*-hexylboronic acid, *t*BuCH₂CH₂B(OH)₂. This procedure was adapted from H. C. Brown et al.⁹ To a flame-dried flask under dinitrogen atmosphere was added dichloromethane (20 mL) and 3,3-dimethyl-1-butene (2.00 mL, 15.5 mmol). Dibromoborane-dimethyl sulfide adduct (1.0 M solution in dichloromethane, 15.5 mL, 15.5 mmol) was added slowly by syringe. The flask was fitted with a reflux condenser and the solution was heated to a reflux under N₂ for 2.5 h. The solution was then cooled to 0°C, opened to air, and H₂O (10 mL) was added in one portion. After stirring for 10 min at 0°C, the layers were separated. The organic fraction was washed with H₂O (2 x 20 mL) and brine (20 mL), dried over MgSO₄, and concentrated by rotary evaporation. The resulting white residue was washed with several portions of hexanes and dried to yield pure *neo*-hexylboronic acid as a white powder (1.21 g, 60%) that requires refrigeration for long-term storage. ¹H NMR (CD₃CN, δ): 5.41 (s, 2H, OH), 1.26 (m, 2H, BCH₂CH₂), 0.85 (s, 9H, CH₃), 0.62 (m, 2H, BCH₂CH₂). ¹¹B{¹H} NMR (CD₃CN, δ): 32.3 (s).

¹ Igau, A.; Gladysz, J. A. *Organometallics* **1991**, *10*, 2327.

² Gaillard, S.; Slawin, A. M. Z.; Nolan, S. P. *Chem. Commun.* **2010**, *46*, 2742.

³ Gardiner, M. G.; Herrmann, W. A.; Reisinger, C.-P.; Schwarz, J.; Spiegler, M. *J. Organomet. Chem.* **1999**, *572*, 239.

⁴ Tamaki, A.; Kochi, J. K. *J. Organomet. Chem.* **1973**, *61*, 441.

⁵ (a) Maishal, T. K.; Basset, J.-M.; Boualleg, M.; Copéret, C.; Veyre, L.; Thieuleux, C. *Dalton Trans.* **2009**, 6956.
(b) Flahaut, A.; Roland, S.; Mangeney, P. *J. Organometal. Chem.* **2007**, *692*, 5754.

⁶ Gunatilleke, S. S.; Barrios, A. M. *J. Inorg. Biochem.* **2008**, *102*, 555.

⁷ Zielinska, A.; Skulski, L. *Tet. Lett.* **2004**, *45*, 1087.

⁸ Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518.

⁹ Brown, H. C.; Bhat, N. G.; Somayaji, V. *Organometallics* **1983**, *2*, 1311.

$^{13}\text{C}\{^1\text{H}\}$ NMR (CD_3CN , δ): 39.4 (BCH_2CH_2), 38.2 (BCH_2CH_2), 31.4 ($\text{C}(\text{CH}_3)_3$), 29.3 ($\text{C}(\text{CH}_3)_3$). *Note*: Combustion analysis gives data consistent with the anhydride (i.e. $(t\text{BuCH}_2\text{CH}_2\text{BO})_3$) rather than the boronic acid. Anal. Calcd. for $\text{C}_{18}\text{H}_{39}\text{B}_3\text{O}_3$: C, 64.36; H, 11.70. Found: C, 64.27; H, 11.60.

Preparation of *syn*- $t\text{BuCHDCHDB}(\text{OH})_2$. An analogous procedure was used to convert (*E*)- $t\text{BuCHD}=\text{CHD}$ to *syn*- $t\text{BuCHDCHDB}(\text{OH})_2$. $^1\text{H}\{^2\text{H}\}$ NMR (CD_3CN , δ): 5.41 (s, 2H, OH), 1.24 (d, $^3J_{\text{HH}} = 4.2$ Hz, 1H, BCHDCHD), 0.86 (s, 9H, CH_3), 0.60 (br, 1H, BCHDCHD). ^2H NMR (CD_3CN , δ): 1.25 (br, 1D), 0.61 (br, 1D). $^{11}\text{B}\{^1\text{H}\}$ NMR (CD_3CN , δ): 32.4 (s). $^{13}\text{C}\{^1\text{H}\}$ NMR (CD_3CN , δ): 39.4 (t, $J_{\text{CD}} = 18.9$ Hz, BCHDCHD), 31.4 ($\text{C}(\text{CH}_3)_3$), 29.3 ($\text{C}(\text{CH}_3)_3$), BCHDCHD not found.

Preparation of *anti*- $t\text{BuCHDCHDB}(\text{OH})_2$. An analogous procedure was used to convert (*Z*)- $t\text{BuCHD}=\text{CHD}$ to *anti*- $t\text{BuCHDCHDB}(\text{OH})_2$. $^1\text{H}\{^2\text{H}\}$ NMR (CD_3CN , δ): 5.41 (s, 2H, OH), 1.23 (d, $^3J_{\text{HH}} = 12.6$ Hz, 1H, BCHDCHD), 0.85 (s, 9H, CH_3), 0.59 (br d, $^3J_{\text{HH}} = 12.0$ Hz, 1H, BCHDCHD). ^2H NMR (CD_3CN , δ): 1.25 (br, 1D), 0.61 (br, 1D). $^{11}\text{B}\{^1\text{H}\}$ NMR (CD_3CN , δ): 32.4 (s). $^{13}\text{C}\{^1\text{H}\}$ NMR (CD_3CN , δ): 38.7 (t, $J_{\text{CD}} = 19.1$ Hz, BCHDCHD), 31.2 ($\text{C}(\text{CH}_3)_3$), 29.2 ($\text{C}(\text{CH}_3)_3$), BCHDCHD not found.

Preparation of $t\text{BuCH}_2\text{CH}_2\text{Au}(\text{IPr})$. Benzene (10 mL) was sparged with N_2 for 40 min, and then IPrAuOH (80.0 mg, 0.133 mmol) and $t\text{BuCH}_2\text{CH}_2\text{B}(\text{OH})_2$ (20.5 mg, 0.158 mmol) were added under flow of N_2 . The resulting cloudy solution became clear over the first few minutes. After stirring overnight under a blanket of N_2 , the mixture was filtered through a pad of Celite and concentrated by rotary evaporation. The white residue was extracted with diethyl ether (5 mL), passed through a pipette-column of basic alumina, and evaporated to dryness. The resulting white residue was extracted with pentane/ Et_2O (1:1, 10 mL), filtered, and concentrated by rotary evaporation to yield $t\text{BuCH}_2\text{CH}_2\text{Au}(\text{IPr})$ as a white powder (55.5 mg, 62%). Crystals suitable for X-ray diffraction were grown by slow evaporation of a concentrated *n*-pentane solution. ^1H NMR (CD_2Cl_2 , δ): 7.52 (t, $J = 7.5$ Hz, 2H, *p*-CH), 7.32 (d, $J = 7.5$ Hz, 4H, *m*-CH), 7.10 (s, 2H, NCH), 2.65 (sept., $J = 6.5$ Hz, 4H, $\text{CH}(\text{CH}_3)_2$), 1.35 (d, $J = 6.5$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.21 (d, $J = 7.0$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.11 (m, 2H, AuCH_2CH_2), 0.62 (s, 9H, $\text{C}(\text{CH}_3)_3$), 0.52 (m, 2H, AuCH_2CH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (CD_2Cl_2 , δ): 202.3, 146.5, 135.6, 130.4, 124.4, 123.2, 46.1, 32.3, 29.5, 29.2, 24.6, 24.2, 15.1. Anal. Calcd. for $\text{C}_{33}\text{H}_{49}\text{AuN}_2$: C, 59.09; H, 7.36; N, 4.18. Found: C, 59.26; H, 7.58; N, 4.10.

Preparation of *syn-t*BuCHDCHDAu(IPr). An analogous procedure was used to convert *anti-t*BuCHDCHDB(OH)₂ to *syn-t*BuCHDCHDAu(IPr). ¹H{²H} NMR (CD₂Cl₂, δ): 7.52 (t, *J* = 7.8 Hz, 2H, *p*-CH), 7.32 (d, *J* = 7.8 Hz, 4H, *m*-CH), 7.10 (s, 2H, NCH), 2.66 (sept., *J* = 7.2 Hz, 4H, CH(CH₃)₂), 1.35 (d, *J* = 6.6 Hz, 12H, CH(CH₃)₂), 1.22 (d, *J* = 7.2 Hz, 12H, CH(CH₃)₂), 1.08 (d, ³*J*_{HH} = 5.4 Hz, 1H, AuCHDCHD), 0.61 (s, 9H, C(CH₃)₃), 0.48 (d, ³*J*_{HH} = 5.4 Hz, 1H, AuCHDCHD). ²H NMR (CD₂Cl₂, δ): 1.08 (br, 1D), 0.50 (br, 1D). ¹³C{¹H} NMR (CD₂Cl₂, δ): 200.5, 146.5, 135.7, 130.5, 124.4, 123.2, 45.5 (t, *J*_{CD} = 19.6 Hz), 32.3, 29.5, 29.3, 24.6, 24.2, 14.5 (t, *J*_{CD} = 18.1 Hz).

Preparation of *anti-t*BuCHDCHDAu(IPr). An analogous procedure was used to convert *syn-t*BuCHDCHDB(OH)₂ to *anti-t*BuCHDCHDAu(IPr). ¹H NMR (CD₂Cl₂, δ): 7.52 (t, *J* = 7.6 Hz, 2H, *p*-CH), 7.32 (d, *J* = 7.6 Hz, 4H, *m*-CH), 7.10 (s, 2H, NCH), 2.65 (sept., *J* = 6.8 Hz, 4H, CH(CH₃)₂), 1.35 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.22 (d, *J* = 6.4 Hz, 12H, CH(CH₃)₂), 1.07 (d, ³*J*_{HH} = 11.2 Hz, 1H, AuCHDCHD), 0.61 (s, 9H, C(CH₃)₃), 0.48 (d, ³*J*_{HH} = 11.2 Hz, 1H, AuCHDCHD). ²H NMR (CD₂Cl₂, δ): 1.09 (br, 1D), 0.53 (br, 1D). ¹³C{¹H} NMR (CD₂Cl₂, δ): 202.3, 146.5, 135.7, 130.4, 124.4, 123.2, 45.5 (t, *J*_{CD} = 18.8 Hz), 32.3, 29.5, 29.2, 24.6, 24.2, 14.5 (t, *J*_{CD} = 17.5 Hz).

Stereochemistry of C-I reductive elimination. Crystalline iodine (1 eq.) was added to a CDCl₃ solution of a (IPr)Au(*neo*-hexyl) complex (1 eq., ~ 25 mM), stirred for 10 min, and transferred to an NMR tube. In the case of unlabeled *t*BuCH₂CH₂Au(IPr), ¹H NMR and GC-MS analyses indicated clean, quantitative conversion to *t*BuCH₂CH₂I and (IPr)AuI.¹⁰ In the cases of *neo*-hexyl-*d*₂ derivatives, ¹H{²H} NMR analysis indicated overall retention of stereochemistry, with *anti-t*BuCHDCHDAu(IPr) being converted to *anti-t*BuCHDCHDI (³*J*_{HH} = 12.8 Hz) and *syn-t*BuCHDCHDAu(IPr) to *syn-t*BuCHDCHDI (³*J*_{HH} = 4.8 Hz).

In situ characterization of *cis*-(IPr)AuF₂(*neo*-hexyl). CDCl₃ was added to solid XeF₂ (1 eq.) and *t*BuCH₂CH₂Au(IPr) (1 eq.). After stirring for 10 min, the clear solution was transferred to an NMR tube and analyzed by NMR spectroscopy. The ¹⁹F NMR parameters of the resulting species were found to be extremely similar to those reported previously for *cis*-(IPr)AuMeF₂.¹¹ δ = -194.7 (d, ²*J*_{FF} = 82.8 Hz, monomer), -212.4 (d, ²*J*_{FF} = 67.8 Hz, monomer).

¹⁰ Scott, V. J.; Labinger, J. A.; Bercaw, J. E. *Organometallics* **2010**, 29, 4090.

¹¹ Mankad, N. P.; Toste, F. D. *J. Am. Chem. Soc.* **2010**, 132, 12859.

Stereochemistry of C-C reductive elimination. CDCl_3 was added to solid XeF_2 (1 eq.) and a $(\text{IPr})\text{Au}(\text{neo-hexyl})$ complex (1 eq., ~ 25 mM). After stirring for 5 min, phenylboronic acid (2.5 eq.) was added in one portion. After an additional 5 min of stirring, the solution was transferred to an NMR tube. In the case of unlabeled $t\text{BuCH}_2\text{CH}_2\text{Au}(\text{IPr})$, ^1H NMR and GC-MS analyses indicated quantitative conversion to products, with the product mixture consisting of ~1:1 *neo*-hexylbenzene and 3,3-dimethyl-1-butene. The main IPr-containing byproduct was $(\text{IPr})\text{AuPh}$.¹² In the cases of *neo*-hexyl- d_2 derivatives, $^1\text{H}\{^2\text{H}\}$ NMR analysis indicated overall retention of stereochemistry, with *anti*- $t\text{BuCHDCHDAu}(\text{IPr})$ producing *anti*- $t\text{BuCHDCHDPh}$ ($^3J_{\text{HH}} = 12.4$ Hz) and *syn*- $t\text{BuCHDCHDAu}(\text{IPr})$ producing *syn*- $t\text{BuCHDCHDPh}$ ($^3J_{\text{HH}} = 5.0$ Hz).

Preparation of $\text{DIMEs}(\text{AuMe})_2$. To a flame-dried Schlenk tube under flow of N_2 was added $\text{DIMEs}\cdot 2\text{HBr}$ (0.319 g, 0.584 mmol), sodium *tert*-butoxide (0.117 g, 1.22 mmol), and methylgold(I) triphenylphosphine (0.405 g, 0.854 mmol). Tetrahydrofuran (10 mL) was added by syringe. The tube was sealed with a Teflon valve and heated to 75°C for 18 h with stirring. After cooling to room temperature, volatiles were removed by rotary evaporation. Benzene (20 mL) was added, and the resulting mixture was filtered through a short pad of basic alumina. The alumina pad was washed with additional benzene (3 x 5 mL), and the combined filtrates were concentrated to tacky yellow solids. Washing with several portions of hexanes provided a fine white powder. Recrystallization by diffusion of pentane vapors into a concentrated dichloromethane solution yielded the desired product as colorless blocks suitable for X-ray diffraction. Yield: 0.200 g (58% based on Au). Analysis by NMR spectroscopy indicated that methylgold(I) triphenylphosphine was present as a minor impurity (typically <10%), and this material was utilized without further purification. ^1H NMR (CDCl_3 , δ): 8.11 (d, $J = 1.8$ Hz, 2H, $\text{C}_{\text{imid}}\text{-H}$), 6.98 (s, 4H, $\text{C}_{\text{mesityl}}\text{-H}$), 6.84 (s, 2H, CH_2), 6.81 (d, $J = 1.8$ Hz, 2H, $\text{C}_{\text{imid}}\text{-H}$), 2.35 (s, 6H, *para*- CH_3), 2.02 (s, 12H, *ortho*- CH_3), 0.19 (s, 6H, Au-CH_3). ^{13}C NMR (CDCl_3 , δ): 200.7 ($\text{C}_{\text{carbene}}$), 139.5, 134.8, 134.5, 129.5, 122.8, 120.2, 61.8 (CH_2), 21.4 (*para*- CH_3), 18.0 (*ortho*- CH_3), -0.62 (Au-CH_3).

Preparation of $\text{DIMEs}(\text{AuCl})_2$ (6). A solution of hydrochloric acid (4 N in 1,4-dioxane, 0.17 mL, 0.68 mmol) was added to a stirring solution of $\text{DIMEs}(\text{AuMe})_2$ (0.200 g, 0.247 mmol) in dichloromethane (5 mL), immediately resulting in methane bubbles. The solution was stirred at room temperature for 0.5 h and then concentrated by rotary evaporation to yield a white powder. Recrystallization from dichloromethane/diethyl ether (-30°C) in two crops gave the desired product as feathery needles. Yield: 0.140 g (67%). Blade-shaped crystals suitable for X-ray diffraction were obtained by diffusing diethyl

¹² Hashmi, A. S. K., Lothschütz, C., Döpp, R., Rudolph, M., Ramamurthi, T. D., and Rominger, F. *Angew. Chem., Int. Ed.* **2009**, 48, 8243.

ether vapors through a small hole into a dichloromethane solution. ^1H NMR (CDCl_3 , δ): 8.08 (d, $J = 1.8$ Hz, 2H, $\text{C}_{\text{imid}}\text{-H}$), 6.97 (s, 4H, $\text{C}_{\text{mesityl}}\text{-H}$), 6.96 (d, $J = 2.0$ Hz, 2H, $\text{C}_{\text{imid}}\text{-H}$), 6.66 (s, 2H, CH_2), 2.34 (s, 6H, *para*- CH_3), 1.97 (s, 12H, *ortho*- CH_3). ^{13}C NMR (CDCl_3 , δ): 173.8 ($\text{C}_{\text{carbene}}$), 140.6, 134.6, 134.3, 129.9, 123.7, 121.5, 63.4 (CH_2), 21.3 (*para*- CH_3), 17.9 (*ortho*- CH_3). Anal. Calcd. for $\text{C}_{25}\text{H}_{28}\text{Au}_2\text{Cl}_2\text{N}_4$: C, 35.35; H, 3.32; N, 6.60. Found: C, 35.23; H, 3.26; N, 6.46.

Preparation of $[(\text{PhCH}_2)(\text{Ph})_2\text{P}]\text{AuCl}_3$ (2). This compound was prepared from $[(\text{PhCH}_2)(\text{Ph})_2\text{P}]\text{AuCl}$ and PhICl_2 according to the procedure for preparing $\text{Ph}_3\text{PAuCl}_3$ reported by Teets and Nocera.¹³ Analytically pure material was obtained by recrystallization from dichloromethane/*n*-pentane. ^1H NMR (CDCl_3): 7.67 – 7.50 (m, 10H), 7.32 (t, $J = 7.6$ Hz, 1H), 7.12 (t, $J = 7.6$ Hz, 2H), 6.81 (d, $J = 6.0$ Hz, 2H), 4.39 (d, $^2J_{\text{HP}} = 13.2$ Hz, 2H, PCH_2Ph). $^{31}\text{P}\{^1\text{H}\}$ NMR (CDCl_3): 40.0 (s). Anal. Calcd. for $\text{C}_{19}\text{H}_{17}\text{AuCl}_3\text{P}$: C, 39.37; H, 2.96. Found: C, 38.14; H, 3.09.

¹³ Teets, T. S.; Nocera, D. G. *J. Am. Chem. Soc.* **2009**, *131*, 7411.

Cyclic voltammetry. Electrochemical measurements were carried out in a one-compartment cell using a BASI Epsilon potentiostat. A glassy carbon electrode was used as the working electrode and platinum wire was used as the auxiliary electrode. The reference electrode was a silver wire immersed in a solution of 0.01 M AgNO₃ and 0.1 M tetrabutylammonium hexafluorophosphate in a glass tube fitted with a porous Vycor tip. The ferrocenium/ferrocene couple was used as an external reference. All experiments were conducted in dichloromethane solution with 0.1 M tetrabutylammonium hexafluorophosphate as a supporting electrolyte at 100 mV/s scan rates.

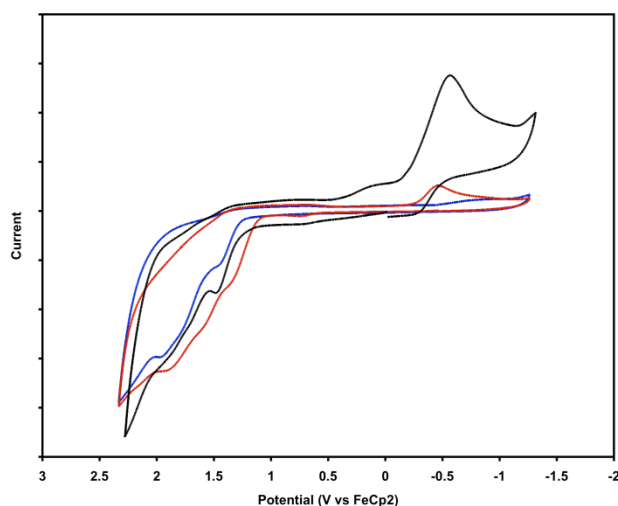


Figure S1. Cyclic voltammetry data for complexes **15** (blue), **17** (black), and **18** (red).

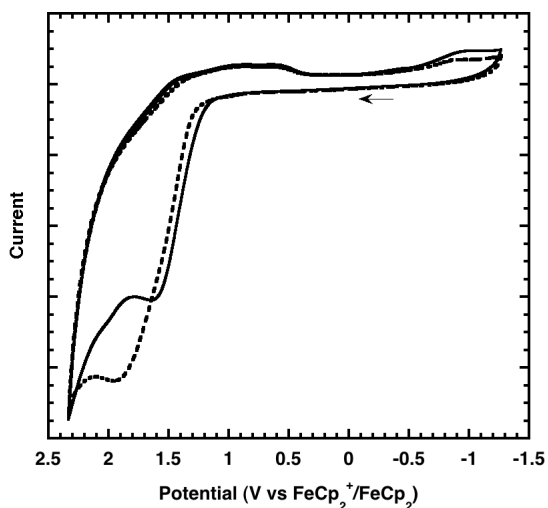


Figure S2. Cyclic voltammograms of complexes **19** (dashed) and **20** (solid).

X-ray crystallography. Low-temperature diffraction data were collected at the UC-Berkeley CHEXRAY crystallographic facility. Measurements were made with a Bruker-AXS Smart Apex CCD detector with graphite-monochromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). The structures were solved by direct methods using SHELXS¹⁴ and refined against F^2 on all data by full-matrix least squares with SHELXL-97¹⁵ using established methods.¹⁶ All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). Details of the data quality and a summary of the residual values of the refinements are listed below.

¹⁴ Sheldrick, G. M. *Acta Cryst.* **1990**, *A46*, 467.

¹⁵ Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112.

¹⁶ Müller, P. *Crystallography Reviews* **2009**, *15*, 57.

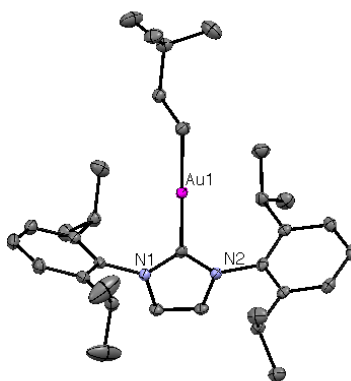


Figure S3. Solid-state structure of (IPr)Au(*neo*-hexyl) (50% ellipsoids). Hydrogen atoms have been omitted for clarity.

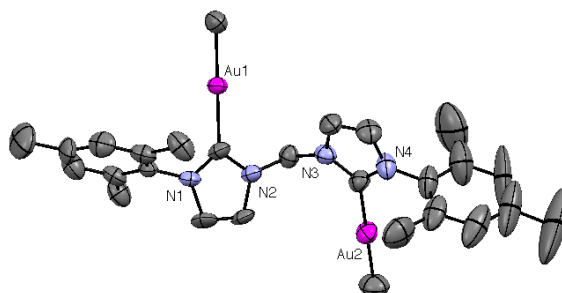


Figure S4. Solid-state structure of DIMes(AuMe)₂ (50% ellipsoids). Hydrogen atoms have been omitted for clarity.

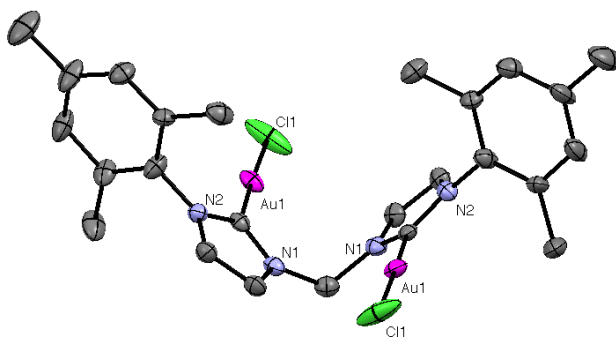


Figure S5. Solid-state structure of DIMes(AuCl)₂ (50% ellipsoids). Hydrogen atoms have been omitted for clarity. Half the molecule was generated by symmetry operations.

Table S1. Crystal data and structure refinement for (IPr)Au(*neo*-hexyl).

Empirical formula	C ₃₃ H ₄₉ AuN ₂	
Formula weight	670.71	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.8072(4) Å	α = 92.008(2)°.
	b = 10.5644(4) Å	β = 94.622(2)°.
	c = 15.4385(7) Å	γ = 95.187(2)°.
Volume	1586.36(11) Å ³	
Z	2	
Density (calculated)	1.404 Mg/m ³	
Absorption coefficient	4.658 mm ⁻¹	
F(000)	680	
Crystal size	0.15 x 0.05 x 0.02 mm ³	
Theta range for data collection	1.32 to 25.40°.	
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -18 ≤ l ≤ 18	
Reflections collected	45192	
Independent reflections	5834 [R(int) = 0.0236]	
Completeness to theta = 25.40°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5834 / 0 / 336	
Goodness-of-fit on F ²	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0128, wR2 = 0.0315	
R indices (all data)	R1 = 0.0135, wR2 = 0.0319	
Largest diff. peak and hole	0.747 and -0.494 e.Å ⁻³	

Table S2. Crystal data and structure refinement for DIMes(AuMe)₂.

Empirical formula	C ₂₇ H ₃₄ Au ₂ N ₄	
Formula weight	808.52	
Temperature	158(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 39.063(17) Å	α = 90°.
	b = 9.791(4) Å	β = 111.636(5)°.
	c = 16.102(7) Å	γ = 90°.
Volume	5724(4) Å ³	
Z	8	
Density (calculated)	1.876 Mg/m ³	
Absorption coefficient	10.259 mm ⁻¹	
F(000)	3056	
Crystal size	0.50 x 0.15 x 0.15 mm ³	
Theta range for data collection	2.44 to 25.35°.	
Index ranges	-46 ≤ h ≤ 46, -11 ≤ k ≤ 11, -19 ≤ l ≤ 19	
Reflections collected	25453	
Independent reflections	5241 [R(int) = 0.0735]	
Completeness to theta = 25.35°	99.9 %	
Absorption correction	None	
Max. and min. transmission	0.3083 and 0.0795	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5241 / 0 / 306	
Goodness-of-fit on F ²	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.0787	
R indices (all data)	R1 = 0.0716, wR2 = 0.0901	
Largest diff. peak and hole	1.708 and -1.193 e.Å ⁻³	

Table S3. Crystal data and structure refinement for DIMes(AuCl)₂.

Empirical formula	C ₂₅ H ₂₈ Au ₂ Cl ₂ N ₄	
Formula weight	849.35	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I-42d	
Unit cell dimensions	a = 12.3331(7) Å	α = 90°.
	b = 12.3331(7) Å	β = 90°.
	c = 43.691(3) Å	γ = 90°.
Volume	6645.6(7) Å ³	
Z	8	
Density (calculated)	1.698 Mg/m ³	
Absorption coefficient	8.997 mm ⁻¹	
F(000)	3184	
Crystal size	0.10 x 0.10 x 0.05 mm ³	
Theta range for data collection	1.72 to 34.97°.	
Index ranges	-19 ≤ h ≤ 19, -19 ≤ k ≤ 19, -70 ≤ l ≤ 70	
Reflections collected	197338	
Independent reflections	7304 [R(int) = 0.0358]	
Completeness to theta = 34.97°	100.0 %	
Absorption correction	None	
Max. and min. transmission	0.6618 and 0.4665	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7304 / 0 / 153	
Goodness-of-fit on F ²	1.662	
Final R indices [I>2sigma(I)]	R1 = 0.0636, wR2 = 0.1901	
R indices (all data)	R1 = 0.0659, wR2 = 0.1918	
Absolute structure parameter	0.03(2)	

Largest diff. peak and hole

11.123 and -2.282 e.Å⁻³

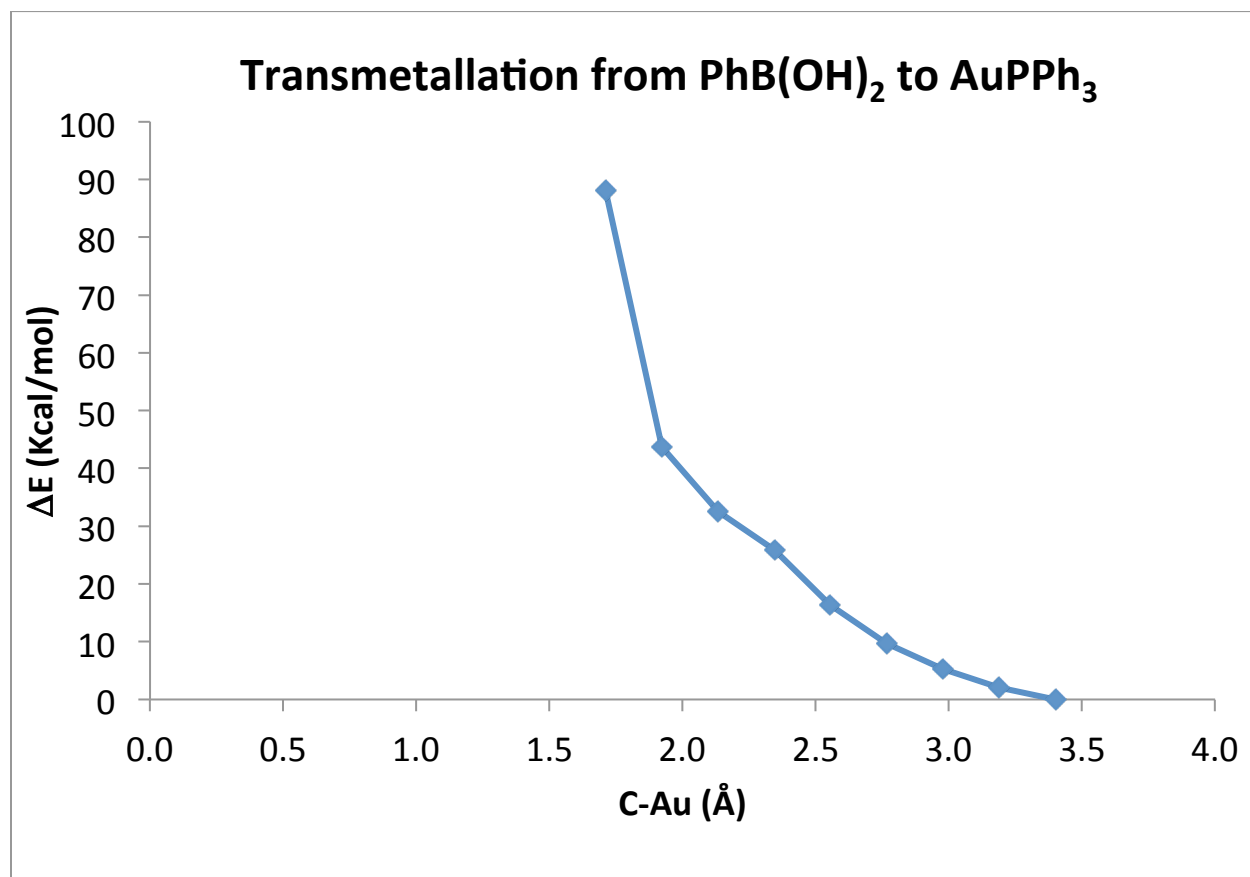
(I) Absolute Energies (In Hartrees) Of All Optimized Molecules

<i>Name</i>	<i>Energy (a.u.)</i>	<i>Name</i>	<i>Energy (a.u.)</i>
1-Cl	-1730.914924	1-Br	-1283.895862
2-Cl	-2432.873848	2-Br	-1985.856635
3-Cl	-4064.303502	3-Br	-3170.237463
4-Cl	-3362.385808	4-Br	-2468.344749
5-Cl	-3362.36865	5-Br	-2468.328917
6-Cl	-3362.376641	6-Br	-2468.345866
7-Cl	-1631.419286	7-Br	-1184.402627
8-Cl	-3262.878987	8-Br	-2368.846724
9-Cl	-3536.748677	9-Br	-2642.715306
10-Cl	-4064.323783	10-Br	-3170.284258
11-Cl	-4238.673221	11-Br	-3344.629179
12-Cl	-4063.948154	12-Br	-3169.919541
13-Cl	-4471.930757	13-Br	-3577.887654
14-Cl	-4472.136765	14-Br	-3578.088991

<i>Name</i>	<i>Energy (a.u.)</i>
10-Cl-dppm	-3640.649696
11-Cl-dppm	-3697.158903
12-Cl-dppm	-3640.266395
13-Cl-dppm	-4048.291748
14-Cl-dppm	-4048.452299

<i>Name</i>	<i>Energy (a.u.)</i>
P(Ph)3Au Br F TFA cycle	-1985.490163
TS Br NMe3	-2160.222353
P P(Ph)3AuBrFTFAB(OH)2Ph TS	-2393.516346
P(Ph)3Au Cl F TFA cycle	-2432.501734
TS Cl NMe3	-2607.245988
P(Ph)3AuCl F TFA B(OH)2Ph	-2840.53339

(II) Relaxed Coordinates Scan of Transmetallation



(III) XYZ of Intermediates and Transition State Structures

BIMETALLIC PATHWAY

1) Ligand on Au is P(Ph)₃

a. Catalyst L-Au-Cl

1-Cl				2-Cl			
P1	0.1230664015	-0.0601046853	-0.0257453461	C1	-0.3921537075	0.8759039465	0.1162366309
C2	0.1524962473	-0.2964264292	1.7393005885	C4	-0.3767464986	0.3473431179	1.5455124473
C13	1.7106762390	-0.2718546672	-0.7814082883	N10	0.9371179740	1.1192899700	-0.4127223445
C24	-0.6952833769	1.4292643762	-0.5412712273	C7	-1.7368565882	0.5468182438	2.2055600148
Au35	-1.3157175974	-1.8225929624	-0.7839145168	C12	1.6854392915	2.2424303560	-0.3113506946
C5	-1.0476289313	-0.4501996351	2.4461862874	C22	-1.8779732336	-0.1610928722	3.5012473341
C4	1.3799629382	-0.2553345254	2.4129721005	O13	2.8404678458	2.3308622385	-0.6398850898
C16	2.4570545455	-1.4326281252	-0.5205011707	C14	0.9575620803	3.4885891878	0.2576232328
C15	2.2360134974	0.7540005440	-1.5823757650	C19	-2.2630699869	0.4223505628	4.6665732659
C27	-1.0912470763	2.3721988983	0.4097492874	Au58	0.1442909352	0.4977601518	4.9442597944
C26	-0.9895404901	1.6064909928	-1.8984029351	F15	1.7905460848	4.5088534612	0.3263532071
Cl36	-3.2849172502	-0.6787034291	-0.4539069711	F16	0.4935660680	3.2632781325	1.4981939630
F13	0.2644933407	-2.9850907087	-1.0744316448	F17	-0.0821856208	3.8337886220	-0.5004685045
C6	-1.0109590015	-0.5515489948	3.8231698039	P24	2.3753611813	1.0296513012	5.6898733055
C7	1.3953516898	-0.3552767751	3.7930257844	Cl59	0.1300721284	-1.6209729636	5.8888872398
C17	3.7277786197	-1.5454516039	-1.0468040921	F60	0.0916472171	2.3512558605	4.1736107336
C18	3.5093832463	0.6194073624	-2.1005398366	C25	3.3983797982	1.4157216636	4.2711117402
C28	-1.7651238288	3.5062963623	-0.0097490012	C36	3.1179620277	-0.2770413862	6.6635985144
C29	-1.6659207026	2.7399147673	-2.2991204919	C47	2.0676684130	2.4765832596	6.7024065379
C3	0.2068081492	-0.5063080115	4.4940180512	C28	2.9752624183	2.4040192358	3.3704625452
Cl4	4.2500064417	-0.5266138282	-1.8365677023	C27	4.6351126769	0.7831621578	4.1022806603
C25	-2.0555038177	3.6855959666	-1.3549918864	C39	3.4811100294	-0.0399569459	7.9898518495
H9	-1.9977407935	-0.5000463886	1.9201182994	C38	3.3512852677	-1.5257008406	6.0781973419
H8	2.3090001196	-0.1279931246	1.8673786496	C50	1.0719772563	2.4053331712	7.6806171527
H20	2.0239941882	-2.2448083358	0.0505479418	C49	2.8103448057	3.6422590339	6.5261172717
H19	1.6659724688	1.6565327906	-1.7740673165	C29	3.7993882204	2.7507291392	2.3160767449
H31	-0.8716899867	2.2251097769	1.4624035000	C30	5.4374814866	1.1332370387	3.0293717189
H30	-0.7185305832	0.8469627218	-2.6275494968	C40	4.0922225861	-1.0477349091	8.7188389146
H10	-1.9344352790	-0.6770524195	4.3767458765	C41	3.9640621014	-2.5203404789	6.8148303471
H21	2.3404376375	-0.3156774127	4.3226489653	C51	0.8336146175	3.5008147370	8.4894345576
H11	4.3090210954	-2.4402639302	-0.8567005256	C52	2.5611068347	4.7333111601	7.3441578922
H22	3.9281265957	1.4120640556	-2.7098473448	C26	5.0186212486	2.1081514181	2.1355765342
H22	-0.0714060999	4.2492413738	0.7177825924	C37	4.3320794356	-2.2815822480	8.1343800159
H33	-1.9083131495	2.8827612174	-3.3458748817	C48	1.5765115887	4.6636420932	8.3182011865
H12	0.2281795457	-0.5945968169	5.5749440764	H2	-0.9002459561	0.1715170731	-0.5506378479
H23	5.2458944886	-0.6289135398	-2.2545882804	H3	-0.9716156478	1.8007873522	0.0693489938
H34	-2.5987570341	4.5685963335	-1.6738783799	H5	-0.0819262518	-0.7110912646	1.5632276216
				H6	0.3735801619	0.9089364370	2.1169582534
				H11	1.4539669475	0.3374442990	-0.7972611674
				H8	-1.9287408392	1.6187737157	2.3319718261
				H9	-2.5236822584	0.1494895504	1.5435368168
				H23	-1.7176395067	-1.2410705724	3.4939286525
				H20	-2.4918276856	-0.1803739582	5.5406613192
				H21	-2.4988739076	1.4837126848	4.6983255396
				H32	2.0074862397	2.8803356048	3.4971739847
				H31	4.9786924307	0.0363389122	4.8095261633
				H43	3.3039427542	0.9278754267	8.4472786235
				H42	3.0447663133	-1.7203476568	5.0543496459
				H54	0.4920198518	1.4936298314	7.8123626274
				H53	3.5795903985	3.6972974256	5.7625075132
				H33	3.4910841071	3.5171022447	1.6160696974
				H34	6.3962705182	0.6446521601	2.8962537276
				H44	4.3832390983	-0.8648695994	9.7470232594
				H45	4.1462827081	-3.4896143580	6.3650304006
				H55	0.0635176420	3.4534088475	9.2509549254
				H56	3.1372435999	5.6427168116	7.2159412383
				H35	5.6403754921	2.3740512885	1.2874271464
				H46	4.8068901737	-3.0679272792	8.7110280691
				H57	1.3817681259	5.5239763593	8.9494400194

3-Cl				4-Cl			
C1	-0.9347954906	-1.1568382117	2.7830476248	P1	0.6546865895	2.1887905124	4.9745388712
H2	0.1448358833	-1.0420625394	2.6155726703	C2	0.3871479419	0.6590800385	5.8512702053
H3	-1.3085402924	-0.2596480273	3.2926235031	C3	-0.1534986931	-1.6328097773	7.3037558327
C4	-1.6243708415	-1.3089876145	1.4370278685	C4	-0.9086001739	0.1156352419	5.8291190791
H5	-1.2821347688	-2.2319562880	0.9509344145	C5	1.4103757991	0.0572854748	6.5976216392
H6	-2.7126272259	-1.3957104565	1.5720053931	C6	1.1278138943	-1.0887443544	7.3268129066
C7	-1.2942816347	-0.1167740808	0.5415250892	C7	-1.1684583943	-1.0323650874	6.5597894444
H8	-0.2093437369	-0.0338114775	0.3788273782	H8	-1.6831691697	0.6035095263	5.2361335191
H9	-1.7272333490	-0.2889553046	-0.4591058699	H9	2.4069815176	0.4915425405	6.6262306655
N10	-1.1058549019	-2.2791734822	3.6857958863	H10	1.9096974731	-1.5564413515	7.9190808448
Cl11	-0.2317724969	-3.3064139163	3.7044892721	H11	-2.1654895266	-1.4637257705	6.5484029749
O12	0.7193132220	-3.4549786817	2.9626986266	H12	-0.3648873329	-2.5336415719	7.8745776757
Cl13	-0.4469105184	-4.2857069899	4.8696731049	Cl13	-0.3286414303	3.5014357951	5.6747871133
F14	-0.2171655477	-5.5281774601	4.4984291336	Cl14	-1.6423666955	5.5767549122	6.9453277053
F15	-1.6892447091	-4.2076140191	5.3727536070	Cl15	-0.6478048802	4.6579485670	4.9519942567
F16	0.4013279342	-3.9649801900	5.8541666681	Cl16	-0.6973228769	3.3640278733	7.0213007935
Cl17	-1.2505443003	2.3980352365	0.7648815474	Cl17	-1.3432654852	4.4174166639	7.6530956978
Cl18	-1.8361453523	1.1893063200	0.9984725900	Cl18	-1.3000448089	5.6943436431	5.5992729602
P19	0.4534375077	2.8297887559	5.3381395277	H19	-0.3908362110	4.7286501310	3.8971012955
C20	0.4529990261	1.3210826205	6.3345916025	H20	-0.4667508108	2.4566827589	7.5752256804
C21	0.2979245612	-0.8365094563	8.0912179060	H21	-1.6169641507	4.3277810577	8.7008383748
C22	-0.5880401846	0.3911411925	6.2075716311	H22	-1.5541745951	6.5944724467	5.0467098289
C23	1.4085147725	1.1738970972	7.3523367754	H23	-2.1567280547	6.3942907520	7.4442782581
C24	1.3205054022	0.0985260254	8.2275253750	Au24	-0.1291598730	1.6250064003	2.7710715219
C25	-0.6520146861	-0.6869479305	7.0832284457	F25	-1.7849843485	2.2172011242	3.7220493627
H26	-1.3430923367	0.5454972151	5.4370061820	P26	5.1763319398	2.3916316134	0.3117385094

H27	2.2069875229	1.9019756832	7.4749054422	Au27	3.2534535895	3.3703039096	1.1856286530
H28	2.0563235225	-0.0063569357	9.0207396226	C128	1.2276561520	4.3756739522	1.9970814515
H29	-1.4557453371	-1.4134910456	6.9852192791	C29	4.8138770884	1.4057694986	-1.1682431202
H30	0.2371768224	-1.6790932438	8.7756411769	C30	4.2457771600	-0.0510908082	-3.4719281697
C31	-0.7525513377	3.9675751797	6.0437964357	C31	3.6725597261	1.6975818321	-1.9186258122
C32	-2.5205039960	5.7627996232	7.2062364437	C32	5.6672517009	0.3729297058	-1.5743982455
C33	-1.1049588947	5.1415645513	5.3630476634	C33	5.3820117120	-0.3498301931	-2.7251459379
C34	-1.3062958097	3.6864061817	7.2988092777	C34	3.3922122752	0.9700507640	-3.0694111561
C35	-2.1872141042	4.5917813163	7.8754463123	H35	2.9959322593	2.4883840591	-1.5931357598
C36	-1.9858465527	6.0363437997	5.9518418855	H36	6.5475059355	0.1237949140	-0.9823975026
H37	-0.6911127623	5.3551562425	4.3786311610	H37	6.0444215527	-1.1539576049	-3.0362791596
H38	-1.0443713566	2.7730343776	7.8283868437	H38	2.4998806083	1.1963278590	-3.6472771988
H39	-2.6112253389	4.3795043501	8.8533663060	H39	4.0214846850	-0.6239815535	-4.3684852231
H40	-2.2551821394	6.9495209145	5.4278408145	C40	6.4524391874	3.6120430299	-0.1158153414
H41	-3.2166573361	6.4665448173	7.6625810591	C41	8.4809667228	5.4572039765	-0.6091898671
Au42	-0.4219311747	2.5440031110	3.0732155109	C42	6.5203626546	4.7956594931	0.6245054420
H43	-1.8151565865	3.3203748884	0.8969734675	C43	7.4012150080	3.3601090254	-1.1107153027
H44	-0.3235450474	2.4630986835	0.1921710121	C44	8.4099218901	4.2840842964	-1.3554723815
H45	-2.7955431612	1.1766953999	1.5226473541	C45	7.5362460721	5.7128210391	0.3800320058
F46	-2.0099178114	1.5141525077	3.9077867520	H46	5.7686289456	4.9974269972	1.3899301888
P47	3.3611232786	0.4926628537	1.6449697073	H47	7.3473485712	2.4463877325	-1.7006871780
Au48	2.4053357038	2.6079030100	2.0610950366	H48	9.1426419690	4.0880169344	-2.1344168154
C149	4.1307168069	4.4061325045	1.7036556714	H49	7.5839353660	6.6339262485	0.9557585785
C150	0.7156283139	4.4063257039	2.2940307671	H50	9.2707420773	6.1781223067	-0.8053099257
C51	2.4312214457	-0.4237994602	0.3794047636	C51	6.0036754830	1.2111418290	1.4325737453
C52	1.0634463802	-1.7770365903	-1.6386081586	C52	7.1753408328	-0.6250461170	3.1804698783
C53	2.1931298593	0.2045286631	-0.8508422987	C53	7.2524017764	1.4779956741	1.9952697101
C54	1.9806546848	-1.7273066989	0.5959339359	C54	5.3430768813	0.0178482199	1.7482934010
C55	1.2926267478	-2.3962332661	-0.4145421361	C55	5.9298883790	-0.8965677044	2.6132752817
C56	1.5191611808	-0.4757017127	-1.8565020307	C56	7.8324433392	0.5610895349	2.8699661722
H57	2.5514592696	1.2215369723	-1.0219000202	H57	7.7794618053	2.3985601558	1.7474361699
H58	2.1429848423	-2.2312856237	1.5475926814	H58	4.3671661541	-0.1963540362	1.3117850193
H59	0.9441667287	-3.4107564220	-0.2300931214	H59	5.4165737244	-1.8277251126	2.8433217932
H60	1.3486533408	0.0097373007	-2.8145145489	H60	8.8091768597	0.7715367962	3.2996695912
H61	0.5358158697	-2.3065759839	-2.4283468986	H61	7.6359252805	-1.3428055015	3.8551270891
C62	5.0574332625	0.5925594352	1.0180297308	C62	2.3710342100	2.6249598476	4.8601623138
C63	7.7249595471	0.6285909999	0.2365325018	C63	5.0550688911	3.3027493597	4.7762201566
C64	5.9410732614	1.5074527784	1.5965615568	C64	3.3175488396	1.6654977870	4.4662791042
C65	5.5110444874	-0.3001846104	0.0409419277	C65	2.7685021085	3.9336992582	5.1781250597
C66	6.8452699424	-0.2778168824	-0.3462625468	C66	4.1141815687	4.2640747131	5.1344050849
C67	7.2732121687	1.5197276691	1.2044552433	C67	4.6591634562	2.0044492458	4.4533687340
H68	5.5764284895	2.2388053710	2.3170574723	H68	3.0021730813	0.6720353736	4.1466311969
H69	4.8264875131	-0.1055917461	-0.4126298628	H69	2.0311126806	4.6811399256	5.4597193679
H70	7.1977515243	-0.9704016733	-1.1065132858	H70	4.4273421262	5.2744074154	5.3821300638
H71	7.9569294409	2.2408948791	1.6449917488	H71	5.4003027720	1.2602249503	4.1748900101
H72	8.7675410425	0.6457850170	-0.0719914610	H72	6.1113365586	3.5625041967	4.7397138984
C73	3.4297691451	-0.6060059124	3.0896429423	C73	1.6048734488	0.5292057519	1.6683780721
C74	3.3581954939	-2.4624323122	5.1681028927				
C75	4.4674002108	-1.5299350550	3.2402389822				
C76	2.3713993964	-0.6048906310	4.0014140644				
C77	2.3315931949	-1.5341737679	5.0318821993				
C78	4.4279829590	-2.4521157972	4.2802782013				
H79	5.2994537932	-1.5366320389	2.5377938937				
H80	1.5616110878	0.1204192270	3.8865446826				
H81	1.4880809232	-1.5444328142	5.7190151446				
H82	5.2337728332	-3.1737755967	4.3894104607				
H83	3.3194920237	-3.1990496898	5.9671261816				
C84	2.1047412096	3.5279529795	5.3602379045				
C85	4.6896302478	4.5617774138	5.2948892104				
C86	3.2030495036	2.6716323310	5.1636848602				
C87	2.3122253493	4.9041820354	5.5147150055				
C88	3.6036860056	5.4116149455	5.4820958876				
C89	4.4871773137	3.1908100120	5.1484796161				
H90	3.0565498168	1.5992062684	5.0367683212				
H91	1.4711769644	5.5764588413	5.6687833887				
H92	3.7623859296	6.4799208139	5.5995466174				
H93	5.3327369497	2.5218267895	5.0040144163				
H94	5.6963591526	4.9688197805	5.2587043923				
H95	-1.9131145082	-2.3161624953	4.2925802219				

5-CI				6-CI			
P19	0.5713312024	2.8932779980	5.5068418636	P1	0.5148243295	2.3883108454	5.7978120708
C20	0.4808001733	1.5678858601	6.7295318339	C2	0.4429222961	1.0427446906	7.0005777327
C21	0.1492344128	-0.3856904309	6.6696036898	C3	0.1041870444	-0.9095856417	8.9439718307
C22	-0.3582533487	0.4808504823	6.4751464399	C4	-0.4642197210	-0.0031908964	6.7800803853
C23	1.1597901069	1.6804415143	7.9543691748	C5	1.1783755342	1.1119577665	8.1907962496
C24	0.9810245064	0.7009339806	8.9227065362	C6	1.0007373193	0.1331736486	9.1608909545
C25	-0.5149115588	-0.4950956896	7.4507327278	C7	-0.6226310270	-0.9771583282	7.7573661474
H26	-0.8841381925	0.4209489803	5.5186996480	H8	-1.0243127867	-0.0486130303	5.8415484920
H27	1.8095240736	2.5302190791	8.1560022031	H9	1.8741569065	1.9302335196	8.3656637310
H28	1.4908366526	0.7900621475	9.8787001969	H10	1.5601153340	0.1899694871	10.0914785276
H29	-1.1699566511	-1.3411066958	7.2618770741	H11	-1.3247440822	-1.7905964768	7.5932470941
H30	0.0135564294	-1.1490349975	9.4317223769	H12	-0.0321400845	-1.6720274664	9.7074198723
C31	-0.8701941519	3.9514357671	5.7284884969	C13	-0.9839495747	3.3679493694	5.9844660149
C32	-3.0111529346	5.6457162422	6.1996729008	C14	-3.2630981982	4.8950500587	6.3738784746
C33	-1.6477641809	4.3957961699	4.6578552764	C15	-1.6710882235	3.8757457951	4.8803264995
C34	-1.1688039179	4.3456247484	7.0397228515	C16	-1.4400302017	3.6155295483	7.2860300891
C35	-2.2366353640	5.1989469266	7.2673575685	C17	-2.5771129143	4.3875135416	7.4740118904
C36	-2.7208618462	5.2433029267	4.9026611627	C18	-2.8139282636	4.6387827454	5.0828818763
H37	-1.4119245408	4.0933025245	3.6406880338	H19	-1.3057439709	3.6911307218	3.8715364777
H38	-0.5703223158	3.9874086264	7.8771382932	H20	-0.9117723788	3.2050947438	8.1459425727
H39	-2.4677263187	5.5127110757	8.2812693680	H21	-2.9334088384	4.5862110684	8.4814515281
H40	-3.3289513733	5.5904981356	4.0720774833	H22	-3.3538947729	5.0347680531	4.2272372751
H41	-3.8498254918	6.3115705549	6.3837419494	H23	-4.1583530025	5.4928704128	6.5259639535
Au42	0.4792254624	1.9744783073	3.3058925176	Au24	0.4186984821	1.3673911257	3.6506291847
F46	-1.3050027377	1.0486025937	3.6790765216	F25	-1.3117585876	0.2903108882	3.9278237694
P63	3.4741687284	0.7048352784	2.6348203401	P26	3.4017474706	0.4905822101	2.6864966976
Au64	2.8973094465	2.9969297958	2.8681049755	Au27	2.6235315578	2.7182091568	3.0427008160
C65	4.9377753206	4.2711049152	2.7084360453	C128	4.6585386356	3.9674030624	2.7078923031
C166	0.8796676183	4.4041591134	2.1860429153	C129	1.1539288388	4.6163619209	2.9122820637
C67	1.9340162851	-0.0805715002	2.0544983625	C30	1.8849318796	-0.3648974181	2.1329713984
C68	-0.5049186890	-1.1144743447	1.1454801016	C31	-0.5144615394	-1.5475451557	1.3009595705
C69	1.1047383052	0.6808067590	1.1876381606	C32	0.9417776909	0.3740837044	1.3689940024
C70	1.5293862906	-1.3585150515	2.4384502825	C33	1.6145625901	-1.6995866901	2.4464818067
C71	0.3198320040	-1.8669793848	1.9790739097	C34	0.4236858612	-2.2810457504	2.0256435938
C72	-0.1080756925	0.1483876163	0.7355696933	C35	-0.2518919211	-0.2298124157	0.9589318071
H73	1.4654103750	1.6228180031	0.7679975347	H36	1.1943067316	1.3705566524	0.9975809264
H74	2.1541363180	-1.9567637126	3.0975013138	H37	2.3316683821	-2.2819162794	3.0221597951
H75	0.0156425367	-2.8658816966	2.2778198502	H38	0.2219147277	-3.3201726907	2.2730089238
H76	-0.7334375302	0.7386765171	0.0717224055	H39	-0.9693384501	0.3463693523	0.3813204178
H77	-1.4553590912	-1.5203689646	0.8119119535	H40	-1.4502070113	-2.0101194712	1.00110

H85	4.1968714245	-1.7530001760	1.3595037125	H48	3.6032818754	-1.4550737874	0.5277967097
H86	5.9492629550	-2.3508524753	-0.2271189625	H49	5.3361768698	-1.8710418534	-1.1705970836
H87	7.2437177391	1.7440841903	-0.4165384278	H50	7.6186691002	1.4553836011	0.3115033834
H88	7.4739938530	-0.6074635601	-1.1654396656	H51	7.3497845543	-0.4264166621	-1.2833987183
C89	3.9724691342	-0.0390408441	4.1948464212	C52	3.9521209356	-0.2884867595	4.2267880583
C90	4.8230867276	-0.9067490962	6.6910722666	C53	4.8252711213	-1.2205721375	6.7064353700
C91	5.3373940423	-0.0849846750	4.4868919300	C54	5.3182531550	-0.3216969120	4.5209403829
C92	3.0330098733	-0.4054575214	5.1644220358	C55	3.0240233314	-0.7201327250	5.1847991764
C93	3.4627276788	-0.8509734922	6.4058520012	C56	3.4629686898	-1.1932253184	6.4147543184
C94	5.7571112066	-0.5211226184	5.7354791166	C57	5.7476884449	-0.7858075350	5.7598864797
H95	6.0696923134	0.2201167640	3.7407684422	H58	6.0478800491	0.0101041698	3.7839415387
H96	1.9648505845	-0.3322902180	4.9637218909	H59	1.9524321073	-0.6795881911	4.9842687564
H97	2.7289511311	-1.1412315980	7.1549696109	H60	2.7329965949	-1.5265726969	7.1503612683
H98	6.8184775791	-0.5628282955	5.9613946349	H61	6.8112787269	-0.8110948348	5.9827082612
H99	5.1576987014	-1.2516955844	7.6659637084	H62	5.1680355638	-1.5834858942	7.6719586669
C100	2.0807640258	3.8348866272	5.7699072737	C63	1.9790463583	3.3776766893	6.1393211494
C101	4.4352152306	5.2770940298	6.0871095230	C64	4.2777088139	4.8976814935	6.5129210193
C102	3.2893433003	3.1629813760	6.0437997685	C65	3.2333448662	2.7491004545	6.2129976060
C103	2.0686822683	5.2306730376	5.6379305245	C66	1.8824808959	4.7670452513	6.2539674129
C104	3.2473592800	5.9432315842	5.8025972306	C67	3.0348986312	5.5191464123	6.4461434979
C105	4.4548986509	3.8905925710	6.2123983002	C68	4.3752593282	3.5115944426	6.4022450714
H106	3.3130632943	2.0764947950	6.1317036255	H69	3.3160506694	1.6654927288	6.1251336759
H107	1.1419304582	5.7499788213	5.4008622844	H70	0.9159263330	5.2598826179	6.1723486402
H108	3.2400257098	7.0237437088	5.6956843320	H71	2.9606329781	6.5999021340	6.5293707697
H109	5.3876496254	3.3728949125	6.4199876217	H72	5.3455627281	3.0229731747	6.4487618453
H110	5.3568144413	5.8405390499	6.2011562252	H73	5.1756047946	5.4952194813	6.6456195001
7-CI				8-CI			
P1	0.000000000000	0.000000000000	0.000000000000	P1	0.3578817287	2.5335168300	6.3451515859
C2	0.000000000000	0.000000000000	1.820601363000	C2	0.5343357407	1.6835163502	7.9492011855
C13	1.757731691450	0.000000000000	-0.4737800642498	C3	0.6804817182	0.4115489528	10.4292895148
C24	-0.6203846755325	1.6446831032216	-0.4723052907098	C4	-0.3281781059	0.6269811535	8.2506930092
Au35	-1.2009027745384	-1.7405472033858	-0.9261936421147	C5	1.4781004829	2.0928902781	8.8962549556
C5	0.1050289183014	-1.2291011414752	2.4691606234293	C6	1.5486635699	1.4575790508	10.1307895994
C4	-0.0627827515675	1.1749718379869	2.5647686326742	C7	-0.2568292493	-0.0028451115	9.4881189055
C16	2.7666993959706	0.3690715759035	0.411587620494	H8	-1.0530155440	0.2963123991	7.5056524664
C15	2.0760504624837	-0.3495885366671	-1.7848318930263	H9	2.1623595167	2.9083911225	8.6633421566
C27	-2.0011060987430	1.8183107817113	-0.5482854886763	H10	2.2860138803	1.7812243976	10.8621214149
C26	0.2296690004481	2.7203688508299	-0.7136644135782	H11	-0.9334268571	-0.8234117625	9.7152436589
C36	-2.4094812907910	-3.4961710802610	-1.8593178406243	H12	0.7379080462	-0.0839226499	11.3957898695
C6	0.160945382561	-1.2804120549580	3.8521756050618	C13	-0.7278396838	3.9605675970	6.6514634312
C7	-0.0149235067385	1.1166791473256	3.9501640168064	C14	-2.3086550684	6.2199116243	7.0139518579
C17	4.0858959851751	0.3908480448518	-0.0174365578975	C15	-1.4302800101	4.5015434787	5.5708339656
C18	3.3939959807440	-0.3185123187237	-2.2096248474698	C16	-0.8244633455	4.5498309945	7.9149501556
C28	-2.5272902762262	3.0631547810673	-0.8517692650449	C17	-1.6171786453	5.6769906178	8.0928214541
C29	-0.3029428331542	3.9631060997126	-1.0249596399835	C18	-2.2137734482	5.6345314214	5.7560559809
C3	0.1001502947292	-0.1074141700162	4.5924416012311	C19	-1.1364855596	4.0550157505	4.5802954952
C14	4.3986816839064	0.0509911487696	-1.3254735322156	H20	-0.285086236	4.1260314628	8.7610325969
C25	-1.6779153275227	4.1351358935268	-1.0907506090844	H21	-1.6952498700	6.1332965420	9.0771402684
H9	0.1317508451764	-2.1439598074164	1.8817121415962	H22	-2.7498939053	6.0585469504	4.9106337283
H8	-0.1579928496669	2.1348041292601	2.0639073202990	H23	-2.9262462061	7.1042386413	7.1560144700
H20	2.5240912621557	0.6305823271942	1.4382442495216	Au24	-0.3703634887	1.1310393997	4.6413294527
H19	1.2842464142126	-0.6568425346745	-2.4636098922453	C125	-1.0612973071	-0.4015090984	2.9685681694
H31	-2.6572571741890	0.9680634999095	-0.3783640793640	P26	2.9545371255	0.2955104553	2.3360212702
H30	1.3072353482088	2.5865001296721	-0.6673405089686	Au27	1.6478295484	2.2156969578	2.5327915526
H10	0.2403283868508	-2.2388882131079	4.3541367560311	C128	0.4928074292	4.2847077353	2.5930334155
H11	-0.0710645076098	2.0324090088614	4.5297777330669	C30	2.2782581839	-0.9739969595	1.2301116614
H21	4.8730112358249	0.6713894226100	0.6749186442325	C31	1.2170393315	-2.8779224357	-0.4981585650
H22	3.6394374726653	-0.5942644920293	-3.2297926051765	C32	1.3598354341	-0.5939941188	0.2507553465
H32	-3.6024058792507	3.1947476302206	-0.9130451922427	C33	2.6539834337	-2.3155839097	1.3495595790
H33	0.3603161749364	4.7996388235134	-1.2199157020900	C34	2.1251544139	-3.2633787027	0.4834130514
H12	0.1333516371447	-0.1489021508414	5.6763642439211	C35	0.8347580875	-1.5462359474	-0.6138944681
H23	5.4323103332567	0.0653089575772	-1.6559065346749	H36	1.0349873400	0.4445790589	0.1885656585
H34	-2.0903316120941	5.1079538446435	-1.3383474684194	H37	3.3470434441	-2.6210556346	2.1332181869
				H38	2.4133421624	-4.3074957397	0.5826351179
				H39	0.1092127601	-1.2484709727	-1.3665228361
				H40	0.7946005964	-3.6238873814	-1.1676756965
				C41	4.6168205886	0.1749714527	1.7126363480
				C42	7.2163769583	1.3750883270	0.9541478104
				C43	5.1359988294	1.9798342350	2.0072548320
				C44	5.4037542847	-0.2119857830	1.0253355605
				C45	6.6985590451	0.1210099911	0.6455347076
				C46	6.4352654617	-2.3034103248	1.6346373537
				H47	4.5161907762	2.7072844336	2.535069965
				H48	5.0012030515	-1.1944924632	0.7823239321
				H49	7.3057968722	-0.6025719657	0.1062675805
				H50	6.8336078324	3.2882470674	1.8688143346
				H51	8.2308120096	1.6315065074	0.6566156657
				C52	3.2758358406	-0.5844686118	3.9038732429
				C53	3.6262486462	-1.7678692719	6.4055414438
				C54	4.5335036546	-0.5839115777	4.5094709201
				C55	2.1976813519	-1.2066732471	4.5446195674
				C56	2.3749626817	-1.7886097210	5.7937293293
				C57	4.7055286414	-1.1761579256	5.7579426536
				H58	5.3819153777	-0.1168097687	4.0097266239
				H59	1.2165153421	-1.2315811704	4.0662310707
				H60	1.5272036305	-2.2570435526	6.2896854384
				H61	5.6878878502	-1.1712205465	6.2258269443
				H62	3.7608396097	-2.2192659239	7.3862198433
				C63	2.0109123250	3.2202531481	6.0096064218
				C64	4.5465088240	4.1614511932	5.3445345058
				C65	3.0802682706	2.3262817715	5.8807091934
				C66	2.2145353829	4.581509687	5.7919662149
				C67	3.4826067797	5.0476796307	5.4587724435
				C68	4.3448103193	2.7992394274	5.5382366420
				H69	2.9230819081	1.2559110687	6.0274670981
				H70	1.3802030472	5.2770809150	5.8580570644
				H71	3.6339573444	6.1094147169	5.2795915259
				H72	5.1721489359	2.0969888404	5.4639437390
				H73	5.5367555139	4.5295516182	5.0821237027
9-CI				10-CI			
P1	0.3395887139	2.6138280514	6.3756373251	C1	-1.2725682492	-2.9358872421	2.3053209133
C2	0.5378104886	1.7398429408	7.9547383537	H2	-0.1820867319	-3.0822330363	2.3279341784
C3	0.7571292974	0.4017238108	10.3848862447	H3	-1.5884339479	-2.6378738448	3.3138905465
C4	-0.2874199363	0.6470862332	8.2294299731	C4	-1.6065327613	-1.8684168007	1.2686592458
C5	1.4782011106	2.1576351543	8.9017825846	H5	-1.2640443768	-2.2258524956	0.2892037267
C6	1.5843039137	1.487089517	10.1141012273	C6	-2.6950847429	-1.7306608741	1.2002632807
C7	-0.1781344034	-0.0180373728	9.4447377646	H7	-0.9070763360	-0.5433720713	1.5844517883
H8	-1.0131042433	0.3158950629	7.4855208000	H8	0.1468110937	-0.7718274459	1.8065812663
H9	2.1320553773	3.0025592734	8.6873602393	H9	-0.8880745189	0.1156430968	0.7060536172
H10	2.3165695579	1.8132809892	10.8491078885	C10	-1.8780358067	-4.2192061869	2.0075333974
H11	-0.8223479463	-0.8679268926	9.6561066724	N11	-1.2871036377	-5.0625990770	1.1350477629
H12	0.8446163897	-0.1219177258	11.3339450318	O12	-0.23		

C18	-2.2006655838	5.7311598746	5.7668927269	C18	-1.5493086879	0.1717957167	2.7288209860
H19	-1.3279075286	4.1486926561	4.5929846713	P19	1.2090149543	2.5957936207	6.0042300509
H20	-0.3067309819	4.1987672546	8.7845446152	C20	1.5635645844	1.4254254605	7.3383450516
H21	-1.7113068424	6.2104822954	9.0959158138	C21	1.8743443640	-0.2148757196	9.5619947870
H22	-2.7351673156	6.1583909946	4.9223409379	C22	0.5684305996	0.4928665585	7.6599745897
H23	-2.9242161241	7.1917633462	7.1702585651	C23	2.7036570158	1.5475457643	8.1426986695
Au24	-0.4011362715	1.2490485888	4.6432464302	C24	2.8552582179	0.7210934597	9.2493177739
Cl25	-0.9839213640	-0.1412851130	2.8143148783	C25	0.7335478984	-0.3227411820	8.7721083385
P26	2.9337867832	0.1539472548	2.3715460781	H26	-0.3368694387	0.4378284270	7.0496875321
Au27	1.5768301614	2.0507341617	2.5705602622	H27	3.4589414201	2.3002470725	7.9297535194
F28	2.6926579521	2.8843362949	0.5926813063	H28	3.7366461922	0.8217708893	9.8780067896
Cl29	0.5938598976	4.2706697777	2.4970303639	H29	-0.0421359083	-1.0400914272	9.0294445485
C30	2.3114840517	-1.0935723568	1.2227423580	H30	1.9941236882	-0.8525841522	10.4349193600
C31	1.3901577522	-2.9743081392	-0.6021915561	C31	0.0335930940	3.7941384390	6.6866158229
C32	1.4323966001	-0.7079479935	0.2088598127	C32	-1.6976045011	5.6639441764	7.7887017708
C33	2.7186886566	-2.4269051106	1.3303070402	C33	-0.9048831193	4.4355773382	5.8733241270
C34	2.2588565812	-3.3623959528	0.4131218045	C34	0.0985068389	4.0823328564	8.0547891544
C35	0.9761040075	-1.6501496553	-0.7036965661	C35	-0.7653929303	5.0231084546	8.5982139202
H36	1.0825176468	0.3233063790	0.1586258917	C36	-1.7672425687	5.3705940763	6.4308375189
H37	3.3879190258	-2.7324507780	2.1344168749	H37	-0.9515045518	4.2219453867	4.8053874489
H38	2.5713298465	-4.4012370772	0.4969220550	H38	0.8157773208	3.5724765155	8.6956852834
H39	0.2787841195	-1.3547054564	-1.4834308991	H39	-0.7145062894	5.2501655823	9.6600231923
H40	1.0228834603	-3.7123040924	-1.3112756683	H40	-2.4969132980	5.8709450461	5.7997986627
C41	4.5721532726	0.6715192175	1.7558403574	H41	-2.3771169314	6.3944339451	8.2205492781
C42	7.0927165118	1.5213623683	0.9054782966	Au42	-0.0564835766	1.5745267238	4.2578151948
C43	5.1139814719	1.8680412452	2.2392754107	H43	-2.5569320425	1.8865861123	3.4976406595
C44	5.2952194880	-0.0890147732	0.8368948636	H44	-1.7252178366	2.1167549704	1.8422641322
C45	6.5502376485	0.3408338010	0.4105562580	H45	-1.8485539309	-0.4100311161	3.6061747849
C46	6.3728721568	2.2854183163	1.8245500487	F46	-1.5310818121	0.9655667652	5.6061793364
H47	4.5433545222	2.4684313495	2.9511922568	P63	3.1343997781	0.4743842347	2.3885949456
H48	4.8799090806	-1.0186790066	0.4505756294	Au64	1.6908482055	2.3834877105	2.4109895257
H49	7.1091990662	-0.2570304207	-0.3053506280	Cl65	2.8713572962	3.2702661940	0.4912443048
H50	6.7988688248	3.2041086810	2.2265339711	Cl66	0.1614745299	4.2379311715	2.4303716937
H51	8.0787479281	1.8452688781	0.5801838370	C67	2.5703920938	-0.7064532175	1.1382578863
C52	3.2390825073	-0.6895300696	3.9498840598	C68	1.7193095551	-2.4944252549	-0.8138642023
C53	3.5761382289	-1.8708252113	6.4474512482	C69	2.1980661751	-0.2315970389	-0.1249618963
C54	4.5096374118	-0.7519971148	4.5259872465	C70	2.5469695624	-2.0813943947	1.4086792181
C55	2.1380790930	-1.2420118876	4.6168838555	C71	2.1190506174	-2.9703899128	0.4318033807
C56	2.3107420470	-1.8248313938	5.8652414733	C72	1.7747968670	-1.1318531257	-1.0955723552
C57	4.6737721122	-1.3449818128	5.7746381513	H73	2.2345076787	0.8369919452	-0.3413598722
H58	5.3728880354	-0.3415762879	4.0033563935	H74	2.8550369037	-2.4602214367	2.3817859185
H59	1.1483241042	-1.2136271640	4.1566293728	H75	2.0654786358	-4.0338738017	0.6456223831
H60	1.4526196786	-2.2469749799	6.3833729647	H76	1.4784364696	-0.7628769319	-0.2740638082
H61	5.6642659208	-1.3969136295	6.2206496664	H77	1.3591865778	-3.1970634764	-1.5616318493
H62	3.7073763943	-2.3262350607	7.4261246243	C78	4.8538549730	0.8749963916	1.9899304006
C63	1.9986128720	3.2656769904	5.9905214514	C79	7.5400005625	1.3636605011	1.4809467304
C64	4.5446588846	4.1606951307	5.2946337190	C80	5.3857197749	2.1420523562	2.2262543932
C65	3.0621710039	2.3591871562	5.9002927526	C81	5.6649366103	-0.1476719750	1.4842941764
C66	2.2132616701	4.6154200918	5.7186402670	C82	7.0077749317	0.1011828934	1.2342799627
C67	3.4854272311	5.0581677794	5.36571018360	C83	6.7311866194	2.3808830082	1.9767833568
C68	4.3325255102	2.8099216962	5.5682295251	H84	4.7463980631	2.9463836373	2.5829449624
H69	2.898693501	1.2975772780	6.0948367437	H85	5.2495921741	-1.1347944429	1.2844662717
H70	1.3860205032	5.3213486123	5.7681520677	H86	7.6376529174	-0.6909695413	0.8375531188
H71	3.6475052806	6.1137054452	5.1588130045	H87	7.1423435144	3.3727220057	2.1527175647
H72	5.1581262348	2.1006340641	5.5191363143	H88	8.5901371880	1.5569648350	1.2753173251
H73	5.5425729073	4.5133032870	5.0378280700	C89	3.1677808299	-0.4417784203	3.9603309557
N74	3.2111203637	4.1838287670	-0.2819706571	C90	3.1949418698	-1.8761170641	6.3549456501
C75	1.9663222219	4.6388610990	-0.9007500188	C91	4.3560961574	-0.5850629381	4.6789732169
C76	3.7068464209	5.0463248797	0.7925992883	C92	1.9928390814	-1.0289354139	4.4492000192
C77	4.2239461951	3.6065952702	-1.1590154582	C93	2.0074339904	-1.7440646360	5.6374487307
H78	4.6703769544	4.4143968841	-1.7539435307	C94	4.3635859963	-1.2977900154	5.8760169457
H79	4.9886016766	3.1263230969	-0.5397914803	H95	5.2791351060	-0.1445988304	4.3031303716
H80	3.7495843095	2.8758005619	-1.8165347004	H96	1.0596508848	-0.9469620735	3.8882420763
H81	4.0256331454	5.9975378148	0.3474437748	H97	1.0896394603	-2.1972453589	6.0064869433
H82	2.8870174695	5.1909985935	1.5063841206	H98	5.2925400695	-1.4059530787	6.4304325059
H83	4.5519222668	4.5460673405	1.2730609710	H99	3.2044100033	-2.4306458316	7.2902738741
H84	2.1692787293	5.5789530894	-1.4297317749	Cl00	2.7210126241	3.4743101380	5.5422997999
H85	1.6188580708	3.8781416288	-1.6017022400	Cl01	5.0193774708	4.8496515403	4.7676284533
H86	1.2334751130	4.7930607374	-0.0995348837	Cl02	3.9596442961	2.8185304328	5.5225521342
				Cl03	2.6379077964	4.8156600798	5.1504827389
				Cl04	3.7853287730	5.4925415653	4.7550533775
				Cl05	5.1044966032	3.5147587857	5.15795866978
				Cl06	4.0318445477	1.7667572999	5.7963439546
				H107	1.6784860532	5.3293312343	5.1448301484
				H108	3.7125403755	6.5307140848	4.4433192706
				H109	6.0659019228	3.0046287353	5.1606762304
				H110	5.9161165111	5.3891023377	4.4723691450
				H100	-2.7706316788	-4.4737781846	2.4063901772
11-Cl				12-Cl			
C17	-0.9463358199	-0.7857377282	4.1304457272	C1	-2.2782516052	-2.2603593291	0.9705274074
C18	-0.8965390513	-0.9514931913	2.6903441862	H2	-3.3422972369	-2.2576905504	1.2331990057
P19	1.2226064725	2.8937857942	5.7704906665	H3	-2.1051792670	-3.1425661940	0.3387673924
C20	2.0556242237	2.6631435348	7.3689250396	C4	-1.7929217945	-0.9665096080	0.3230115977
C21	3.0901677425	2.3655433249	9.9371730725	H5	-1.8367845012	-1.0085873599	-0.7691008424
C22	1.5223333018	1.6956097216	8.2290622053	H6	-2.4134385455	-0.1188488705	0.6402511573
C23	3.0982940457	3.4880348428	7.8042604861	C7	-0.3686529553	-0.8071506263	0.8538990399
C24	3.6157132991	3.3316351367	9.0849649441	H8	0.3195367331	-1.4767393149	0.3188577387
C25	2.0434708845	1.5544103703	9.5094971545	H9	0.0121682837	0.2188191661	0.7611651506
H26	0.6889142643	1.0762746094	7.8901664162	N10	-1.4508699777	-2.3790892725	2.1787022557
H27	3.5018429785	4.2621104149	7.1543896364	Cl11	-1.5892175891	-3.4839772821	2.9404895775
H28	4.4243887246	3.9764910997	9.4211092112	O12	-2.4026734977	-4.3649106765	2.7322509786
H29	1.6215605599	0.8088493395	10.179997363	C13	-0.5939965498	-3.6533830042	4.1098251772
H30	3.4916322410	2.2527192999	10.9419349883	F14	-0.5078524932	-2.5631588820	4.8870161621
C31	-0.2208122742	3.9386814078	6.1342071585	F15	0.6424273512	-3.8938551391	3.6332887757
C32	-2.3949709291	5.5732901736	6.7315152735	F16	-0.9390753441	-4.6712113194	4.8729564718
C33	-1.4825663963	3.6395295009	5.6175534354	Cl17	-1.0451747391	-0.1948587358	3.2372685312
C34	-0.0522892608	5.0593331202	6.9552652504	C18	-0.4855663145	-1.2641361333	2.3097723454
C35	-1.1365818191	5.8742729602	7.2476769673	P19	1.3823306287	2.5240387680	6.0315823529
C36	-2.5657251657	4.4584710580	5.9192258851	C20	1.8657387240	1.8469015877	7.6572130794
H37	-1.6238844881	2.7745082790	4.9712679528	C21	2.3676350989	0.7983292312	10.1938928069
H38	0.9272064374	5.2908523783	7.3730327886	C22	1.0978431865	0.7811146302	8.1399115140
H39	-1.0008378345	6.7437002637	7.8863102167	C23	2.8729858581	2.3938560308	8.4598001924
H40	-3.5470630727	4.2191555090	5.5174723827	C24	3.1269890151	1.8630979361	9.7190409383
H41	-3.2444065415	6.2094762406	6.9678777918	C25	1.3508613341	0.2674425345	9.4074973619
Au42	0.3105569188	0.8442906612	4.8334140007	H26	0.2875593099	0.3825184480	7.5232506677
H43	-0.6894329388	-1.6742938064					

C72	3.2553436257	-3.1012139539	0.3695990777	H39	-0.3491554107	6.3894246612	8.5873439281
H73	3.1173411699	-0.9528833662	0.2636168235	H40	-2.9445288766	4.8696851555	5.5172588343
H74	3.7911618783	-2.6394234038	4.1796716313	H41	-2.4906990831	6.4939353045	7.3368770967
H75	3.7524311058	-4.9035805150	3.2072253101	Au42	0.2499002869	0.9325167576	4.4811611066
H76	3.1244156576	-3.2322270279	-0.7019784048	H43	-1.6620042252	-0.6132649747	4.0373974216
H77	3.4137446417	-5.2116015134	0.7699228283	H44	-1.5905970525	0.5891732192	2.6977501385
C78	4.8613624803	0.8316625525	2.0540778350	H45	0.4669063324	-1.6701156365	2.6696601822
C79	7.0412415533	1.9417733386	0.7367924952	F46	-0.9933856168	0.3442237128	6.0247980240
C80	4.7746287184	2.1223246863	1.5341211557	P63	3.3888951032	0.1304355486	2.7791441039
C81	6.0420387634	0.0914123898	1.9072934208	Au64	1.6616714234	1.7101297279	2.3865486548
C82	7.1297895236	0.6512008836	1.2534022504	C165	2.7396621629	2.5183532116	0.2960899023
C83	5.8690293632	2.6742065246	0.8774442039	C166	-0.2094960707	3.2080910952	2.2085316017
H84	3.8511292800	2.6914327549	1.6206397953	C67	3.1709137801	-1.3163013224	1.6979596406
H85	6.1080276911	-0.9231199254	2.3005526053	C68	2.9080062318	-3.4428709820	-0.0774957602
H86	8.0450775859	0.0762312693	1.1376503932	C69	3.1200851524	-1.0732168229	0.3188423315
H87	5.7948049791	3.6767591919	0.4623464361	C70	3.0960897353	-2.6240413931	2.1812524290
H88	7.8912668899	2.3735959829	0.2137109055	C71	2.9516103387	-3.6830189204	1.2904149834
C89	3.9183494295	-0.0532908167	4.6820901924	C72	3.0008755824	-2.1397188544	-0.5613097338
C90	4.5377178882	-0.1568158233	7.4059662826	H73	3.1658144743	-0.0474625908	-0.0541896857
C91	5.1066714232	0.5069563375	5.1549372082	H74	3.1457245651	-2.8262688078	3.2489377648
C92	3.0516313789	-0.6850544803	5.5844080120	H75	2.8738047814	-4.6976363980	1.6741138705
C93	3.3603647647	-0.7366610067	6.9363642625	H76	2.9671650889	-1.9495468099	-1.6314678353
C94	5.4093067480	0.4555730273	6.5141981230	H77	2.7997408681	-4.2740044605	-0.7708337996
H95	5.7940642149	0.9956962119	4.4656783933	C78	5.0279899465	0.7769458941	2.3425734431
H96	2.1247961617	-1.1424820509	5.2317651374	C79	7.5804077301	1.7060904786	1.7589764405
H97	2.6712919493	-1.2183533594	7.6265697566	C80	5.2888068656	2.1455153570	2.3633887728
H98	6.3326262514	0.9031339814	6.8741797883	C81	6.0470114109	-0.1288479248	2.0288752317
H99	4.7687756879	-0.1801186542	8.4681236357	C82	7.3211842778	0.3382756545	1.7384504950
C100	2.3102887475	3.8790868405	4.6984330801	C83	6.5687144570	2.6051155064	2.0741255925
C101	3.9353937456	5.3180603321	2.9397696107	H84	4.4921952748	2.8535161874	2.5840337716
C102	3.6927983132	3.6590401482	4.6740424174	H85	5.8414834643	-1.1988040206	2.0082303550
C103	1.7470107560	4.8143757099	3.8235724455	H86	8.1112763386	-0.3658647767	1.4883726833
C104	2.5590164296	5.5221760479	2.9442670441	H87	6.7666929316	3.6747769953	2.0806884093
C105	4.4996785370	4.3865787666	3.8082724122	H88	8.5770431514	2.0715078216	1.5206545210
H106	4.1413211021	2.9219602776	5.3392335753	C89	3.5561502306	-0.4861275055	4.4870651723
H107	0.6714534071	4.9830542709	3.8215342394	C90	3.7397869849	-1.3261043942	7.1448661760
H108	2.1111046074	6.2430944125	2.2650865065	C91	4.6933618559	-0.1904520546	5.2406164474
H109	5.5751931661	4.2176983386	3.8053302645	C92	2.5163290614	-1.2180552872	5.0748675177
H110	4.5689411893	5.8852975121	2.2614720717	C93	2.6096282716	-1.6395244154	6.3927096795
H78	-1.0536023760	-0.0285437895	2.1306568752	C94	4.7777025118	-0.6062713202	6.5679635672
C86	0.0053502983	-1.9922642458	2.0873899541	H95	5.5110853855	0.3772857906	4.7979614350
H80	0.2684186938	-1.7240009096	1.0541855718	H96	1.6167954889	-1.4626129011	4.5114907023
H81	0.9412826094	-2.0455576085	2.6573069091	H97	1.7835059577	-2.1948194100	6.8325243276
C84	-0.7172795425	-3.3374162115	2.1238956610	H98	5.6614017321	-0.3584247278	7.1523535313
H83	-0.1611877248	-4.1081686797	1.5794839460	H99	3.8020383313	-1.6323992727	8.1867547924
H89	-0.8322301220	-3.6785108494	3.1611115197	C100	2.7923890515	3.4963443817	5.3964857360
C85	-2.0859342014	-3.0789984591	1.5176741039	C101	4.8819278626	5.0116242295	4.3232685497
N86	-2.5349567725	-1.766859186	2.0171264709	C102	4.128077462	3.1486883659	5.628507532
C87	-3.5627891199	-1.5816216353	2.9270481577	C103	2.5204355099	4.5872504361	4.5620526239
O88	-3.9272782714	-0.4746431400	3.2545956892	C104	3.5614922780	5.3358385054	4.0261828363
C95	-4.2353501953	-2.8195448627	3.5514150376	C105	5.1604427965	3.9116636900	5.1279381904
F90	-3.3068571849	-3.6016534716	4.1152704295	H106	4.3517538846	2.2794319037	6.2671771008
F91	-5.1088191220	-2.4682422253	4.4663612463	H107	1.4901593274	4.8477490324	4.3212301007
F92	-4.8639738654	-3.5302935266	2.6061664243	H108	3.3357620497	6.1772519180	3.3758427855
H93	-2.7087782987	-0.8844417821	1.0784652413	H109	6.1921609845	3.6361776485	5.3402616149
H94	-2.0024265513	-2.9976555025	0.4229222603	H110	5.6946195827	5.6099386352	3.9159124187
H100	-2.8030966954	-3.8753361284	1.7290872333				
N96	-2.9651249556	-0.0834230816	0.0871721758				
C97	-1.7261519207	0.2667360135	-0.6350172497				
C98	-3.8852734628	-0.8522615628	-0.7654708677				
C99	-3.6308574472	1.1353071140	0.5938773826				
H101	-1.9673094360	0.8219993286	-1.5517330511				
H102	-1.0866561730	0.8966208555	-0.0056506702				
H103	-1.1839875178	-0.6460054286	-0.9065361785				
H104	-4.2720795111	-0.2262209563	-1.5807259622				
H105	-3.3621492772	-1.7113894833	-1.1978327544				
H111	-4.7265321247	-1.2111926131	-0.1608624077				
H112	-3.8619897172	1.8046236723	-0.2459576353				
H113	-4.5513297328	0.8588599941	1.1137510067				
H114	-2.9653686065	1.6462229327	1.2958985086				
13-CI				14-CI			
C1	-2.3308725088	-2.1504878004	1.3963852411	C1	-5.0041062581	-2.0373525863	1.2340652236
H2	-3.3830915923	-2.4199108928	1.5344145864	H2	-5.3290410445	-1.9467760613	2.2775794661
H3	-1.8839900024	-2.8841122462	0.7085241286	H3	-5.6793895089	-2.7555544895	0.7483013411
C4	-2.1077434736	-0.7190696968	0.9438033496	C4	-4.9234768876	-0.7059513630	0.4994702073
H5	-2.3823843438	-0.6147774991	-0.1447838040	H5	-5.8435526827	-0.4896608293	-0.0528835966
H6	-2.8784620200	-0.0616768365	1.3664988657	H6	-4.7616468848	0.1120228156	1.2104531875
C7	-0.7446603557	-0.3807777593	1.5326641381	C7	-3.7121084501	-0.8649939079	-0.4197520711
H8	-0.0540342440	-0.8579606986	0.9473115647	H8	-4.0041139895	-1.3914775136	-1.3378879770
H9	-0.5460879263	0.6962709234	1.5644810452	H9	-3.2662562515	0.0929689113	-0.071936332
N10	-1.6170683788	-2.2204836814	2.6820987569	N10	-3.6315982861	-2.5659687001	1.1837445270
C11	-1.6674594135	-3.3909849612	3.3535539227	C11	-3.4446404903	-3.7765466497	1.7587058645
O12	-2.3732114793	-4.3292701673	3.0317806851	O12	-4.3258900594	-4.4009854674	2.3195824246
C13	-0.7181526677	-3.5715106184	4.5602366797	C13	-2.0271131044	-4.3902835689	1.7458570799
F14	-0.8084168255	-2.5890286626	5.4668511845	F14	-1.2353204791	-3.7563480508	2.6210769233
F15	0.5603524906	-3.5873762742	4.1354459817	F15	-1.4247737295	-4.3211776637	0.5443737981
F16	-0.9590272020	-4.7126751080	5.1715550644	F16	-2.0750349003	-5.6642252699	2.0874771035
C17	-1.2635564351	-0.1091700230	4.0462674016	C17	-1.6971820626	-0.9307780460	1.1880035425
C18	-0.7780573194	-1.0220634986	2.9246971835	C18	-2.7219440245	-1.7328926239	0.3666931095
P19	1.5866670341	2.6756754153	6.5405948774	P19	0.2565683752	2.8193982512	5.7608042907
C20	2.4458862012	2.0735166349	8.1209961695	C20	0.3941821048	2.4951668839	7.5471399664
C21	3.2680104242	1.1205081167	10.6125606640	C21	0.4949721094	2.0160503418	10.2879932603
C22	1.7544628390	1.0232290872	8.7344330031	C22	-0.2323975549	1.3694326183	8.0849080137
C23	3.5381966479	2.6554034934	8.7740286513	C23	1.0729668811	3.3828222508	8.3882590497
C24	3.9527642787	2.1705986021	10.0089987539	C24	1.1206458873	3.1408777670	9.7550796056
C25	2.1656013627	0.5577766201	9.9791955074	C25	-0.1800336417	1.1316565146	9.4543891593
H26	0.8927992093	0.5784607915	8.2289736686	H26	-0.7582722207	0.6634814541	7.4408492717
H27	4.0655900257	3.4946454455	8.3236017371	H27	1.5626173018	4.2625258264	7.9704357164
H28	4.8067390190	2.6250532846	10.5071487908	H28	1.6498348288	3.8317900129	10.4079527716
H29	1.6212437357	-0.2566631560	10.4530815073	H29	-0.6673036513	0.2465185326	9.8574537005
H30	3.5917199820	0.7466284381	11.5818016841	H30	0.5382962160	1.8297863972	11.3591862717
C31	0.5807152443	3.9744985791	7.0700165449	C31	-1.0521697269	4.0729807899	5.5968108569
C32	-1.2073031846	5.9785025005	7.8133337905	C32	-3.0664902824	5.9783538407	5.2867633579
C33	-0.5755068894	4.1963245899	6.3187328133	C33	-1.3368360899	4.5919978113	4.3285535842
C34	0.8371759603	4.7640152209	8.1958902104	C34	-1.7908418891	4.5000905817	6.7031735402
C35	-0.0543264288	5.7619501988	8.5633719114	C35	-2.7975257936	5.4474266072	6.5435609995
C36	-1.4664357954	5.1972823655	6.6945542437	C36	-2.3317964007	5.5514090209	4.1833259378

B47	-2.9140884988	0.4132024660	5.9981797185	H47	-0.4985682598	-1.6780947923	6.3949042574
O48	-2.5263798072	1.7142748672	6.1577799500	O48	-2.5206067813	-2.8560169129	5.4679028923
H49	-2.0035917850	1.8127527800	6.9829034336	H49	-1.7166671126	-2.8825685722	4.9308918527
O50	-2.9282386578	-0.5425551847	6.9671223075	F50	-3.4622411194	-1.9047271690	7.3329731447
H51	-2.0520944975	-0.4928890171	7.3919583349	P51	3.6907461137	-0.2147300733	2.9497130953
C52	-3.4686743656	0.0220685600	4.5706447852	Au52	2.1286435869	1.4579383124	2.4739325255
C53	-5.3637823927	-0.5836363076	2.5619789294	Cl53	0.7222441132	3.1865523495	1.6514198607
C54	-3.9904401586	1.0239891175	3.7167104638	C54	3.1139209139	-1.8589968846	2.4402817303
C55	-3.9667634327	-1.2856545295	4.3925113591	C55	2.0673407754	-4.3247629972	1.6678780904
C56	-4.8868617991	-1.5903966920	3.3990369412	C56	2.1817256336	-1.9344726050	1.4023044300
C57	-4.9078864994	0.7276660988	2.7232267080	C57	3.5346658397	-3.0282383694	3.0773034550
H58	-3.6578787854	2.0531815921	3.8594102815	C58	3.0099837806	-4.2565146749	2.6892179401
H59	-3.6420546617	-2.0594479702	5.0882843158	C59	1.6627196197	-3.1628889542	1.0170807095
H60	-5.2444506526	-2.6128110276	3.2878579600	H60	1.8286154890	-1.0180352541	0.9265393680
H61	-5.2900032620	1.5196979695	2.0822833929	H61	4.2477154482	-2.9762247477	3.899530569
H62	-6.0968861884	-0.815379864	1.7917169971	H62	3.3259143031	-5.1623911907	3.2016460928
P63	3.2745676568	0.2469352588	3.1101507466	H63	0.9119338344	-3.2104799867	0.2313739560
Au64	1.52401101828	1.8408080629	2.8467571240	H64	1.6330203352	-5.2820164503	1.877280303
Cl65	2.3349653664	2.6681074733	0.6230134307	C65	5.2216991326	0.1072781835	2.0155421832
Cl66	-0.4792392557	3.2222689843	2.8478025266	C66	7.6092058631	0.6645288324	0.6981188576
C67	2.9010196733	-1.1742779282	2.0332363424	C67	5.5565574660	1.4265278120	1.7004079825
C68	2.3374897859	-3.2411821952	0.2539811995	C68	6.0859047065	-0.9325429921	1.6642977996
C69	2.7391109974	-0.8989580026	0.6678976579	C69	7.2759263412	-0.6514138719	1.0048404161
C70	2.8007033760	-2.4867160748	2.4856687152	C70	6.7515813471	1.7026496381	1.0459935254
C71	2.5025224135	-3.5148144972	1.6055134466	C71	4.8736498094	2.2356981522	1.9660577161
C72	2.4690210554	-1.9353748893	-0.2141853851	H72	5.8217095049	-1.9624941429	1.9022273012
H73	2.8006134896	0.1313808301	0.3089390284	H73	7.9449925850	-1.4627287201	0.7274160991
H74	2.9472741982	-2.7166895487	3.5486258471	H74	7.0076246577	2.7304517061	0.7995236616
H75	2.4015851883	-4.5316605189	1.9780378148	H75	8.5406688694	0.8808955504	0.179467331
H76	2.3454707332	-1.7181849270	-1.2726072639	C76	4.2464619476	-0.3663213517	4.6856191223
H77	2.1079093413	-0.0475529079	-0.4390734731	C77	4.9659178423	-0.3763570123	7.3893584282
C78	4.8741965114	0.8483849369	2.4923565516	C78	5.5238258740	0.0426582664	5.0771928053
C79	7.3637871626	1.7029324988	1.6021285890	C79	3.3390882238	-0.8044174049	5.6586113528
C80	5.1337872946	2.2108285300	2.3663912301	C80	3.6991202102	-0.8065459722	7.0005850147
C81	5.8601234299	-0.0894880017	2.1630101628	C81	5.8783098465	0.0357478290	6.4244729781
C82	7.1029286108	0.3396977709	1.7209315884	H82	6.2457909813	0.3755278761	4.3320559927
C83	6.3823289032	2.6327592035	1.9203442685	H83	2.3452841309	-1.1398214585	5.3615784157
H84	4.3590452525	2.9404175406	2.5954131764	H84	2.9798552913	-1.1410459284	7.7456119389
H85	5.6522992390	-1.1557654785	2.2535623754	H85	6.8747710693	0.3591386910	6.7183970628
H86	7.8679124492	-0.3895684045	1.4646137900	H86	5.2428895390	-0.3702631428	8.4411281099
H87	6.5796956864	3.6972191046	1.8145073756	C87	1.8308137640	3.6408332894	5.3337614498
H88	8.3357499834	2.0387277117	1.2468682892	C88	4.3036982410	4.7512787083	4.6565738522
C89	3.6300560905	-0.3941316059	4.7886811016	C89	3.0036760201	2.8873886545	5.4607586783
C90	4.0880065860	-1.1605694869	7.4459433312	C90	1.9076916700	4.9540498732	4.8733174912
C91	4.8288780809	-0.0645686769	5.4253425412	C91	3.1409963310	5.5023898013	4.5318932815
C92	2.6719878633	-1.1355945053	5.4954324398	C92	4.2329554129	3.4432229477	5.1305525938
C93	2.9018515881	-1.5200059998	6.8087055267	H93	2.9590878812	1.8593894634	5.8243822867
C94	5.0511155132	-0.4432345995	6.7487069520	H94	1.0048153695	5.5516667555	4.7660140267
H95	5.5895107038	0.5071111276	4.8945761142	H95	3.1877175643	6.5249360298	4.1643675509
H96	1.7257809904	-1.4135711448	5.0306477996	H96	5.1351496583	2.8430993253	5.2407332079
H97	2.1332653792	-2.0777748060	7.3399331677	H97	5.2648620231	5.1850222991	4.3895087144
H98	5.9822343283	-0.1608591482	7.2362074121	C98	-3.5472954411	1.8605763240	3.8993600112
H99	4.2549002204	-1.4352743950	8.4849183594	C99	-2.9855249891	2.3066112847	2.7076406308
C100	3.0736263119	3.6219835511	5.6924006785	C100	-2.3532632221	1.4130870060	1.8486807596
C101	5.0079951654	5.0991933189	4.3139235363	C101	-2.2972566829	0.0523773709	2.1522423692
C102	4.4283474352	3.2899533972	5.7989541239	C102	-2.8632573208	-0.3872888021	3.3539774370
C103	2.6954944217	4.6728852513	4.8476594177	C103	-3.4783832516	0.5067079519	4.2253710858
C104	3.6585784362	5.4016858144	4.1597373898	H104	-4.0268929288	2.5681721558	4.5749095792
C105	5.3891661525	4.0350418781	5.1239141739	H105	-3.0260794147	3.3626424519	2.4473984534
H106	4.7367413345	2.4467829059	6.4149880109	H106	-1.8829287616	1.7809524818	0.9369121115
H107	1.6421260240	4.9215597402	4.7197379376	H107	-2.8265902488	-1.4437666782	3.6115447271
H108	3.3483250376	6.2115271823	3.5041084489	H108	-3.9119287788	0.1375788287	5.1545905653
H109	6.4411654572	3.7730174856	5.2237190880	H109	-1.0609960692	-0.3934109859	0.4675481530
H110	5.7613924712	5.6827816116	3.7886647956	H110	-1.0406274299	-1.6259246245	1.7291068647

2) Ligand on Au is P(Ph)₃

b. Catalyst L-Au-Br

1-Br				2- Br			
P1	0.0966214736	-0.0313568975	-0.0261578894	C1	-0.3321043725	0.8781288491	0.1224364620
C2	0.1172709343	-0.2553465258	1.7411684375	C4	-0.3462963544	0.4067432206	1.5742276823
Cl3	1.6887110126	-0.2160139705	-0.7822303553	N10	1.0106750610	1.0534025456	-0.4024620445
Cu4	-0.7232789851	1.4650179558	-0.5317917768	C7	-1.7185420745	0.6447111371	2.2051183144
Au35	-1.2587639844	-1.8638425509	-0.7670331857	Cl2	1.7863404787	2.1650731602	-0.3685886683
C5	-1.0923543626	-0.3902624396	2.4358244302	C22	-1.9151375926	-0.0680336261	3.4951140396
C4	1.3367733516	-0.2211572194	2.4276644576	Cl3	2.9596598664	2.1928367340	-0.6730277852
C16	2.4644299728	-1.3534496665	-0.5044010780	C14	1.0816994819	3.4654539697	0.083592661
C15	2.1774133732	0.7973192003	-1.6219543754	C19	-2.2942217207	0.5240027641	4.6654389441
C27	-1.0652565501	2.4209200318	0.4275369296	Au58	0.1143111801	0.5167003699	4.9760698530
C26	-1.0366170182	1.6578266797	-1.8819637100	F15	1.9348387601	4.4733101039	0.0794167074
Br12	-3.4591279535	-0.7229745430	-0.5996277908	F16	0.6045177693	3.3348259770	1.3361455805
F13	0.3495810833	-3.0315924964	-0.8887000943	F17	0.0578270654	3.7715236390	-0.7123456546
C6	-1.0731094504	-0.4774632156	3.8140823566	P24	2.3700720017	0.9961946895	5.7119982830
C7	1.3355928296	-0.3095437478	3.8087324774	Br15	0.0097422641	-1.7569735274	6.0574077712
C17	3.7254329572	-1.4567115471	-1.0553093056	F60	0.0993393875	2.3528458667	4.1629825819
C18	3.4411297143	0.6720680560	-2.164668382	C25	3.3849452303	1.3928397576	4.289493560
C28	-1.7064547341	3.5800374253	0.0238214139	C36	3.1513886267	-0.2973199282	6.7648967832
C29	-1.6796437888	2.8161871266	-2.2671597850	C47	2.0575002300	2.4322530312	6.7365705368
C3	0.1377842305	-0.4399482342	4.4978848161	C28	2.9303305273	2.3450865599	3.3608341466
C14	4.2094195840	-0.4525194557	-1.8865826012	C27	4.6538204691	0.8092849599	4.1514454743
C25	-2.0160478467	3.7738365136	-1.3144056490	C39	3.5613991523	-0.0455381813	7.9891918383
H9	-2.0377453209	-0.4343719656	1.899532316	C38	3.4010978039	-1.5437953775	6.0817647247
H8	2.2727057570	-0.1073325814	1.8909383208	C50	1.1357746921	2.3096110055	7.7864897053
H20	2.0577112528	-2.1588432115	0.5945905261	C49	2.7289870869	3.6371983419	6.5136192484
H19	1.5862237926	1.6831218395	-1.8267701247	C29	3.7572836904	2.7104443085	2.3013947474
H31	-0.8278355503	2.2667245828	1.4751546634	C30	5.4586365889	1.1771773349	3.0824331694
H30	-0.8062171457	0.8920164158	-2.6184022271	C40	4.2313844156	-1.0354340667	8.6977154099
H10	-2.0041768681	-0.5857797156	4.3585413667	C41	4.0741850719	-2.5201285049	6.7973138143
H11	2.2750126174	-0.2758438160	4.3486577683	C51	0.9014284720	3.3931056782	8.6184282987
H21	4.3271881072	-2.3351850768	-0.8534088863	C52	2.4833898720	4.7156462952	7.3545052711
H22	3.8304224877	1.4545081221	-2.8058221203	C26	5.0104515755	2.1194145925	2.1618714740
H32	-1.9694560396	4.3317774012	0.7592855203	C37	4.4871266955	-2.2663997667	8.1048157424
H33	-1.9361353363	2.9706919400	-3.3088732563	C48	1.5741150849	4.5946873301	8.4000166078

H12	0.1461385591	-0.5175729185	5.5797860707	H2	-0.8617768201	0.1645573540	-0.5206791968
H23	5.1962292066	-0.5496021165	-2.3266105334	H3	-0.8762939689	1.8231843747	0.0323024031
H34	-2.5312380438	4.6777053894	-1.6211637306	H5	-0.0601504721	-0.6544951258	1.6371836198
				H6	0.3982844183	0.9855337687	2.1387351959
				H11	1.5225592133	0.2328377130	-0.7064624645
				H8	-1.8755854466	1.7234865862	2.3367193356
				H9	-2.5034875233	0.2792830655	1.5211192997
				H23	-1.7936423170	-1.1558510652	3.4859953750
				H20	-2.5605298322	-0.0773215155	5.5330572293
				H21	-2.4795737475	1.5974343123	4.7047754752
				H32	1.9338039781	2.7703829422	3.4677847179
				H31	5.0162898768	0.0854650840	4.8769521556
				H43	3.3749197536	0.9204306210	8.4522995193
				H42	3.0633271250	-1.7479804275	5.0664252103
				H54	0.6151537851	1.3651044973	7.9552730214
				H53	3.4407030565	3.7297898996	5.6962385441
				H33	3.4253374122	3.4491721894	1.5868286632
				H34	6.4417946476	0.7272821390	2.9717306833
				H44	4.5583285566	-0.8397953404	9.7154028993
				H45	4.2705452799	-3.4861421948	6.3403051948
				H55	0.1918591226	3.3044643048	9.4366157670
				H56	3.0057410020	5.6544084031	7.1911917887
				H35	5.6346344083	2.3963882224	1.3158617910
				H46	5.0105872297	-3.0375890369	8.6644143257
				H57	1.3851365659	5.4441189691	9.0515219961
3- Br				4- Br			
C1	-0.934795490600	-1.156838211700	2.783047624800	P1	0.654686589500	2.188790512400	4.974538871200
H2	0.144835883300	-1.042062539400	2.615572670300	C2	0.387147941900	0.659080038500	5.851270205300
H3	-1.308540292400	-0.259648027300	3.292623503100	C3	-0.153498693100	-1.632809777300	7.303755832700
C4	-1.624370841500	-1.308987614500	1.437027868500	C4	-0.908600173900	0.116635241900	5.829119079100
H5	-1.282134768800	-2.231956288000	0.9509344114500	C5	1.410375799100	0.057285474800	6.597621659200
H6	-2.712627225900	-1.395710456500	1.572005393100	C6	1.127813894300	-1.088744354400	7.326812906600
C7	-1.294281634700	-0.116774080800	0.541525089200	C7	-1.168458394300	-1.032365087400	6.559789444400
H8	-0.209343736900	-0.033811477500	0.378827378200	H8	-1.683168169700	0.603508526300	5.2361133519100
H9	-1.727233349000	-0.288955304800	0.459105869900	H9	2.406981576600	0.491542540500	6.626230665500
N10	-1.105854901900	-2.279173482200	3.685795886300	H10	1.909697473100	-1.556441351500	7.919080844800
C11	-0.231772496900	-3.306413916300	3.704489272100	H11	-2.165489526600	-1.463725770500	6.548402974900
O12	0.719313222000	-3.454978681700	2.962698626600	H12	-0.364887332900	-2.533641571900	7.874577675700
C13	-0.4469110518400	-4.285706989900	4.869673104900	C13	-0.328641430300	3.501435795100	5.674787113300
F14	-0.217165547700	-5.528177460100	4.498429133600	C14	-1.642366695500	5.576754912200	6.945372705300
F15	-1.689244709100	-4.207614019100	5.372753607000	C15	-0.647804880200	4.657948567000	4.951994256700
F16	0.401327934200	-3.964980190000	5.854166668100	C16	-0.697322876900	3.364027873300	7.021300793500
C17	-1.250544300300	2.398035236500	0.764881547400	C17	-1.343265485200	4.417416663900	7.653095697800
C18	-1.836145352300	1.189306320000	0.998472590000	C18	-1.300048408900	5.694343643100	5.599272960200
P19	0.453437507700	2.829788755900	5.338139527700	H19	-0.390836211000	4.728650131000	3.897101295500
C20	0.452999026100	1.321082620500	6.334591602500	H20	-0.466750810800	2.456682758900	7.575225680400
C21	0.297924561200	-0.836509456300	8.091217906000	H21	-1.616964150700	4.327781057700	8.700838374800
C22	-0.588040184600	0.391141192500	6.207571631100	H22	-1.554174595100	6.594472446700	5.046709828900
C23	1.408514772500	1.173897097200	7.352336775400	H23	-2.156728054700	6.394290752000	7.444278258100
C24	1.320505402200	0.098526025400	8.227525375000	Au24	-0.129159873000	1.625006400300	2.771071521900
C25	-0.652014686100	-0.686947930500	7.083228445700	F25	-1.784984348500	2.217201124200	3.722049362700
H26	-1.343092336700	0.545497215100	5.437006182000	P26	5.176331939800	3.391631613400	0.311738509400
H27	2.206987522900	1.901975683200	7.474905442200	Au27	3.253453589500	3.370303090600	1.185628653000
H28	2.056323522500	-0.006356935700	9.020739622600	Br28	1.1625022936195	4.4080087435089	2.0231794609738
H29	-1.455745337100	-1.413491045600	9.985219279100	C29	4.813877088400	1.405769498600	-1.168243120200
H30	0.237176822400	-1.679093243800	8.775641176900	C30	4.245777160000	-0.051090808200	-3.471928169700
C31	-0.752551337700	3.967575179700	0.043796435700	C31	3.672559726100	1.697581632100	-1.918625812200
C32	-2.528053969000	5.762798623200	7.206236443700	C32	5.667251700900	0.372929705800	-1.5743982445500
C33	-1.104958884700	5.141564551300	5.363047663400	C33	5.382011712000	-0.349830193100	-2.725145937900
C34	-1.306295809700	3.686406181700	7.298809277700	C34	3.392212275200	0.970050764000	-3.069411156100
C35	-2.187214104200	4.591781316300	7.875446312300	C35	2.995932259300	2.488384059100	-1.593135759800
C36	-1.985846557700	6.036343799700	5.951841885500	H36	6.547505935500	0.123794914000	-0.982397502600
H37	-0.691111276200	5.355156242500	4.378631161000	H37	6.044421552700	-1.153957604900	-3.036279159600
H38	-1.044371356600	2.773034377600	7.828386843700	H38	2.499880608300	1.196327859000	-3.647277198800
H39	-2.611225338900	4.379504350100	8.853366306000	H39	4.021484685000	-0.623981553500	-4.368485223100
H40	-2.255182139400	6.949520914500	5.427840814500	C40	6.452439187400	3.612043029900	-0.115815341400
H41	-3.216657336100	6.466544817300	7.662581059100	C41	8.480966722800	5.457203976500	-0.609189667100
Au42	-0.421931174700	2.544003111000	3.073215510900	C42	6.520362654600	4.795659493100	0.624505442000
H43	-1.815156586500	3.320374888400	0.896973467500	C43	7.401215008000	3.360109025400	-1.110715302700
H44	-0.323545047400	2.463096883500	0.192171012100	C44	8.409921890100	4.284084296400	-1.355472381500
H45	-2.795543161200	1.176969539900	1.522647354100	C45	7.536246072100	5.712821039100	0.380032005800
F46	-2.009917811400	1.514152507700	3.907786752000	H46	5.768628945600	4.997426997200	1.389930188800
P47	3.361123278600	0.492662853700	1.644996970300	H47	7.347348571200	2.446387732500	-1.700687178000
Au48	2.405353703800	2.607930310000	2.061095036600	H48	9.142641969000	4.088016934400	-2.134416815400
Br49	4.104954670734	4.379281749887	1.7089928748621	H49	7.583935366000	6.633926248500	0.955758578500
Br50	0.715628313900	4.406325703900	2.294030767100	H50	9.270742077300	6.178122306700	-0.805309925700
C51	2.431221445700	-0.423799460200	3.79404762600	C51	6.003675483000	1.211141829900	1.432573745300
C52	1.063446380200	-1.777036590300	-1.638608158600	C52	7.175340832800	-0.625046117000	3.180469878300
C53	2.193129859300	0.204528663100	-0.850842298700	C53	7.252401776400	1.477995674100	1.995269710100
C54	1.980654684800	-1.727306989900	0.595933935900	C54	5.343076861300	0.017848219900	1.748293401000
C55	1.292626747800	-2.396233266100	-0.414542136100	C55	5.929888379000	-0.896567704400	2.613725261700
C56	1.519161180800	-0.475701711200	-1.856502030700	C56	7.832443339200	0.561089534900	2.869961722000
H57	2.551459269600	1.221536972300	-1.021900020200	H57	7.779461805300	2.398560155800	1.747436166900
H58	2.142984842300	-2.231285623700	1.547592681400	H58	4.367166154100	-0.196354036200	1.311785019300
H59	0.944166782700	-3.410756422000	-0.23093121400	H59	5.416573724400	-1.827725112600	2.843321793200
H60	1.348653340800	0.009737300700	-2.814514548900	H60	8.809176859700	0.771536796200	3.299669591200
H61	0.535815689700	-2.306575983900	-2.428346898600	H61	7.635925280500	-1.342805501500	3.855127089100
C62	5.057433262500	0.592559435200	1.018029730800	C62	2.371034210000	2.624959847600	4.860162313800
C63	7.724959547100	0.628590999900	0.236532501800	C63	5.055068891100	3.302749359700	4.776220156600
C64	5.941073261400	1.507452778400	1.596561556800	C64	3.317548839600	1.665497778700	4.466279104200
C65	5.511044487400	-0.300184610400	0.040941927700	C65	2.768502108500	3.933699258200	5.178125059700
C66	6.845269942400	-0.277816882400	-0.346262546800	C66	4.114181568700	4.264074713100	5.134405084900
C67	7.273212168700	1.519727669100	1.204455243300	C67	4.659163456200	2.004449245800	4.453368734000
H68	5.576428489500	2.238805371000	2.317057472300	H68	3.002173081300	0.672035373600	4.146631196900
H69	4.826487513100	-1.015591746100	-0.412629862800	H69	2.031112680600	4.681139925600	5.459719367900
H70	7.197751524300	-0.970401673300	-1.106513285800	H70	4.427342126200	5.274407415400	5.382130063800
H71	7.956929440900	2.240898479100	1.644991748800	H71	5.400302772000	1.260224950300	4.174890010100
H72	8.767541042500	0.645785017000	-0.071991461000	H72	6.111336558600	3.562504196700	4.739713894800
C73	3.429769145100	-0.606005912400	3.089642942300	Br73	1.7173938094104	0.4580756922466	1.5968005903946
C74	3.358195493900	-2.462432312200	5.168102892700				
C75	4.467400210800	-1.529935055000	3.240238982200				
C76	2.371399396400	-0.604890631000	4.001414064400				
C77	2.331593194900	-1.534173767900	5.031882199300				
C78							

H90	3.0565498168000	1.5992062684000	5.0367683212000				
H91	1.471176844000	5.5764588413000	5.668783387000				
H92	3.762385926000	6.4799208139000	5.995466174000				
H93	5.3327369497000	2.5218267895000	5.0040144163000				
H94	5.6963591526000	4.9688197805000	5.2587043923000				
H95	-1.9131145082000	-2.3161624953000	4.2925802219000				
5- Br				6- Br			
P19	0.5713312024000	2.8932779980000	5.5068418636000	P19	0.8248885676	2.3886371747	6.1817081703
C20	0.4880801733000	1.56785858601000	6.7295318339000	C20	1.0284923748	1.2639067395	7.5884668316
C21	0.1492344128000	-0.3856904309000	8.6696036898000	C21	1.1620991992	-0.3594753134	9.8377357801
C22	-0.3582533487000	0.4808504823000	6.4751464399000	C22	0.3877698645	0.0196865656	7.5812824767
C23	1.1597901069000	1.6804415143000	7.9543691748000	C23	1.17077762017	1.7089908743	8.7299209113
C24	0.9810245064000	0.7009339806000	8.9227065362000	C24	1.17723831067	0.8918484832	9.8506960495
C25	-0.5149115588000	-0.4950956896000	7.4507327278000	C25	0.4679819198	-0.7888521260	8.7098951196
H26	-0.8841381925000	0.4209489803000	5.5186996480000	H26	-0.1919147003	-0.2946919778	6.7085640775
H27	1.8095240736000	2.5302190791000	8.1560022031000	H27	2.1812580279	2.6889105526	8.7491801863
H28	1.4908366526000	0.7900621475000	9.8787001969000	H28	2.2982704080	1.2362388210	10.7378140711
H29	-1.1699566511000	-1.3411066958000	7.2618770741000	H29	-0.0267896101	-1.7568414230	8.7103118922
H30	0.0135564294000	-1.1490349975000	9.4317223769000	H30	1.2173655559	-0.9970264064	10.7170231639
C31	-0.8701941519000	3.9514357671000	5.7284864969000	C31	-0.7083327784	3.3043085753	6.4262243511
C32	-3.0111529346000	5.6457162422000	6.1996729008000	C32	-3.1045552518	4.5792497788	6.9940825770
C33	-1.6477641809000	4.3957961699000	4.6575527644000	C33	-1.19120598056	2.7300929991	6.0029290312
C34	-1.1688039179000	4.3452647484000	7.0397228515000	C34	-0.7025422885	4.4971261896	7.1604546436
C35	-2.2366353640000	5.1989469266000	7.2673575685000	C35	-1.9060812464	5.1304267821	7.4382296686
C36	-2.7208618462000	5.2433092657000	4.9026611627000	C36	-3.1060630135	3.3797814254	6.2887604602
H37	-1.4119245048000	4.0933025245000	3.6406880338000	H37	-1.9146124360	1.7671699790	5.4886229984
H38	-0.5703223158000	3.9874086264000	7.8771382932000	H38	0.2299295525	4.9256387115	7.5233200379
H39	-2.4677263187000	5.51271110757000	8.2812693680000	H39	-1.9060617235	6.0581711799	8.0046569850
H40	-3.3289513733000	5.5904981356000	4.0720774833000	H40	-4.0439477843	2.9419672978	9.5578348881
H41	-3.8498254918000	6.3115705549000	6.3837419494000	H41	-4.0430295517	5.0842595890	7.2079552689
Au42	0.4792254624000	1.9744783073000	3.3058925176000	Au42	0.5318498071	1.0066427538	4.2495008909
F46	-1.3050027377000	1.0486025937000	3.6790765216000	F46	-1.0726893051	-0.1059348469	4.9274021583
P63	3.4741687284000	0.7048352764000	2.6348203401000	P63	3.5962452568	0.2961358721	3.1809233729
Au64	2.8973094645000	2.9969297958000	2.86810497755000	Au64	2.4922393992	2.4296292803	3.1672798494
Br28	4.9962439500481	4.3076158289629	2.7038608040695	Br65	4.3000211293	4.0280256768	2.2505311823
Br29	0.8796676183000	4.4041591134000	2.1860429153000	Br66	0.4030890396	3.9005803533	2.6643794447
C67	1.9340162851000	-0.0805571502000	2.0544983625000	C67	2.1907204579	-0.8444453100	2.9226588289
C68	-0.5049186890000	-1.1144743447000	1.1454801016000	C68	-0.0680366689	-2.4695965999	2.5944321061
C69	1.1047383052000	0.6808067590000	1.1876381606000	C69	1.0781655014	-0.3895358795	2.1659770291
C70	1.5293862906000	-1.3585150515000	2.4384502825000	C70	2.1603029249	-2.1240491407	3.4792582653
C71	0.3198320040000	-1.8669793848000	1.9790739097000	C71	1.0371963509	-2.9278083768	3.3078838744
C72	-0.1080756925000	0.1483876163000	0.7355696933000	C72	-0.0432923680	-1.2113404085	2.0094479614
H73	1.4694103750000	1.6228180031000	0.7679975347000	H73	1.1376405881	0.5453873864	1.6027387970
H74	2.1541363180000	-1.9567637126000	3.0975013138000	H74	3.0094542186	-2.4921865222	4.0519700172
H75	0.0156425367000	-2.8658816996000	2.2778198502000	H75	0.1245598767	3.9240942890	3.7427981003
H76	-0.7334375302000	0.7386765171000	0.0717224055000	H76	-0.8914787714	-0.8498753220	1.4344943014
H77	-1.4553590912000	-1.5203689646000	0.8119119535000	H77	-0.9463277393	-3.0998928779	2.4899930085
C78	4.7440766941000	0.3464832973000	1.3997209580000	C78	4.7642444062	0.0166769614	1.8340137230
C79	6.7041476621000	-0.3390594269000	0.4430163578000	C79	6.6098520923	-0.4591524396	-0.1869619727
C80	5.5938489709000	1.3338620106000	0.8982066454000	C80	5.8220458735	0.9113925175	1.6307502307
C81	4.8650991619000	-0.9836335247000	0.9732563414000	C81	4.6264121183	-1.1103378429	1.0152320461
C82	5.8490846037000	-1.3210571627000	0.0547979485000	C82	5.5534561423	-1.3424493472	0.0073299731
C83	6.5770444613000	0.9796779959000	-0.0246880035000	C83	6.7442994765	0.6641300533	0.6238062332
H84	5.5006170251000	2.3668145489000	1.2335287346000	H84	5.9035846408	1.8140930700	2.2341489569
H85	4.1968714245000	-1.7530001760000	1.3595037125000	H85	3.8036728190	-1.8075430607	1.1612671631
H86	5.9492629550000	-2.3508254753000	-0.2771189625000	H86	5.4469420926	-2.2158342100	-0.6305790044
H87	7.2437177391000	1.7440641903000	-0.4165384278000	H87	7.5619700292	1.3613664590	0.4620712174
H88	7.4739938530000	-0.6074635601000	-1.1654396656000	H88	7.3291105900	-0.6423856007	-0.9812220783
C89	3.9724691342000	-0.0390408441000	4.1948464212000	C89	4.3757800053	-0.1536142971	4.7553144764
C90	4.8230867276000	-0.9067490962000	6.6910722666000	C90	5.5606038402	-0.6661149835	7.2306119230
C91	5.3373940423000	-0.0849846750000	4.4868919300000	C91	5.7629435206	-0.0607270446	4.9021182951
C92	3.0330098733000	-0.4054575214000	5.1644220358000	C92	3.5856218476	-0.5003020775	5.8596046890
C93	3.4627276788000	-0.8509734922000	6.4058520012000	C93	4.1779265963	-0.7666159373	7.0868783569
C94	5.7571112066000	-0.5211226184000	5.7354791166000	C94	6.3475001974	-0.3139264683	6.1387655252
H95	6.0969923134000	0.2201167640000	3.7407684422000	H95	6.3913011113	0.1972572338	4.0517832996
H96	1.9648505845000	-0.3322902180000	4.9637218909000	H96	2.5002284582	-0.5623788297	5.7723188977
H97	7.2289511311000	-1.1412315980000	7.1549696109000	H97	3.5504730027	-1.0412355851	7.9333579586
H98	6.8184775791000	-0.5628282955000	5.9613946384000	H98	7.4271356437	-0.2428746573	6.2441670029
H99	5.1576987014000	-1.2516955844000	7.6659637084000	H99	6.0250383958	-0.8672748525	8.1925808088
C100	2.0807640258000	3.8348866272000	5.7699072737000	C100	2.2587364545	3.4893974816	6.1229729824
C101	4.4352152306000	5.2770940258000	6.0871065230000	C101	4.5205843778	5.1018206223	5.92277499912
C102	3.2893433003000	3.1629813760000	6.0437997685000	C102	3.5285115984	2.9692215774	6.4422908247
C103	2.0686822683000	5.2306730376000	5.6379305245000	C103	2.1415377400	4.8079352551	5.6739908158
C104	3.2473592800000	5.9432315842000	5.8025972306000	C104	3.2700848433	5.6107890338	5.5877070317
C105	4.4548986509000	3.8905925710000	6.2123983002000	C105	4.6485592186	3.7806972017	6.3442456595
C106	3.3130632943000	2.0764947950000	6.1317036255000	C106	3.6423072669	1.9374564044	6.7725674016
H107	1.1419304582000	5.7499788213000	5.4008228414000	H107	1.1764262444	5.2021312882	5.3642009025
H108	3.2400257098000	7.0237437088000	5.6956843320000	H108	3.1727724175	6.6333702425	5.2340367375
H109	5.3876496254000	3.3728949125000	6.4199876217000	H109	5.6260936751	3.3768553437	6.5963969276
H110	5.3568144413000	5.8405390499000	6.2011562252000	H110	5.4013848175	5.7335211572	5.8409852483
7- Br				8- Br			
P1	0.0014046072	0.0110743468	0.0062248411	P1	0.4719417848	2.6064727803	6.3188924568
C2	-0.0053827007	0.0061305186	1.8260270792	C2	0.7182321048	1.6338164551	7.8412752406
C13	1.7574823040	0.0076854389	-0.46809093075	C3	0.9947089671	0.1265549572	10.1709646405
C24	-0.6228788397	1.6534564623	-0.4674139803	C4	-0.1409111847	0.5611089137	8.0916813154
Au35	-1.1948491379	-1.7388248776	-0.9258907679	C5	1.7198009268	1.9448177113	8.7654098881
C5	0.1003776582	-1.2254376442	2.4698103075	C6	1.85611221317	1.1909493764	9.9252626322
C4	-0.0783957578	1.1776545857	2.5745009843	C7	-0.0048306547	-0.1866077954	9.2553480004
C16	2.7669931021	0.3789141633	0.4115839702	H8	-0.9109514802	0.3076026662	7.3614404361
C15	2.0703544354	-0.3513450354	-1.7787456366	H9	2.3991793910	2.7742053235	8.5720270997
C27	-2.0045538375	1.8284500781	-0.5230198704	H10	2.6389440246	1.4362499100	10.6395740811
C26	0.2247474725	2.7256106589	-0.7311118840	H11	-0.6778009692	-1.0199093989	9.4438109454
Br12	-2.4816177947	-3.6286375851	-1.9329976149	H12	1.1045058756	-0.4625634926	11.0788522626
C6	0.1452888564	-1.2826546512	3.8529264139	C13	-0.6223883809	3.9853143592	6.7725971652
C7	-0.0408747502	1.1135378921	3.9600159314	C14	-2.2327968423	6.1725544392	7.3733555544
C17	4.0875040924	0.3948142599	-0.0219069115	C15	-1.4006173741	4.5751327384	5.7724818682
C18	3.3686016272	-0.3250707717	-2.2082251796	C16	-0.6567154529	4.4911806395	8.0748536374
C28	-2.5336947175	3.0715668036	-0.8276155375	C17	-1.4639991252</		

H12	0.0980346990	-0.1590894381	5.6817909323	H38	2.3856269354	-4.3855505212	0.8650702857
H23	5.4276978740	0.0569139195	-1.6630498827	H39	0.3977975217	-1.3178414223	-1.3941230170
H34	-2.1015402967	5.1118695566	-1.3372447002	H40	0.9261507113	-3.7128349036	-1.0233911171
				C41	4.7569921845	0.6351422495	1.8433653626
				C42	7.3929475693	1.2111140769	1.1493782938
				C43	5.2807604416	1.9106689341	2.0710859148
				C44	5.5572391710	-0.3468581548	1.2549649484
				C45	6.8708573350	-0.0560364935	0.9075040453
				C46	6.5984253383	2.1937084533	1.7304894872
				H47	4.6496801349	2.6808345796	2.5184934995
				H48	5.1498121518	-1.3390965653	1.0645205104
				H49	7.4894958888	-0.8218968192	0.4451937749
				H50	7.0007602439	3.1880602386	1.9110223377
				H51	8.4218991050	1.4349070764	0.8765312859
				C52	3.2963048187	-0.5397590920	4.0335294498
				C53	3.4965765845	-1.5441031353	6.6297446368
				C54	4.5254644683	-0.5323941720	4.6957078702
				C55	2.1727438598	-1.0870462606	4.6662120234
				C56	2.2751111090	-1.5799279048	5.9611259876
				C57	4.6221257503	-1.0351524284	5.9909293535
				H58	5.4087309695	-0.1238328786	4.2052032448
				H59	1.2124928442	-1.1193568191	4.1474760396
				H60	1.3916671156	-1.9856014880	6.4504070779
				H61	5.5816849899	-1.0213538911	6.5034576384
				H62	3.5700997428	-1.9184328656	7.6485584572
				C63	2.0989252929	3.3511061273	5.9862824451
				C64	4.5988341589	4.3840767492	5.3197106753
				C65	3.1906954128	2.4936456252	5.8125785485
				C66	2.2627500468	4.7242373746	5.8146533836
				C67	3.5130460784	5.2358553442	5.4800595018
				C68	4.4374875306	3.0106491415	5.4901500018
				H69	3.0668301341	1.4172493008	5.9338270676
				H70	1.4121677985	5.3952922783	5.9205625443
				H71	3.6333467982	6.3069839663	5.3373542827
				H72	5.2827473197	2.3349177554	5.3646219215
				H73	5.5744619781	4.7890634876	5.0581607412
9- Br				10- Br			
P1	0.3546084737	2.5840648297	6.4588981575	C1	-1.2725682492000	-2.9358872421000	2.3053209133000
C2	0.5446014350	1.5950056581	7.9698929031	H2	-0.1820873190000	-3.0822303630000	2.3239541784000
C3	0.7430849014	0.0837190690	10.2977937912	H3	-1.5884339479000	-2.6378738448000	3.3138905465000
C4	-0.3432537662	0.5413815360	8.1986106603	C4	-1.6065327613000	-1.8684168007000	1.2686592458000
C5	1.5372192217	1.8863741661	8.9104332216	H5	-1.2640443780000	-2.2258524956000	0.2892037267000
C6	1.6328088016	1.1299295642	10.0718486992	H6	-2.6950847429000	-1.7306608741000	1.2002632807000
C7	-0.2447210676	-0.2101442131	9.3632134942	C7	-0.9070363360000	-0.5433720713000	1.5844517883000
H8	-1.1105906590	0.3094021339	7.4589928659	H8	0.1468110937000	-0.7718274459000	1.8065812663000
H9	2.2378802825	2.7015105616	8.7317149863	H9	-0.8880745189000	0.1156430968000	0.7060536172000
H10	2.4049516918	1.3575697415	10.8029698607	N10	-1.8780358067000	-4.2192061869000	2.0075333974000
H11	-0.9383735518	-1.0285153016	9.5397449948	C11	-1.2871036377000	-5.0625909770000	1.1350477629000
H12	0.8217371982	-0.5068178747	11.2076462825	O12	-0.2390412167000	-4.8585682367000	0.5546153493000
C13	-0.6572568708	4.0309114747	6.8695468472	C13	-2.0285509910000	-6.3889497282000	0.9057337858000
C14	-2.1250587001	6.3260659529	7.4151065052	F14	-2.2892175570000	-6.5370028500000	-0.3839204807000
C15	-1.3454012865	4.6792001292	5.8392412723	H15	-3.1869440552000	-6.4413121710000	1.5797014205000
C16	-0.7095074279	4.5303584496	8.1735582355	F16	-1.2660813463000	-7.3958129244000	1.3087724801000
C17	-1.4460833814	5.6772610690	8.4418697107	C17	-1.9323760811000	1.4805810074000	2.70244407068000
C18	-2.0737417484	5.8296444172	6.1163702069	C18	-1.5493086879000	0.1717957167000	2.7288209860000
H19	-1.2696057809	4.2936262900	4.8196296296	P19	1.2090149543000	2.5957936207000	6.0042300509000
H20	-0.1822655324	4.0214248770	8.9791156414	C20	1.5635645844000	1.4254254605000	7.3383450516000
H21	-1.4924125904	6.064481965	9.4567856436	C21	1.8743443640000	-0.2148757198000	9.5619947870000
H22	-2.6059787346	6.3352184874	5.3145620951	C22	0.5684305996000	0.4928665585000	7.6599745897000
H23	-2.7016921123	7.2227139379	7.6301164646	C23	2.7036570158000	1.5475457643000	8.1426986695000
Au24	-0.4411427541	1.3328360673	4.6563349967	C24	2.8552562179000	0.7210934959000	9.2493177739000
Br25	-1.0672069899	-0.0726211379	2.6266309919	C25	0.7335478984000	-0.3227411820000	8.7721083385000
P26	3.0319077741	0.1427558965	2.3904320910	H26	-0.3368684387000	0.4378284270000	7.0498875321000
Au27	1.5959308509	1.9965017500	2.5879842967	H27	3.4589414201000	2.3002470725000	7.9297535194000
F28	2.6881228100	2.7031609297	0.5848454004	H28	3.7366461922000	0.8217708893000	9.8780067896000
Br29	0.5871617908	4.3863870948	2.4565995138	H29	-0.0421359083000	-1.0400914272000	9.0294445485000
C30	2.4971523991	-1.0889534025	1.1768429334	H30	1.9941236882000	-0.8525841522000	10.4349193600000
C31	1.7118750002	-2.9343145648	-0.7480695040	C31	0.0335930940000	3.7941384390000	6.6866158229000
C32	1.7779254243	-0.6652353451	0.0561372546	C32	-1.6976045011000	5.6639441764000	7.7887017708000
C33	2.8140764854	-2.4406800277	1.3357285045	C33	-0.9048831193000	4.4355773382000	5.8733241270000
C34	2.4221247248	-3.3598336012	0.3694438058	C34	0.0985068389000	4.0823328564000	8.0547891544000
C35	1.3895314615	-1.5892478672	-0.9044469439	C35	-0.7653929303000	5.0231084546000	8.5982139202000
H36	1.5024392317	0.3850891494	-0.0421085619	C36	-1.7672425687000	5.3705940763000	6.4308375189000
H37	3.3602291343	-2.7750837214	2.2171579596	H37	-0.9515045518000	4.2219453867000	4.8053874489000
H38	2.6642588534	-4.4122773771	0.4950234719	H38	0.8157773208000	3.5724765155000	6.8956852834000
H39	0.8142611106	-1.2648196293	-1.7680161544	H39	-0.7145062894000	5.2501655823000	9.6600231923000
H40	1.3960196392	-3.6574789194	-1.4960468483	H40	-2.4969132980000	5.8709450461000	5.7997986627000
C41	4.6837519029	0.7037689982	1.8498808442	H41	-2.3771169314000	6.3944339451000	8.2205492781000
C42	7.2237149246	1.5881240239	1.1097759802	Au42	-0.0564835766000	1.5745226728000	4.2578151948000
C43	5.1294632694	1.9691819457	2.2449056494	H43	-2.5569320425000	1.8865861123000	3.4976406595000
C44	5.5097756610	-0.1096660597	1.0739831261	H44	-1.7252178366000	2.1167549704000	1.8422641322000
C45	6.7762928041	0.3351390984	0.7038250538	H45	-1.8485539309000	-0.4100311161000	3.6061747849000
C46	6.3993278108	2.4052028191	1.8828909370	F46	-1.5310818121000	0.9655667652000	5.6061793364000
H47	4.4783899135	2.6088780207	2.8449826000	P63	3.1343997781000	0.4743842347000	2.3885949456000
H48	5.1659302333	-1.0937245798	0.7575215101	Au64	1.6908482055000	2.3834877105000	2.41098985257000
H49	7.4179299008	-0.3039796180	0.1020102359	Br49	2.8996976562564	3.2915549936464	0.4451571791646
H50	6.7513324572	3.3815779537	2.2132511928	B50	0.1130026360649	4.2967058110788	2.4308985911765
H51	8.2176788597	1.9279878073	0.8278408066	C67	2.57033920938000	-0.7064532175000	1.1382578863000
C52	3.2881810684	-0.7431496173	3.9533034775	C68	1.7193095551000	-2.4944252549000	-0.8138642023000
C53	3.5494779112	-1.9828833989	6.4314761348	C69	2.1980661751000	-0.2315970389000	-0.1249618963000
C54	4.5449146761	-0.8427894098	4.5535408730	C70	2.5469695624000	-2.0813943947000	1.4086792181000
C55	2.1629180706	-1.2853940599	4.5870986957	C71	2.1190506174000	-2.9703899128000	0.4318033807000
C56	2.2975822177	-1.9005092934	5.8243085734	C72	1.7747968670000	-1.1318531257000	-1.0955723552000
C57	4.6708913089	-1.4639469431	5.7929971883	H73	2.2345076787000	0.8369919452000	-0.3413598722000
H58	5.4261054703	-0.4363633942	4.0580338472	C74	2.8550369037000	-2.4602214367000	2.3817859185000
H59	1.1814838108	-1.2173186729	4.1128198568	H75	2.0654786358000	-4.0338738017000	0.6456223831000
H60	1.4206859780	-2.3138476377	6.3173129588	H76	1.4784364696000	-0.7628769319000	-2.0746038082000
H61	5.6499456761	-1.5417294851	6.2601033566	H77	1.3591865778000	-3.1970634764000	-1.5616318493000
H62	3.6508917407	-2.4592748131	7.4038385144	C78	4.8538549730000	0.8749963916000	1.9899304006000
C63	2.0268548472	3.2053416589	6.0893081398	C79	7.5400005625000	1.3636605011000	1.4809467304000
C64	4.5997304918	4.0586236410	5.4454902663	C80	5.3857197749000	2.1420523562000	2.2662654392000
C65	3.0469628130	2.2686520216	5.8824879272	C81	5.6649366163000	-0.1476719750000	1.4842941764000
C66	2.2973414243	4.5659184497	5.9588904633	C82	7.0077749317000	0.1011828934000	1.2342799627000
C67	3.5837222279	4.9883160870	5.6320709164	C83	6.7311866194000	2.3808830082000	1.9767833568000
C68	4.3309621856	2.6967001111	5.5755752345	H84	4.7463980631000	2.9463836373000	2.5829449624000
H69	2.8397018330	1.2010625339	5.9744119305	H85	5.2495921741000	-1.1347944429000	1.2844662717000
H70	1.5040871396	5.2980238569	6.1011009814	H86	7.6376529174000	-0.6909695413000	0.8375531188000
C71	3.7903162632	6.0514249861	5.5329415569	H87	7.1423435144000	3.3727220057000	2.1527175647000
H72	5.1237706092	1.9621121212	5.4382021683	H88			

H80	3.6983630369	2.1309204886	-1.7684594743
H81	3.9759029520	5.7011273367	-0.4155829662
H82	2.8961521498	5.1623398087	0.9309460830
H83	4.5638313658	4.4980141478	0.7859000165
H84	2.1084960252	4.8588093376	-2.0296516760
H85	1.5633080069	3.1676155041	-1.7710430787
H86	1.2040904730	4.4188456777	-0.5322799689
11- Br			
C17	-0.9463358199000	-0.7857377282000	4.1304457272000
C18	-0.8965390513000	-0.9514931913000	2.6903441862000
P19	1.2226064725000	2.8937857942000	5.7704906665000
C20	2.0556242237000	2.6631435348000	7.3689250396000
C21	3.0901677425000	2.3655433249000	8.9371730725000
C22	1.522333018000	1.6956097216000	8.220622053000
C23	3.0982940457000	3.4880348428000	7.8042604861000
C24	3.8157132991000	3.3316351367000	9.0849649441000
C25	2.0434708845000	1.5544103703000	9.5094971545000
H26	0.6889142643000	1.0762746094000	7.8901664162000
H27	3.5018429785000	4.2621104149000	7.1543896364000
H28	4.4243887246000	3.9764910997000	9.4211092112000
H29	1.6215605599000	0.8088493395000	10.1799997363000
H30	3.4916322410000	2.2527192999000	10.9419349883000
C31	-0.2208122742000	3.9368614078000	6.1342071585000
C32	-2.3949709291000	5.5732901736000	6.7315152735000
C33	-1.4825663963000	3.6395295009000	5.6175534354000
C34	-0.0522892608000	5.0593331202000	6.9552652504000
C35	-1.1365818191000	5.8742729602000	7.2476596731000
C36	-2.5657251657000	4.4584710580000	5.9192258851000
H37	-1.6238844881000	2.7745082790000	4.9712679528000
H38	0.9272064374000	5.2908523783000	7.3730327886000
H39	-1.0008378345000	6.7437002637000	7.8863102167000
H40	-3.5470630727000	4.2191555090000	5.5174723827000
H41	-3.2444065415000	6.2094762406000	6.9678777918000
Au42	0.3105569188000	0.8442906612000	4.8334140007000
H43	-0.8894329388000	-1.6742938064000	4.7180612730000
H44	-1.8636794688000	-0.3119415325000	4.4958111468000
F46	-0.6833641878000	0.4697830483000	6.5922939382000
P63	3.4718064851000	0.0550682324000	2.9210577739000
Au64	1.4507873581000	1.2384982177000	2.4652983414000
B32	1.9000364009010	1.3261609937797	0.0279041313403
B33	-0.6353633395639	2.5666635266694	2.2186903833398
C67	3.4391113263000	-1.6488299665000	2.2863097213000
C68	3.4197573348000	-4.2108489768000	1.1958597519000
C69	3.2629716192000	-1.8217554418000	0.9068345563600
C70	3.6222341244000	-2.7617888542000	3.1121046026000
C71	3.8062935219000	-4.0401357891000	2.5627893486000
C72	3.2553436257000	-3.1012139539000	0.3695909777000
H73	3.1173411699000	-0.9528833662000	0.2636168235000
H74	3.7911618783000	-2.6394234038000	4.1796716313000
H75	3.7524311058000	-4.9035805150003	3.2072253101000
H76	3.1244156576000	-3.2322270279000	-0.7019784048000
H77	3.4137446417000	-5.2116015134000	0.7699228283000
C78	4.8613624803000	0.8316625525000	0.2540778350000
C79	7.0412415533000	1.9417733386000	0.7367924952000
C80	4.7746287184000	2.12323246863000	1.53412111557000
C81	6.0420387634000	0.0914123898000	1.9072934208000
C82	7.1297895236000	0.6512008836000	1.2534022504000
C83	5.8690293632000	2.6742065246000	0.8774442039000
H84	3.8511292800000	2.6914327549000	1.6206397953000
H85	6.1080276911000	-0.9231199254000	2.3005526053000
H86	8.0450775859000	0.0762312693000	1.1376503932000
H87	5.7948048791000	3.6767559191000	0.4623464361000
H88	7.8912668899000	2.3735959829000	0.2137109055000
C89	3.9183494295000	-0.0532908167000	4.6820901924000
C90	4.5377178882000	-0.1568158233000	7.4059662828000
C91	5.1066714232000	0.5069563375000	5.1549372082000
C92	3.0516313789000	-0.6850544803000	5.5844080120000
C93	3.3603647647000	-0.7366610067000	6.9363642625000
C94	5.4093067480000	0.4555730273000	6.5141981230000
H95	5.7940642149000	0.9958962119000	4.4656783933000
H96	2.1247961617000	-1.1424820509000	5.2317651374000
H97	2.6712919493000	-1.2183533594000	7.6265697566000
H98	6.3326262514000	0.9031339814000	6.8741797883000
H99	4.7687756879000	-0.1801186542000	8.4681236357000
C100	2.3102887475000	3.8798068405000	4.6984330801000
C101	3.9353937456000	5.3180603321000	2.9397696107000
C102	3.6927938132000	3.6590401482000	4.6470424174000
C103	1.7470107560000	4.8143757099000	3.8235724455000
C104	2.5590164296000	5.5221760479000	2.9442670441000
C105	4.4996785370000	4.3865787666000	3.8082724122000
H106	4.1413211021000	2.9219602776000	5.3392335753000
H107	0.6714534071000	4.9830542709000	3.8215342394000
H108	2.1111046074000	6.2430944125000	2.2650860506000
H109	5.5751931661000	4.2176983386000	3.8053302645000
H110	4.5689411893000	5.8852975121000	2.2614720717000
H78	-1.0536023760000	-0.0285437895000	2.1306568752000
C86	0.0053502983000	-1.9922624458000	2.0873899542000
H80	0.2684186938000	-1.7240009096000	1.0541855718000
H81	0.9412826904000	-2.0455576085000	2.6573069091000
C84	-0.7172795425000	-3.3374162115000	2.1238956610000
H83	-0.1611877248000	-4.1081686797000	1.5794839460000
H89	-0.8322301220000	-3.6785108494000	3.1611115197000
C85	-2.0859342014000	-3.0789984591000	1.5176741039000
N86	-2.5349567725000	-1.7668859186000	2.0171264709000
C87	-3.5627893199000	-1.5816216353000	2.9270481577000
O88	-3.9272782714000	-0.4746431400000	3.2545956892000
C95	-4.2353501953000	-2.8195448627000	3.5514150376000
F90	-3.3068571849000	-3.6016534716000	4.1152704295000
F91	-5.1088191220000	-2.468242253000	4.4663612463000
F92	-4.8639738654000	-3.5302935266000	2.6061664243000
H93	-2.7087782987000	-0.8844417821000	1.0784652413000
H94	-2.0024265513000	-2.9976555025000	0.4229222603000
H100	-2.8030966954000	-3.8753361284000	1.7290872333000
N96	-2.9651249556000	-0.0834230816000	0.0871721758000
C97	-1.7281519207000	0.2667360135000	-0.6350172497000
C98	-3.8852734628000	-0.8522615628000	-0.7654708677000
C99	-3.6308574472000	1.1353071140000	0.5938773826000
H101	-1.9673094360000	0.8219993286000	-1.5517330511000
H96	1.0596508848000	-0.9469620735000	3.8882420763000
H97	1.0896344503000	-2.197245389000	6.006489433000
H98	5.2925400695000	-1.4056530787000	6.4304325059000
H99	3.2044100033000	-2.4306458316000	7.2902738741000
C100	2.7210126241000	3.4743101380000	5.5422997999000
C101	5.0193774708000	4.8496515403000	4.7676284533000
C102	3.9596442961000	2.8185304328000	5.5225521342000
C103	2.6379077964000	4.8156600798000	5.1504827389000
C104	3.7853287730000	5.4925415653000	4.7550533775000
C105	5.1044966032000	3.5147587857000	5.1579586978000
H106	4.0318445477000	1.7667572999000	5.7963439546000
H107	1.6784860532000	5.3293312343000	5.1448301484000
H108	3.7125403755000	6.5307140848000	4.4433192706000
H109	6.0659019228000	3.0046287353000	5.1606762304000
H110	5.9161165111000	5.3891023377000	4.4723691450000
H100	-2.7706316788000	-4.4737781848000	2.4063901772000
12- Br			
C1	-2.5682409716	-1.9050654355	1.7568927416
H2	-3.5983629919	-1.8695345647	2.1295086680
H3	-2.5008928398	-2.7678595538	1.0800333565
C4	-2.0954982348	-0.6069057228	1.1073475416
H5	-2.2410262371	-0.6103401030	0.0232767342
H6	-2.649824733	0.2525712104	1.5052572681
C7	-0.6231612701	-0.5166559199	1.5055598849
H8	-0.0132453155	-1.1867764328	0.8840099257
H9	-0.2164667679	0.4988057455	1.4107364113
N10	-1.6266537326	-2.1065391031	2.8671705038
C11	-1.7387476276	-2.2312508097	3.6042577420
O12	-2.6069763368	-4.0697097365	3.4490494396
C13	-0.6421122030	-3.4863881606	4.6632727460
F14	-0.4453619385	-2.4402272611	5.4807277259
F15	0.5351008466	-3.7364043541	4.0604582890
F16	-0.9474834341	-4.5311249854	5.4065916187
C17	-1.0641695397	0.0108521047	3.9656402060
C18	-0.6163900739	-1.0268300478	2.9478682464
P19	1.6742788998	2.7008469490	6.5252020723
C20	2.2911267146	1.9963766256	8.0972301389
C21	3.0174987130	0.9145213584	10.5674073225
C22	1.6031078548	0.8912523067	8.6089175973
C23	3.3124845877	2.5838034649	8.8512374280
C24	3.6840521427	2.0323688578	10.0718506637
C25	1.9667175043	0.3613803238	9.8436350430
H26	0.7621855507	0.4755130066	8.0485917244
H27	3.8183684221	3.4789036260	8.4928632434
H28	4.4880635946	2.4885069026	10.6457907415
H29	1.4226898894	-0.4952887212	10.2370524873
H30	3.3060817844	0.4902300620	11.5268585532
C31	0.5057426673	3.9803846885	7.1064573159
C32	-1.3265506499	5.8059111519	8.1399229398
C33	-0.8061581262	3.5761331973	7.3743111043
C34	0.9005667641	5.2932074862	7.3732753232
C35	-0.0171213489	6.2024779261	7.8854016076
C36	-1.7148440994	4.4938742538	7.8901572329
H37	-1.1001144515	2.5379294037	7.2038719714
H38	1.9242552292	5.6101693048	7.1776556564
H39	0.2931089459	7.2257197882	8.0861817860
H40	-2.7351209648	4.1777189377	8.0952709325
H41	-2.0434935512	6.5210046790	8.5371955579
Au42	0.3582320759	1.1374910395	5.0715688941
H43	-1.5604534509	-0.4368753903	4.8306356447
H44	-1.6914990627	0.7941729744	3.5246295907
H45	0.3523208518	-1.4725639094	3.2038001717
F46	-0.7375312726	0.5157366597	6.7313706030
P63	3.3156725752	0.2635050002	3.0978727085
Au64	1.5974963445	1.9093971889	2.8499455624
Br65	2.4922403517	2.8751620415	0.5324313479
Br66	-0.4502334063	3.5073606268	2.9176225511
C67	2.9473442931	-1.1695612262	2.0378669208
C68	2.4678458319	-3.2675013354	

H102	-1.0866561730000	0.8966208555000	-0.0056506702000
H103	-1.1839875178000	-0.6490542860000	-0.90653161785000
H104	-4.2720795111000	-0.2262209563000	-1.5807258622000
H105	-3.3621492772000	-1.7113894833000	-1.1978327544000
H111	-4.7265321247000	-1.2111926131000	-0.1608624077000
H112	-3.8619897172000	1.8046236723000	-0.2459576353000
H113	-4.5513297328000	0.8588599941000	1.1137510067000
H114	-2.9653686065000	1.6462229327000	1.2958985086000
13- Br			
C1	-2.3309655370	-2.1504759584	1.3963504107
H2	-3.3831846205	-2.4198990508	1.5343797560
H3	-1.8840830486	-2.8841004042	0.7084892982
C4	-2.1078365018	-0.7190578548	0.9437685192
H5	-2.1383314630	-0.6147656571	-0.1448186344
H6	-2.8785550482	-0.0616649945	1.3664640353
C7	-0.7447533839	-0.3807659173	1.5326293077
H8	0.0539412158	-0.8579488566	0.9472767343
H9	-0.5461809545	0.6962827654	1.5644462148
N10	-1.6171614070	-2.2204718394	2.6820639265
C11	-1.6675524417	-3.3909731192	3.3535190923
O12	-2.3733045075	-4.3292583253	3.0317455847
C13	0.7182456959	-3.5714927764	4.58077118493
F14	-0.8085098537	-2.5890168206	5.4668163541
F15	0.5602594624	-3.5873644322	4.1354111513
F16	-0.9591022302	-4.7126632660	5.1715202340
C17	-1.2636484633	-0.1091581810	4.0462325712
C18	-0.7781503476	-1.0220516566	2.9246623531
P19	1.7585740059	2.6756872573	6.5405600470
C20	2.4457931730	2.0735284769	8.1209611391
C21	3.2679173960	1.1205199587	10.6125258336
C22	1.7543698108	1.0232409292	8.7343981727
C23	3.5381036197	2.6554153354	8.7773938209
C24	3.9526712505	2.1706104441	10.0089639235
C25	2.1655083345	0.5577884621	9.9791606770
H26	0.8927061811	0.5784726335	8.2289388382
H27	4.0654969975	3.4946572875	8.3235669067
H28	4.8066459908	2.6250651266	10.5071139604
H29	1.6211507075	-0.2566513140	10.4530466769
H30	3.916269538	0.7466402801	11.5817668537
C31	0.5806222161	3.9745104211	7.0699817145
C32	-1.2073962128	5.9785143425	7.8132989601
C33	-0.5755987176	4.1963364319	6.3186979829
C34	0.8370829321	4.7640270629	8.1958553800
C35	-0.0544194570	5.7619620408	8.6533707810
C36	-1.4685288236	5.1972942075	6.9645194133
H37	-0.7851835678	3.5953723977	5.4334390564
H38	1.7320101704	4.5917848798	8.7924825183
H39	0.1493754339	6.3712511104	9.4413115566
H40	-2.3666031533	5.3575379013	6.1059281120
H41	-1.9068490688	6.7580924803	8.1073203964
Au42	0.4471256725	1.0218379110	5.1538459615
H43	-1.3824376883	-0.5927240114	5.0044531717
H44	-1.6076470018	0.8870734465	3.7964974582
H45	0.2256803427	-1.3754783044	3.2025365148
F46	-0.5195265876	0.1083860786	6.8947204140
B47	-2.914084998	0.4132024660	5.9981797185
O48	-2.5263799072	1.7142748672	6.1577799500
H49	-2.0035917850	1.8127527800	6.9629034336
O50	-2.9282366578	-0.5425551847	6.9671223075
H51	-2.0520944975	-0.4928890171	7.3919583349
C52	-3.4686743656	0.0220685600	4.5706447652
C53	-5.3637823927	-0.5836363076	2.5619789294
C54	-3.9904401586	1.0239891175	3.7167104638
C55	-3.9667634327	-1.2856545295	4.3925111391
C56	-4.8868617991	-1.5903996920	3.3990369412
C57	-4.9078864994	0.7276660988	2.7232267080
H58	-3.8578787854	2.0531815921	3.8594102815
H59	-3.6420546617	-2.0594479702	5.0882843158
H60	-5.2444506526	-2.6128110276	3.2878579600
H61	-5.2900323620	1.5196879695	2.0822833929
H62	-6.096861984	-0.8153879864	1.7917189971
P63	3.2744746286	0.2469471008	3.1101159162
Au64	1.5239171546	1.8408204449	2.8467222936
Br65	2.3280071206	2.6590754315	0.6472881701
Br66	-0.5176932551	3.2487358543	2.8477877150
C67	2.9009266451	-1.1742660862	2.0332015120
C68	2.3373967577	-3.2411703532	0.2539463691
C69	2.7390179692	-0.8989461606	0.6678628275
C70	2.8006103478	-2.4867042328	2.4956338848
C71	2.5024293853	-3.5148026552	1.6054786162
C72	2.4689280272	-1.9353630573	-0.2142202155
H73	2.8005204614	0.1313926721	0.3089041980
H74	2.9471811700	-2.7166777067	3.5485910167
H75	2.4014921601	-4.5316486769	1.9780029844
H76	2.3453777050	-1.7181730850	-1.2726420943
H77	2.1078163131	-0.4475410659	-0.4391083035
C78	4.8741034832	0.8483967789	2.4923217212
C79	7.3636941344	1.7029443408	1.6020937586
C80	5.1336942664	2.2108403720	2.3663563997
C81	5.8603034017	-0.0894761597	2.1629753324
C82	7.1028355826	0.3397116129	1.7208967580
C83	6.3822358750	2.6327710455	1.9203094381
H84	4.3589522243	2.9404293826	2.5953763460
H85	5.8522062108	-1.1557536365	2.2535275450
H86	7.8878194210	-0.3895565625	1.4645789596
H87	6.5796026582	3.6972309466	1.8144725452
H88	8.3556569552	2.0387395537	1.2468334588
C89	3.6299630623	-0.3941197639	4.7886462712
C90	4.0879135578	-1.1605576449	7.4459085008
C91	4.8287850527	-0.0645568349	5.4253077108
C92	2.6718948351	-1.1355826633	5.4953976094
C93	2.9017585599	-1.5199941578	6.8086706963
C94	5.0510224850	-0.4432227575	6.7486721216
H95	5.5894176756	0.5071229696	4.8945412838
H96	1.7256879622	-1.4135593028	5.0306129692
H97	2.1331623510	-2.0777629640	7.3398983373
H98	5.9821404001	-0.1608473062	7.2361725817
H99	4.2548071922	-1.4352625530	8.4848835290
C100	3.0735332837	3.6219953931	5.6923658481
C101	5.0079021372	5.0992051609	4.3138887059
C102	4.4282544070	3.2899652392	5.7989192935
C103	2.6954013935	4.6728970933	4.8476245873
C104	3.6584854080	5.4016976564	4.1597025594
C105	5.3890731243	4.0350537201	5.1238793435
H106	4.7366483063	2.4467947479	6.4149531805
H107	1.6420329958	4.9215715822	4.7197031072
H108	3.3482302094	6.2115390243	3.5040736185
14- Br			
C1	-5.0041062581000	-2.0373525863000	1.2340652236000
H2	-5.3290410445000	-1.9467760613000	2.27759794661000
H3	-5.6793895089000	-2.7555544895000	0.7483013411000
C4	-4.9234768876000	-0.7059513630000	0.4994702073000
H5	-5.8435526827000	-0.4896608293000	-0.0528835966000
H6	-4.7616468848000	0.1120228156000	1.2104531875000
C7	-3.7121084501000	-0.8649939079000	-0.4197520711000
H8	-4.0041139895000	-1.3914775136000	-1.3378879770000
H9	-3.2662562515000	0.0929689113000	-0.7119396332000
N10	-3.6315982861000	-2.5659687001000	1.1837445270000
C11	-3.4446404903000	-3.7765466497000	1.7587058645000
O12	-4.3258900594000	-4.4009854674000	2.3195824246000
C13	-2.0271131044000	-4.3802835689000	1.7485870799000
F14	-1.2353204791000	-3.7563480508000	2.6210769233000
F15	-1.4247737286000	-4.3211776637000	0.5443737981000
F16	-2.0750349003000	-5.6642252699000	2.0874771035000
C17	-1.6971820626000	-0.9307780460000	1.1880035425000
C18	-2.7219440245000	-1.7328926239000	0.3666931095000
P19	0.2565683752000	2.8193982512000	5.7608042907000
C20	0.3941821048000	2.4951668839000	7.5471399664000
C21	0.4949721094000	2.0160503418000	10.2879932603000
C22	-0.2323975549000	1.3694326183000	8.0849080137000
C23	1.0729668811000	3.3828222508000	8.3882590497000
C24	1.1206458873000	3.1408777670000	9.7550796056000
C25	-0.1800336417000	1.1316565146000	9.543891593000
H26	-0.7582722207000	0.6634814541000	7.4408492717000
H27	1.5626173018000	4.2625258264000	7.9704357164000
H28	1.6498348288000	3.8317900129000	10.4079527716000
H29	-0.6673036513000	0.2465185326000	9.8574537005000
C30	0.5382962160000	1.8297863972000	11.3591862717000
C31	-1.0521697269000	4.0729807899000	5.5968108569000
C32	-3.0664902824000	5.9783538407000	5.2867633579000
C33	-1.3368306089900	4.5919978113000	4.3285535842000
C34	-1.7908418891000	4.5000905817000	6.7031735402000
C35	-2.7975257936000	5.4474266072000	6.5435609995000
C36	-2.3317964007000	5.5514090209000	4.1833259378000
H37	-0.7780964354000	4.2417719285000	3.4571581779000
H38	-1.5831718279000	4.0950553348000	7.6921925053000
H39	-3.3707880203000	5.7724853917000	7.4096013825000
H40	-2.5403751839000	5.9592466818000	3.196108096000
H41	-3.8504570485000	6.722669966000	5.1659070696000
Au42	0.0096154159000	0.7568528742000	4.6825651771000
H43	-2.1628729626000	-2.3806795175000	-0.3161294955000
Br44	0.2318203929991	-1.6605415663457	4.1853876219495
B45	-2.3774329694000	-2.1140102898000	6.5938572292000
O46	-1.2121102245000	-1.5853770127000	7.0418003656000
H47	-0.4985682598000	-1.6780947923000	6.3949042574000
O48	-2.5206067813000	-2.8560169129000	5.4679028923000
H49	-1.7166671126000	-2.8825685722000	4.9308918527000
F50	-3.4622411994000	-1.9047271690000	7.3329731447000
P51	3.6907461137000	-0.2147300733000	2.9497130953000
Au52	2.1286435869000	1.4579383124000	2.4739325255000
Br53	0.6603225835380	3.2626604733824	1.6152059376125
C54	3.1139209139000	-1.8589968846000	2.4402817303000
C55	2.0673407754000	-4.3247629972000	1.6678780904000
C56	2.1817256336000	-1.9344726050000	1.4023044300000
C57	3.5346658397000	-3.0282383694000	3.0773034550000
C58	3.0099837806000	-4.2565146749000	2.6892179401000
C59	1.6627196197000	-3.1628889542000	1.700707095000
H60	1.8286154890000	-1.0180352541000	0.9265936880000
H61	4.2477154482000	-2.9762247477000	3.8999350669000
H62	3.3259143031000	-5.1623911907000	3.2016480928000
H63	0.9119338344000	-3.2104799867000	0.2317379860000
H64	1.6330203352000	-5.2820164503000	1.3877280303000
C65	5.2216991326000	0.1072781835000	2.0155421832000

H109	6.4410724290	3.7730293276	5.2236842576	H109	-1.0609960692000	-0.3934109859000	0.4675481530000
H110	5.7612994430	5.6827934536	3.7886299652	H110	-1.0406274299000	-1.6259246245000	1.7291068647000

3) Ligand: DPPM

Catalyst L-Au-Cl

10-Cl-dppm				11-Cl-dppm			
C1	6.0427246388	-0.2538552598	10.8392027000	C1	9.9539748999257	0.9021808476667	7.8428395979771
H2	6.9576233688	-0.6233087537	11.3196394409	H2	9.6530192753257	0.2658305997667	8.8622901636771
H3	6.0313406591	0.8319607567	10.9753744102	H3	10.9505266409257	1.3082986140667	8.0440857870771
C4	6.0462441308	-0.5667432781	9.3491552976	C4	9.8232163245257	0.1826006222667	6.5149708285771
H5	5.9433439783	-1.6463600000	9.1665828642	H5	10.2114153430257	0.8112280845667	5.7008219915771
H6	5.1604571501	-0.0818056472	8.9115618415	H6	10.3933186153257	-0.7507360916333	6.5043436537771
C7	7.3055690763	-0.0111287218	8.6794335165	C7	8.3221690072257	-0.0516081185333	6.3406098774771
H8	7.5053284662	0.9925947658	9.0630530940	H8	8.0632710052257	-0.3240187312333	5.3088471172771
H9	8.1592562443	-0.6626945967	8.9214878533	H9	7.9955150465257	-0.8631218244333	7.0011608864771
N10	4.9043471740	-0.8562858028	11.5200712980	N10	8.9626243821257	2.0062940947667	7.7825396324771
H11	4.9455438223	-1.8525811527	11.7085107911	C11	8.3824572601257	2.4357247313667	9.0420179535771
C12	3.6738309840	-0.3514354917	11.7611404048	O12	8.1721801418257	1.6679396446667	9.9273634159771
O13	2.7273448670	-1.0034680933	12.1551796136	C13	8.2428946619257	3.9609358045667	9.1561140692771
C14	3.4875725739	1.1560897234	11.4861994569	F14	7.4030006322257	4.3127908855667	10.0855202657771
F15	2.2604226925	1.5367293180	11.7939359784	F15	7.9123955701257	4.5119468981667	7.9826100815771
F16	3.6568826697	1.3836602067	10.1615409512	F16	9.4708167632257	4.4085273480667	9.4627739231771
F17	4.3522333783	1.9158798869	12.1424927173	P17	2.8815913509257	1.7081125832667	6.4950772678771
P18	2.4966915682	0.9719095625	5.8267783259	C18	1.7902169942257	1.2900342261667	6.0763794500771
C19	1.4084284087	0.4145994389	7.1468522656	C19	0.1325023386257	0.7035019265667	8.2307670701771
C20	-0.3021058598	-0.4021296495	9.1735155640	C20	0.4088778775257	1.4997499153667	5.9748137074771
C21	0.0292521156	0.6360295677	7.0266908505	C21	2.3336915119257	0.7811325777667	7.2587773741771
C22	1.9215731232	-0.2343135588	8.2719522597	C22	1.5018781749257	0.4889148475667	8.3348301554771
C23	1.0632701471	-0.6360123397	9.2907251658	C23	-0.4145597225743	1.2083241144667	7.0524718317771
C24	-0.8204618281	0.2261414503	8.0424711124	H24	-0.0251253848743	1.8904080778667	5.0541804915771
H25	-0.3825781672	1.1224694470	6.1424229006	H25	3.4083194914257	0.6145364992667	7.3398506896771
H26	2.9913560009	-0.4280818123	8.3506124252	H26	1.9263588367257	0.0932794836667	9.2537075281771
H27	1.4578463751	-1.1203886709	10.1822521789	H27	-1.4857362764743	1.3787152461667	6.9757563808771
H28	-1.8898511404	0.4017844862	7.9546923295	H28	-0.5165568453743	0.4754197640667	9.0728990985771
H29	-0.9705314357	-0.7150099936	9.9719609124	C29	2.3297388294257	0.8073079712667	3.2303348000771
C30	2.0909497073	0.0928249958	4.3101979738	C30	1.5852659954257	-0.5880257490333	6.90461575731771
C31	1.4997148325	-1.2675236107	1.9667466870	C31	1.4306124517257	-0.2572918756333	3.3274941189771
C32	1.3655936486	-1.1001380337	4.3656316605	C32	2.8760979425257	1.1545758378667	1.9896473599771
C33	2.5457580759	0.5888321561	3.0830177792	C33	2.4946628918257	0.4620764604667	0.8506465553771
C34	2.2424392998	-0.0903134118	1.9136352235	C34	1.0598616236257	-0.9498397907333	2.1809701338771
C35	1.0664262423	-1.7720149990	3.1878897793	H35	1.0188477457257	-0.5464376795333	4.2922717033771
H36	1.0401073608	-1.5030169417	5.3226706816	H36	3.6194207609257	1.9475949928667	2.9126052493771
H37	3.1502621045	1.4942509801	3.0337752959	H37	2.9184460451257	0.7328020824667	-0.1127148281229
H38	2.5898397078	0.2940626052	0.9584372182	H38	0.3583321830257	-1.7767152941333	2.2554753638771
H39	0.4972099089	-2.6969194537	3.2259240693	H39	1.2932315322257	-1.1335050853333	0.0523373327771
H40	1.2650557762	-1.7993678768	1.0481903733	Au40	5.2491179812257	1.8037461217667	5.1806089331771
Au41	4.7994487644	0.8308826157	6.4154892740	C41	5.9575728038257	0.2358999273667	3.4633205691771
C42	4.8337222453	-1.4370741880	5.4461055609	C42	7.6105577089257	1.2247513042667	6.7003629031771
C43	7.1787199675	0.0323661473	7.2000738603	H43	6.8740735202257	1.1918645137667	7.5051881175771
H44	7.1397988687	-0.925307412	6.6716768750	C44	7.3080802674257	2.2076649777667	5.6612878511771
C45	7.1380969271	1.1842852411	6.4558209015	H45	7.8888009432257	2.1013264633667	4.7398519103771
H46	7.2364939559	1.1275218770	5.3706281354	H46	7.2797778921257	3.2363495362667	6.0277036435771
H47	7.2564323705	2.1439544026	6.9562791715	P47	2.9445077688257	4.5156408680667	5.8134259364771
P48	2.4966557807	3.8071704634	6.8976926429	C48	3.4757185161257	6.1247130977667	5.2038654196771
C49	2.6866245073	5.4553572898	6.2121248953	C49	4.4055425416257	8.5864968717667	4.3262084692771
C50	3.1728562693	7.9951377981	5.2051035306	C50	2.9142797810257	7.2978972349667	5.7121092180771
C51	2.0242738579	6.5565724017	6.7598275056	C51	4.5226510654257	6.1834895984667	4.2771952281771
C52	3.6165837033	5.6311808601	5.1805334502	C52	4.9797758931257	7.4159277473667	3.8352529263771
C53	3.8522141145	6.9006606846	4.6753384525	C53	3.3807496208257	8.5272934665667	5.2635201129771
C54	2.2663561914	7.8236999005	6.2453965342	H54	2.1260138509257	7.2513731728667	6.4604254874771
H55	1.3341142983	6.4266804014	7.5906328816	H55	4.9966314077257	5.2698384676667	3.9142735335771
H56	4.1798508803	4.7837943576	4.7867946712	H56	5.7901790783257	7.4661259041667	3.1128303257771
H57	4.5739040132	7.0402069631	3.8749783067	H57	2.9444266776257	9.4424594746667	5.65475758919771
H58	1.7505329647	8.6819948524	6.6674280334	H58	4.7680238217257	9.5515690304667	3.9813423181771
H59	3.3619529865	8.9902971596	4.8108501410	C59	1.3623444839257	4.6893289378667	6.6730459811771
C60	0.9922662543	3.7615665706	7.9444451484	C60	-1.1374758171743	4.9501388661667	7.8634134823771
C61	-1.3199095251	3.6611133369	9.4767373110	C61	1.1945559174257	4.3520942644667	0.0160271432771
C62	1.0512686649	3.2951744070	9.2573529106	C62	0.2743485787257	5.1651435528667	9.9264756022771
C63	-0.2277954065	4.1780426478	7.3939718914	C63	-0.9705873535743	5.2956179100667	6.5242260496771
C64	-1.3796313335	4.1311533727	8.1663778958	C64	-0.0593531474743	4.4813127069667	8.6039301707771
C65	-0.1109975499	3.2395738656	10.0177791881	H65	2.0401169788257	4.0068209532667	8.60663522720771
H66	1.9976977993	2.9813679755	9.6879418252	H66	0.3986820966257	5.4590168138667	4.8837800494771
H67	-0.2791272049	4.5579731327	6.3730833677	H67	-1.8095237705743	5.6757814886667	5.9467783776771
H68	-2.246776901	4.4683555959	7.7480265342	H68	-0.1875516376743	4.2184538262667	9.6508789977771
H69	-0.0625354249	2.8698824573	11.0388583317	H69	-2.1135571126743	5.0554224589667	8.3310036450771
H70	-2.224883423	3.6281009373	10.0796501777	Au70	4.6214031238257	3.5635304692667	7.1233672130771
Au71	4.4208343681	3.0716635233	7.9081384820	C71	4.3098554500257	5.4146131243667	8.6806665537771
C72	4.0774723190	4.9617477712	9.3808551893	C72	2.5532692633257	3.4899992584667	4.3264559393771
C73	2.0919937868	2.7257158757	5.4515862933	H73	3.2276223666257	3.7903853949667	3.5143010469771
H74	2.7489330142	3.0420095563	4.6318912710	H74	1.5222143241257	3.6686470752667	3.9951695385771
H75	1.0539749884	2.8392871465	5.1092792937	F75	6.0055315946257	2.6614543854667	8.3295692395771
F76	6.1344755343	2.5475947291	8.8075776026	H76	9.3940518369238	3.0516279402337	7.0452150769974
				N77	9.8254402924981	4.0774451502669	6.0394302829202
				H78	10.1384493482973	4.9092512780126	6.5192468070547
				H79	10.5815719293605	3.7061256956833	5.4822168495005
				H80	9.0471804470607	4.3086565865216	5.4386367370788

12-Cl-dppm				13-Cl-dppm			
C1	9.9270744192	1.9050468846	7.1577951737	C1	-3.3064752319	-2.8889567575	1.7093310577
H2	10.7097434462	1.7453150085	7.9114522195	H2	-4.2321968607	-2.6370255816	2.2430767256
H3	10.3275017478	2.6208410472	6.300514908	H3	-3.4666586707	-3.8588722318	1.2205019880
C4	9.4293389202	0.6014415236	6.5307321903	C4	-2.8424588655	-1.7912593533	0.7488784492
H5	9.1687431510	0.7519095182	5.4756245871	H5	-3.1181685615	-2.0076833211	-0.2873874279
H6	10.1906901135	-0.1837221111					

P17	2.5610122542	0.6707833689	5.4654684949	C17	-1.4911745169	-0.8076994705	3.3353985470
C18	1.3491897310	0.2055658886	6.7382095375	C18	-1.1606197618	-1.9920174204	2.4420570330
C19	-0.3799617034	-0.3899294721	8.8431772490	P19	1.8563185322	1.7431321376	5.1720763824
C20	0.0081984877	0.6052606800	6.6831510366	C20	2.7447039747	0.9156714545	6.5317200839
C21	1.8125763046	-0.4998938348	7.8531727420	C21	4.0696000791	-0.3799784672	8.6036640164
C22	0.9510347116	-0.7859702758	8.9067305908	C22	2.2381349362	-0.2854097192	7.0337356603
C23	-0.8538929818	0.2975955453	7.7281220505	C23	3.8978302383	1.4795404113	7.0858027909
H24	-0.3660381250	1.1835219490	5.8381010502	C24	4.5617690939	0.8290266001	8.1162969809
H25	2.8609408623	-0.788694136	7.9237035531	C25	2.9098436204	-0.9287053412	8.0696645978
H26	1.3343804949	-1.2998356054	9.7845644651	H26	1.3047529257	-0.6843532758	6.6333345029
H27	-1.8923728696	0.6190084863	7.6838138185	H27	4.2751107622	2.4361020891	6.7210638390
H28	-1.0505494081	-0.6059073311	9.6717152281	H28	5.4591890677	1.2678646115	8.5467753858
C29	2.1440896550	-0.1419071380	3.8973213159	H29	2.5197991458	-1.8662362078	8.4600470898
C30	1.6622285261	-1.3136474447	1.4263137393	H30	4.5904003653	-0.8885065335	9.4123499726
C31	0.8563997951	-0.5785251953	3.5737007376	C31	1.1374272507	3.2445948697	5.8801432758
C32	3.1994102399	-0.3101658008	2.9924130369	C32	-0.1741679534	5.4012774201	7.0359174658
C33	2.9457144526	-0.8911864919	1.7543928859	C33	1.7191639393	4.5112359092	5.8364803701
C34	0.6196546398	-1.1631686869	2.3368703454	C34	-0.0980181805	3.0529294914	6.5102776760
H35	0.0435640892	-0.4815371127	4.2915437644	C35	-0.7480641023	4.1343255951	7.0894854772
H36	4.2144005054	-0.0150874716	3.2779233667	C36	1.0564628809	5.5890137051	6.4137764271
H37	3.7630447463	-1.0282899479	1.0504134174	H37	2.6840108137	4.6663409597	5.3534616113
H38	-0.3804971954	-1.5087056092	2.0851406902	H38	-0.5531064859	2.0592806151	6.5440573356
H39	1.4725269869	-1.7755676813	0.4599892778	H39	-1.7129333632	3.9738586082	7.5663691420
Au40	4.9496802966	1.1353470301	6.0530718063	H40	1.5015210579	6.5806173612	6.3733476861
F41	5.8558493964	0.4340014336	4.2380216247	H41	-0.6901795847	6.2512379238	7.4769307087
C42	7.5471623661	1.6087650527	7.6270600569	Au42	0.0892169945	0.3783266409	4.0701378536
H43	6.9454281068	1.5827245759	8.5378699780	H43	-1.8470581095	-1.1334687817	4.3170483905
C44	6.7517222893	2.1574547921	6.4587388872	H44	-2.1812370911	-0.0903777793	2.8740043689
H45	7.2544495771	2.0270451078	5.4931362973	H45	-0.1796820759	-2.4218123685	2.6769776701
H46	6.4503507702	3.1999738394	6.6065666057	F46	-0.5759159464	-0.1469375373	6.0012015523
P47	2.7360443033	3.4744233898	6.6245245513	B47	-2.9382101826	0.1237654025	6.7688174099
C48	3.8700764129	4.7830140617	6.0975726260	O48	-2.4904397004	1.1442947034	7.5778860574
C49	5.7425240005	6.7611366982	5.5421948613	H49	-1.9773850893	0.8358544723	8.3283753719
C50	4.3812016450	5.5738562147	7.1338803389	O50	-2.9919010752	-1.1895977616	7.1488768437
C51	4.2990581698	4.9841600337	4.7859312578	H51	-2.5239653744	-1.3933596780	7.9606162794
C52	5.2351672642	5.9761575028	4.5126994387	C52	-3.6117282105	0.4999452132	5.4099730058
C53	5.3136384507	6.5617817910	6.8515334168	C53	-4.7792979423	1.1469545187	2.9397913987
H54	4.0625796090	5.3981008687	8.1634865417	C54	-3.3786474612	1.7400361119	4.8066071577
H55	3.9222076640	4.3727917793	3.9683616495	C55	-4.4475391754	-0.4098485126	4.7508853541
H56	5.5727836117	6.1293551817	3.4906483532	C56	-5.0351717513	-0.0881477075	3.5316441693
H57	5.7194037176	7.1635197288	7.6608539175	C57	-3.9463528769	2.0614278623	3.5776625408
H58	6.4824529824	7.5277025024	5.3245403584	H58	-2.7267239181	2.4598960946	5.3038360118
C59	1.2199742383	4.2916568601	7.1910819382	H59	-4.6275887147	-1.3870451974	5.2002338452
C60	-1.1930613991	5.4690342452	7.8990614428	H60	-5.6964142218	-0.8007864331	3.0389208787
C61	0.3865826384	3.6617495649	8.1173104623	H61	-3.7299423758	3.0190607691	3.1093227036
C62	0.8505435712	5.5159672098	6.6271247390	H62	-5.2239783830	1.3956851953	1.9775730559
C63	-0.3573862984	6.1019574738	6.9845275561	C63	3.1690250555	2.2523527903	3.9659371152
C64	-0.8226617594	4.2518611906	8.4615840521	H64	4.1679090953	2.3647466805	4.4059202800
H65	0.6943325848	2.7299045379	8.5880091089	H65	2.8683143516	3.2082859049	3.5115540815
H66	1.5085136500	6.0148092853	5.9164891533	P66	3.1474791382	0.9951212777	2.6124142753
H67	-0.6421813572	7.0583339663	6.5524411029	Au67	0.9673677847	1.3544070774	1.7365545613
H68	-1.4672566517	3.7649918661	9.1896991614	C68	1.9436131611	2.5570242706	-0.1829627974
H69	-2.1348381467	5.9335816685	8.1828100522	C69	-1.2785384523	1.9382803052	1.2343546321
Au70	3.8354970759	2.1382911545	8.2368027048	C70	3.4561040779	-0.5962485045	3.4274115384
C71	2.9133082826	3.2956475604	10.1967060342	C71	3.8550353437	-2.9945168228	4.7792378696
C72	2.1936434335	2.4710658583	5.1593682970	C72	2.5840173732	-1.6670344824	3.2284720530
H73	2.7890904262	2.7474819874	4.2797201984	C73	4.5527013065	-0.7426863336	4.2849124542
H74	1.1392820683	2.6778587987	4.9376391649	C74	4.7461812758	-1.9387970568	4.9610571740
C75	4.9372081514	0.3757462851	9.4465157476	C75	2.7791062827	-2.8649476420	3.9087700382
				H76	1.7475901031	-1.5557194993	2.5379349600
				H77	5.2500546520	0.0813549279	4.4356267149
				H78	5.5852739768	-2.0419893741	5.6452761721
				H79	2.0800227718	-3.6852677421	3.7670504589
				H80	4.0030092052	-3.9258595838	5.3213601138
				C81	4.6155707926	1.3148628280	1.5985842863
				C82	6.8735068027	1.7928290403	0.0418602824
				C83	4.9587016598	2.6239238991	1.2471216592
				C84	5.3940214139	0.2459383791	1.1469521697
				C85	6.5207955978	0.4885690696	0.3703521593
				C86	6.0909831654	2.8577226883	0.4796395757
				H87	4.3311666683	3.4593775264	1.5497491445
				H88	5.1269144481	-0.7767510066	1.4070771835
				H89	7.1248936368	-0.3464914148	0.0238204415
				H90	6.3558965035	3.8769587121	0.2103443596
				H91	7.7569027636	1.9807652981	-0.5637465916
14-Cl-dppm							
C1	6.8293465013	1.5298223908	9.4046796642				
H2	7.5536869435	0.7819299429	9.7383763477				
H3	5.9952093646	1.5401818990	10.1174647286				
C4	7.4333247119	2.9180545629	9.2312864880				
H5	7.4620664591	3.4771298481	10.1725253681				
H6	8.4601892573	2.8374221313	8.8496352749				
C7	6.5284355777	3.5514982699	8.1830349580				
H8	5.5820930689	3.8717652849	8.6461129047				
H9	6.9630952682	4.4248450947	7.6859466370				
N10	6.3337798052	1.2169109140	8.0540699660				
C11	6.2980701856	-0.0014501194	7.4602265004				
O12	6.2011090193	-0.1851671622	6.2632322433				
C13	6.4165090590	-1.2111610374	8.4068204400				
F14	6.0200157714	-2.3158146313	7.8092040029				
F15	5.7056100185	-1.0557164409	9.5283888018				
F16	7.7045613618	-1.3722320423	8.7696237416				
P17	-0.7923998382	0.1956425641	4.7805961931				
C18	-1.2701584448	-0.2000992518	6.4917385467				
C19	-1.8723598678	-0.8882903213	9.1307555601				
C20	-2.0779627509	0.6349535267	7.2737338721				
C21	-0.7612395721	-1.3756920958	7.0496066342				
C22	-1.0657012641	-1.7189355180	8.3610517082				
C23	-2.3769961266	0.2891529003	8.5858410487				
H24	-2.4698913695	1.5714705506	6.8784010849				
H25	-0.0892172399	-2.0045961732	6.4656980491				
H26	-0.6481352442	-2.6266550019	8.7883120697				
H27	-2.9975930814	0.9497197703	9.1869063006				
H28	-2.0974076873	-1.1499919844	10.1617519751				
C29	-2.2018855430	-0.2253113926	3.6991478875				
C30	-4.3260459359	-0.5645552531	1.9274217183				
C31	-3.5153665849	-0.2383593787	4.1749616732				
C32	-1.9564829301	-0.3975461475	2.3348102645				
C33	-3.0183654240	-0.5607927432	1.4522138437				
C34	-4.5724498609	-0.4081299817	3.2883656210				
H35	-3.7126168473	-0.1150296327	5.2392504955				
H36	-0.9294240260	-0.3980720814	1.9663081153				
H37	-2.8227498882	-0.6877082432	0.3901565302				
H38	-5.5937082635	-0.4151767484	3.6626520901				
H39	-5.1558302833	-0.6907105022	1.2358548891				
Au40	1.3725837759	-0.4772269175	4.1462432064				
C41	3.5645264026	-0.6964054308	3.3518022604				

C42	6.2522425903	2.4133975404	7.2011475056
H43	7.0506137854	2.3518225661	6.4419028161
C44	4.9082504026	2.5464773120	6.4860270700
P45	0.5776127109	2.8825589290	5.4942986013
C46	1.3896802243	3.6249556291	4.0358464181
C47	2.4474668556	4.5542875233	1.6323856671
C48	0.8904223248	4.7964690007	3.4583114746
C49	2.4267500881	2.9280977902	3.4147889108
C50	2.9447542193	3.3914070038	2.2088992414
C51	1.4219352311	5.2569855656	2.2611707970
H52	0.0943381652	5.3574993081	3.9457153623
H53	2.8334107504	2.0166913947	3.8562042661
H54	3.7490960997	2.8341860121	1.7334799590
H55	1.0346322380	6.1727740695	1.8193191581
H56	2.8606515689	4.9182144965	0.6942991526
C57	-0.1433358894	4.2579546687	6.4507128308
C58	-1.0825141400	6.4401478913	7.9220184271
C59	0.5585806049	4.7079144745	7.5728587479
C60	-1.3299099324	4.9021727013	6.0818837124
C61	-1.7958430153	5.9863809304	6.8164260674
C62	0.0923592353	5.7986872096	8.2989790795
H63	1.4659897247	4.1940046844	7.8903424302
H64	-1.8931044937	4.5705361162	5.2096431156
H65	-2.7173374753	6.4822699665	6.5195716243
H66	0.6501541003	6.1418511875	9.1670069301
H67	-1.4469615458	7.2907345169	8.4932511491
Au68	1.7786781448	1.3152174969	6.7698586137
C69	2.8344215033	-0.4357643589	7.9656437871
C70	-0.87299081158	2.0406337853	4.6889838334
H71	-0.8934701839	2.3022655720	3.6234182227
H72	-1.8173531522	2.3855624347	5.1260141193
B73	3.6906322143	2.5906021673	10.3329840564
F74	3.1763020918	3.2471140653	9.2730839287
O75	3.6311297142	1.2583778283	10.4547535338
H76	3.2963618097	0.7493256275	9.6915000380
O77	4.2935384296	3.3664722533	11.2728025535
H78	4.6223824287	2.8225213557	11.9936121533
C79	4.9424748490	6.1144954016	4.0837833014
C80	5.6977083164	5.0065995460	3.7088900486
C81	5.6659172152	3.8476255724	4.4745467086
C82	4.8907895247	3.7812193280	5.6348922360
C83	4.1419892295	4.8991868754	6.0038054631
C84	4.1593520140	6.0562552488	5.2312865219
H85	4.9584072288	7.0183093044	3.4774556584
H86	6.3032918476	5.0422545748	2.8047540555
H87	6.232555430	2.9677051896	4.1671210625
H88	3.5380341480	4.8535527291	6.9121204419
H89	3.5571700435	6.9141106368	5.5263840013
H90	4.1238630731	2.6099856644	7.2539814279
H91	4.7090931971	1.6456572618	5.8842908725

(II) MONOMETALLIC PATHWAY

1. Catalyst Au-Br

P(Ph) ₃ Au Br F TFA cycle				TS Br NMe ₃			
C1	-2.2891255999	1.6475205608	1.3292138361	C1	-0.6063749865	0.8431071224	0.0256210136
C2	-3.0073029574	2.2406883896	2.5329758694	C2	-2.0300447717	1.2634604676	0.4608314885
N3	-1.3084399722	0.7475521060	1.9463169067	N3	0.3030895289	0.5389375036	1.1230697026
C4	-3.0571870924	1.0832028707	3.5376682769	C4	-2.3278628102	1.1486318103	1.9527260353
C5	0.0277880463	0.8032672599	1.8209974271	C5	1.1271383925	1.3700517091	1.7656577378
C6	-2.0274891644	0.0475517090	3.0324722073	C6	-1.9368721674	-0.1071793489	2.6355227568
O7	0.8488957523	0.1431444701	2.4419467543	O7	1.9122528547	1.0012037020	2.6408388782
C8	0.5709167982	1.8012673342	0.7721545605	C8	1.1140025677	2.8520832472	1.3483186028
C9	-1.2370156721	-0.6521127083	4.1051455265	C9	-2.0531390010	-0.3030843652	3.9878262178
Au10	0.1435333931	0.5866043254	5.1267230113	Au10	0.0009959473	0.5856617359	4.7556500340
F11	1.8862302524	1.6772243230	0.6683431452	F11	1.8422067863	3.5863530491	2.1653409693
F12	0.3048701429	3.0632502331	1.1268509407	F12	-0.1228926676	3.3547655746	1.3093193520
F13	0.0451782410	1.5927212894	-0.4419591041	F13	1.6332751563	2.9569801467	0.1161019074
P14	1.7092819139	2.2251599134	6.1902210449	P14	1.8023105292	1.6408432871	5.9702670377
Br15	0.7783486968	-1.4955300239	6.4177802142	Br15	0.5167268365	-1.6297362526	5.8819461581
F16	-0.505314269	2.2782234725	4.1779190737	F16	-0.4777799806	2.3711928103	3.9645181652
H20	-2.9695630620	1.0402482871	0.7124162453	H17	-0.6596607283	-0.0813115836	-0.5652181752
H21	-1.8259409058	2.3906808964	0.6837906171	H18	-0.1742030563	1.5976088550	0.4935949011
H22	-2.3902437970	3.0466355580	2.9417740521	H19	-2.2108729776	2.3037095497	0.1721182899
H23	-3.9935421346	2.6377993248	2.2731696268	H20	-2.7576228893	0.6649368195	-0.1020564326
H25	-2.7897591255	1.4255824248	4.5422904735	H21	0.5648216572	-0.5098308972	1.2134241460
H26	-4.0496130479	0.6203649399	3.5894072030	H22	-1.8615950119	1.9700713222	2.5225248307
H27	-2.5867535299	-0.7638225835	2.5260811491	H23	-3.4091551353	1.2825530111	2.1161672139
H28	-0.6101519892	-1.4645151435	3.7340663959	H24	-1.5770280081	-0.9466489239	2.0325315680
H29	-1.9216335745	-1.0230200178	4.8761733805	H25	-1.9809136693	-1.3086895578	4.3975454847
C35	3.3348861308	5.1577094278	3.0454802019	H26	-2.6176045706	0.4290530767	4.5728796244
C36	3.0850203043	5.6063989013	4.3388355072	C27	3.1544948210	5.6579837397	4.3027930840
C37	2.5714838256	4.7322527644	5.2884683893	C28	1.8148060788	5.4481843330	4.6226408104
C38	2.3101074790	3.4032603623	4.9448792324	C29	1.3906662857	4.2034568971	5.0584658926
C39	2.5530301463	2.9571698521	3.6439988391	C30	2.3254491824	3.1654706295	5.1907381402
C40	3.0676818090	3.8377367465	2.6988954034	C31	3.6697649973	3.3717127237	4.8571188990
H41	3.7329005051	5.8441429081	2.3012295517	C32	4.0776618995	4.6227642170	4.4161773539
H42	3.2875888547	6.6406013794	4.6083899342	H33	3.4813875341	6.6368945597	3.9603887363
H43	2.3736449282	5.0805437404	6.3020442816	H34	1.0965497160	6.2573337878	4.5223096382
H44	2.3284245923	1.9268154125	3.3617326651	H35	0.3434798112	4.0214896335	5.2813414670
H45	3.2441440921	3.4897687605	1.6845267517	H36	4.3963430245	2.5704715822	4.9649676961
C42	-0.8470455262	4.7768822637	9.0499305018	H37	5.1221940796	4.7915273963	4.1681520569
C43	-1.3066169352	4.4405747795	7.7795747693	C38	0.2301838795	2.7427822450	10.1311384839
C44	-0.5236346295	3.6660524945	6.9338197158	C39	1.1738423876	3.5457707864	9.4978889099
C45	0.7350933120	3.2269987561	7.3639710412	C40	1.6196944991	3.2245806693	8.2234949409
C46	1.1972728555	3.5689489495	8.6358147141	C41	1.1208170055	2.0813566509	7.5822134337
C47	0.4028257708	4.3426404485	9.4758963177	C42	0.1766858864	1.2721016023	8.2234102864
H48	-1.4663910773	5.3798728789	9.7104722641	C43	-0.2662379017	1.6088117528	9.4956063973
H49	-2.2838531658	4.7824592557	7.4458066285	H44	-0.1217835127	3.0038007402	11.1260522540
H50	-0.8651158017	3.3966597252	5.9325406539	H45	1.5634658420	4.4296121957	9.9961501510
H51	2.1764818128	3.2313311261	8.9715436366	H46	2.3554802254	3.8571571875	7.7309273730
H52	0.7644057185	4.6071807398	10.4671167484	H47	-0.2037859010	0.3767962410	7.7342579053
C49	5.3972232226	0.8574530391	8.5864033278	H48	-1.0035138815	0.9827192879	9.9909428174
C50	5.5569844325	1.7774667177	7.5572066837	C49	5.3130287472	-1.2369822393	6.4301625039
C51	4.4563673855	2.1994659626	6.8192977915	C50	4.6781420241	-0.7399176965	7.5630230869
C52	3.1861790326	1.6960065768	7.1093833104	C51	3.6114301830	0.1401584111	7.4337408761
C53	3.0321063524	0.7595344133	8.1385012512	C52	3.1961537068	0.5277581162	6.1565680342
C54	4.1339768770	0.3491189965	8.8764067579	C53	3.8265542889	0.0223014231	5.0111590417
H55	6.2600033556	0.5305857401	9.1626348885	C54	4.8892928628	-0.8556905003	5.1583562153
H56	6.5432776258	2.1736154057	7.3264780502	H55	6.1434084503	-1.9305431679	6.5376999324
H57	4.5869937119	2.9234640032	6.0172280573	H56	5.0113929007	-1.0404549996	8.5525754918
H58	2.0465649732	0.3483321689	8.3547859872	H57	3.1075963427	0.5222111316	8.3194349899
H59	4.0066178563	-0.3771453993	9.6756227912	H58	3.4729496553	0.3109874021	4.0215233435
				H59	5.3879356619	-1.2508168417	4.2768662106
				N60	1.1099260608	-2.0145225908	1.0817132467
				C61	0.1895664341	-3.0207786757	0.5595609954
				C62	2.2412209252	-1.8286519475	0.1757306126
				C63	1.5783284777	-2.3915621898	2.4137678046
				H64	2.9044763204	-1.0537066896	0.5770207959
				H65	2.8200936410	-2.7590436193	0.0499064724
				H66	1.8825463766	-1.5049680654	-0.8087505589
				H67	-0.6727646054	-3.1260381440	1.2288753407
				H68	-0.1679651794	-2.7277561211	-0.4343426820
				H69	0.6730702968	-4.0093901956	0.4730915857
				H70	0.7217684231	-2.5334784924	3.0842730537
				H71	2.1633479309	-3.3268913483	2.3916592663
				H72	2.1956511611	-1.5838998155	2.8252423330
P P(Ph) ₃ AuBrFTFAB(OH) ₂ Ph TS							
C1	-3.0682231975	-3.5353174495	2.6343193263				
H2	-3.9421615905	-3.4449056149	3.2906610527				
H3	-2.9808152051	-4.5932016366	2.3534259274				
C4	-3.1041882909	-2.6022333592	1.4255127089				
H5	-3.5302354893	-3.0859840497	0.5416864825				
H6	-3.7154279534	-1.7159441185	1.6468014281				
C7	-1.6435420889	-2.1938689161	1.2426260094				
H8	-1.0722370543	-3.0047666573	0.7717133641				
H9	-1.5012945957	-1.2851961728	0.6493312723				
N10	-1.8495210730	-3.1352557647	3.3529584330				
C11	-1.4710195570	-3.8743389110	4.4170166032				
O12	-2.0832119875	-4.8415204219	4.8305621900				
C13	-0.1999073806	-3.4177492464	5.1654119228				
F14	0.8829865008	-3.3674254321	4.3685143410				
F15	0.0770023991	-4.2425820557	6.1593205855				
F16	-0.3745213124	-2.1941556642	5.6750253182				
C17	-1.6350459904	-0.6702587705	3.2592327306				
C18	-1.1708449671	-2.0062276566	2.6859867449				

P19	1.7496633266	1.8198721107	5.1697221102
C20	3.2946269546	2.2931710695	4.3411311014
C21	5.6110905696	3.1218927079	3.0347127074
C22	4.5469225677	2.0335672658	4.9031376249
C23	3.2092460751	2.9615121953	3.1145842023
C24	4.3655361584	3.3787187545	2.4690913079
C25	5.7010247884	2.4479876779	4.2472836716
H26	4.6191487765	1.5111584540	5.8556926721
H27	2.2342244233	3.1457656597	2.6640715089
H28	4.2941217517	3.8973088278	1.5161187948
H29	6.6741367064	2.2444287084	4.6881722408
H30	6.5158439744	3.4444860927	2.5243584860
C31	2.2365070891	0.7262329514	6.5379731522
C32	2.9685452586	-1.0468089342	8.5598475831
C33	2.3682954127	-0.6379884670	6.2645119893
C34	2.4722830901	1.1986933204	7.8294952711
C35	2.8406763745	0.3111813912	8.8355458277
C36	2.7310458225	-1.5215797070	7.2725426667
H37	2.1636353522	-1.0156879293	5.2613027287
H38	2.3627331248	2.2606041457	8.0474659146
H39	3.0235426871	0.6826615137	9.8414153186
H40	2.8106858633	-2.5842710746	7.0532532002
H41	3.2458994256	-1.7384925562	9.3519134729
C42	1.1061335152	3.3451848606	5.9236646112
C43	-0.0309761781	5.6287579774	7.0381426945
C44	1.8069717653	4.5526260333	5.9040227366
C45	-0.1655875612	3.2825998233	6.5062322433
C46	-0.7282243746	4.4236065094	7.0618268957
C47	1.2341714355	5.6906372531	6.4636625985
H48	2.7955973579	4.6069897706	5.4502082766
H49	-0.7119335616	2.3389212949	6.5125939234
H50	-1.7230245842	4.3604845163	7.4993505395
H51	1.7797052212	6.6315879136	6.4455406723
H52	-0.4762082859	6.5249385638	7.4651535795
Au53	-0.0597521916	0.5440415324	3.9699604528
H54	-2.2020870780	-0.7655225215	4.1902922525
H55	-2.1644799884	-0.0347884230	2.5407245642
H56	-0.0876549219	-2.1360684027	2.7636221992
F57	-0.8270211057	0.3798090860	5.8502617451
Br58	0.7893081285	0.6887777470	1.5947704911
B59	-3.2593206743	0.6954893464	6.1791405314
O60	-2.9123044606	1.5458260566	7.1983475101
H61	-2.4954140088	1.0980348932	7.9380089965
O62	-3.3659233395	-0.6675034217	6.2954192779
H63	-2.8129948594	-1.0492892673	6.9803403957
C64	-3.7262841469	1.3228903385	4.8230109131
C65	-4.4163255470	2.3841445200	2.3141875985
C66	-3.2196283671	2.5566183806	4.3978045168
C67	-4.5947108940	0.6376323360	3.9645366631
C68	-4.9478407596	1.1649185769	2.7275191851
C69	-3.5479387397	3.0785797436	3.1496789410
H70	-2.5439985861	3.1082467600	5.0528910257
H71	-4.9870360107	-0.3317488889	4.2738685400
H72	-5.6341103598	0.6232175959	2.0784358457
H73	-3.1293264312	4.0308120595	2.8299121880
H74	-4.6801448648	2.7929103329	1.3407610976

2. Catalyst Au-Cl

P(Ph)3Au Cl F TFA cycle				TS Cl NMe3			
C1	-3.1058154103	1.5718077709	2.1664647684	C1	-0.5456526611	0.8282518559	-0.0229679081
C2	-3.7830794556	1.1328974994	3.4510603341	C2	-2.0102924791	1.0578488808	0.4249626517
N3	-1.7475648742	1.0552894797	2.3099425396	N3	0.3997967692	0.6074864204	1.0619714659
C4	-3.1376745563	-0.2232218217	3.7503351931	C4	-2.2579720477	1.1095886950	1.9285868285
C5	-0.5989618137	1.7438276262	2.2417908289	C5	1.149897101	1.4764420239	1.7443462159
C6	-1.8607372485	-0.3019438359	2.8845218327	C6	-1.9029775971	-0.1031727555	2.7134190347
O7	0.5164302581	1.2652958923	2.2383038281	O7	1.9068010199	1.1469099558	2.6552418887
C8	-0.7025177346	3.2911136403	2.1997389905	C8	1.0758998697	2.9497566490	1.3055142072
C9	-0.6663098188	-0.8939067097	3.5907421157	C9	-2.1748946521	-0.2494428154	4.0439067788
Au10	0.3175751041	0.3666365456	4.9789727363	Au10	-0.0330675801	0.6463370459	4.7309526337
F11	0.4858958089	3.8209106638	2.4374514911	F11	1.7358376600	3.7284593313	2.1377066763
F12	-1.5479702601	3.7952573052	3.1081677180	F12	-0.1869053027	3.3807380245	1.2229521440
F13	-1.1196254153	3.7097539054	0.9973440029	F13	1.6238032938	3.0701210689	0.0894862090
P14	1.6745591260	2.0986814384	6.1890617310	P14	1.8004787697	1.6321402100	5.9532426198
C15	2.0069714908	-1.2469550639	5.0770612235	C15	0.4401512224	-1.4165495744	5.7410104768
F16	-1.2053049208	1.6993797841	4.9549069410	F16	-0.4701015186	2.4289249529	3.9391444752
H20	-3.5581008292	1.0797332650	1.2920931163	H17	-0.4809759230	-0.0718044419	-0.6468656691
H21	-3.1252825188	2.6437436921	1.9885940588	H18	-0.2021280192	1.6566277890	-0.6486403448
H22	-3.5319070549	1.8417616819	4.2434819164	H19	-2.3640820635	2.0058900911	0.0055099027
H23	-4.8697976118	1.0785215785	3.3494911044	H20	-2.6442180170	0.2784801070	-0.0173089328
H25	-2.8780814405	-0.3055736813	4.8083789525	H21	0.5847679010	-0.3889612084	1.2846855653
H26	-3.8012149539	-1.0575301532	3.5008483947	H22	-1.7291244000	1.9576377912	2.3941488844
H27	-2.0580107075	-0.9848848755	2.0379528366	H23	-3.3224779556	1.3229937944	2.1069017946
H28	0.1482182219	-1.1541858639	2.9156401788	H24	-1.4140213808	-0.9389797950	2.2000285892
H29	-0.9793078702	-1.7781188620	4.1543914876	H25	-2.0510842591	-1.2129759516	4.5336399618
C35	3.9549810637	4.2950686687	2.8543406517	H26	-2.7734943636	0.5040088696	4.5604586391
C36	3.5593435986	5.0000425885	3.9836682688	C27	3.1770114764	5.6704831222	4.3757153063
C37	2.8794699839	4.3537773017	5.0027845203	C28	1.8387175746	5.4699925353	4.7073861547
C38	2.5966183416	2.9916735155	4.8958792444	C29	1.4038761105	4.2194436599	5.1146126848
C39	2.9967807574	2.2886116991	3.7618015004	C30	2.3279584378	3.1682862212	5.2086317166
C40	3.6749387429	2.9422901240	2.7451309373	C31	3.6697418196	3.3636889863	4.8592730703
H41	4.4752333916	4.8074937806	2.0511446401	C32	4.0877957264	4.6204006945	4.4459501917
H42	3.7740487739	6.0606670040	4.0665636000	H33	3.5123942493	6.6543877814	4.0565422873
H43	2.5541962947	4.9108747863	5.8775801996	H34	1.1299025096	6.2907363323	4.6383070363
H44	2.7590251469	1.2345919858	3.6562165829	H35	0.3569902698	4.0457714277	5.3469868525
H45	3.9633161219	2.3918318091	1.8561362539	H36	4.3851156080	2.5482957006	4.9328035450
C42	-0.7983770313	5.3675669585	8.2654679745	H37	5.1305640015	4.7821643776	4.1861493755
C43	-0.9768958401	5.0848542326	6.9172259191	C38	0.2554875469	2.5414580050	10.1687414373
C44	-0.2275775165	4.0937216159	6.3086815089	C39	1.1133248558	3.3410081611	9.5298961028
C45	0.7197215981	3.3844430304	7.0503268743	C40	1.5503454857	3.1727323707	8.2375488206
C46	0.8989659990	3.6698181795	8.4010974273	C41	1.1283411211	2.0060612831	7.5840203296
C47	0.1366212158	4.6603899230	9.0050675768	C42	0.2700429555	1.1085272001	8.2314891010
H48	-1.3921016848	6.1423661511	8.7403700478	C43	-0.1633302041	1.3826568393	9.5209732972
				H44	-0.0891159723	2.7524992991	11.1780470577
				H45	1.4442495366	4.3330919965	10.0380324921

H49	-1.7099617017	5.6335724563	6.3346743367	H46	2.2221322561	3.8711825084	7.7432870086
H50	-0.3803923182	3.8618602713	5.2611941264	H47	-0.0468146973	0.1937710797	7.7332253386
H51	1.6370189117	3.1245841744	8.9830986900	H48	-0.8319008080	0.6875288115	10.0217516850
H52	0.2792292619	4.8816323400	10.0579330044	C49	5.2566427895	-1.3278037891	6.3012058696
C49	4.6380252263	0.5929348403	9.3519928532	C50	4.6451759999	-0.8414325458	7.4514597790
C50	5.0177265416	1.6268419648	8.5085505617	C51	3.5898469232	0.0558434057	7.3530920799
C51	4.1466310246	2.0821105908	7.5300163251	C52	3.1624171298	0.4740168216	6.0886906692
C52	2.8912125217	1.4971280068	7.3947164763	C53	3.7690479675	-0.0214391142	4.9257463244
C53	2.5182060294	0.4491781032	8.2337650615	C54	4.8193756111	-0.9190169657	5.0426949782
C54	3.3887903952	0.0033999789	9.2145953976	H55	6.0784340892	-2.0348985205	6.3846881749
H55	5.3230304329	0.2377732557	10.1153226008	H56	4.9877156184	-1.1639974971	8.4310241938
H56	5.9981063622	2.0808596974	8.6109648945	H57	3.1074184790	0.4301620112	8.2535250374
H57	4.4448842849	2.8896755504	6.8669900699	H58	3.4090238674	0.2905879320	3.9460035268
H58	1.5470312625	-0.0237509955	8.1087273831	H59	5.2973760124	-1.3071282462	4.1466514338
H59	3.0966819164	-0.8144027088	9.8650071224	N60	1.0499865798	-2.1877101915	1.2103856012
				C61	0.2186113141	-3.2251226429	0.6170133795
				C62	2.2603324320	-1.9819550249	0.4245794629
				C63	1.3941065139	-2.5227529713	2.5852211409
				H64	2.8568232473	-1.1768251178	0.8725300673
				H65	2.8838942468	-2.8933508257	0.3779482762
				H66	1.9997750039	-1.6896891298	-0.5999837390
				H67	-0.7049960214	-3.3461761810	1.1955139799
				H68	-0.0482623786	-2.9533893625	-0.4109469931
				H69	0.7338028004	-4.2030369057	0.5898744621
				H70	0.4837506545	-2.6895688467	3.1738198825
				H71	2.0174884692	-3.4336710345	2.6493383985
				H72	1.9410283597	-1.6878955609	3.0440179193
P(Ph)3AuCl F TFA B(OH)2Ph							
C1	-3.1374920777	-3.3963748049	2.5052508461				
H2	-4.0108656879	-3.3119432646	3.1630046709				
H3	-3.0769963833	-4.4435504685	2.1793161865				
C4	-3.1434788206	-2.4129319407	1.3369429648				
H5	-3.5929977377	-2.8420487487	0.4365703201				
H6	-3.7187726390	-1.5140210109	1.6010410081				
C7	-1.6682994071	-2.0550062595	1.1637951950				
H8	-1.1305403724	-2.8700692144	0.6617955902				
H9	-1.4911119217	-1.1311275798	0.6043678330				
N10	-1.9118741995	-3.0583169173	3.2430669157				
C11	-1.5827399912	-3.8205662996	4.3064833505				
O12	-2.2420886916	-4.7631052508	4.7038080462				
C13	-0.2971110974	-3.4328962156	5.0684222956				
F14	0.7892939467	-3.4210185584	4.2766400257				
F15	-0.0629918603	-4.2822539399	6.0530347488				
F16	-0.4162830770	-2.2087505528	5.5962869674				
C17	-1.5939631319	-0.6056875211	3.2315019348				
C18	-1.1867864375	-1.9374174463	2.6109185525				
P19	1.8146705459	1.8168813345	5.1799164066				
C20	3.3711246154	2.2878985850	4.3740461588				
C21	5.6968235492	3.0879041140	3.0715083743				
C22	4.6125889528	2.1105085556	4.9887311597				
C23	3.2997546771	2.8538751171	3.0967963603				
C24	4.4616530991	3.2582061138	2.4527388961				
C25	5.7721434161	2.5117775485	4.3350348432				
H26	4.6719042077	1.6632194553	5.9797664645				
H27	2.3328990991	2.9634366211	2.6057225957				
H28	4.4034480123	3.6979362791	1.4599654020				
H29	6.7380115689	2.3738983679	4.8158295939				
H30	6.6061627716	3.4003248036	2.5628269350				
C31	2.2657516181	0.7707101085	6.5951728193				
C32	2.9329435192	-0.9225311199	8.7026125965				
C33	2.2836022666	-0.6133323305	6.4068531465				
C34	2.5799039337	1.3036353143	7.8468723142				
C35	2.9166797840	0.4555315464	8.8962001368				
C36	2.6154649991	-1.4574803744	7.4578538600				
H37	2.0138676752	-1.0362705817	5.4384876898				
H38	2.5521634892	2.3825063208	7.9999606228				
H39	3.1602700739	0.8722737934	9.8710818508				
H40	2.6083028518	-2.5347140564	7.3058931660				
H41	3.1864784378	-1.5830369839	9.5288562690				
C42	1.1350711080	3.3514945515	5.8873687937				
C43	-0.0232275658	5.6375881583	6.9764467381				
C44	1.8245557545	4.5652741381	5.8554179654				
C45	-0.1391002107	3.2849644091	6.4657445030				
C46	-0.7113939519	4.4273794786	7.0085797749				
C47	1.2413019825	5.7046164939	6.4017712920				
H48	2.8144900716	4.6224296670	5.4046875975				
H49	-0.6787918452	2.3374254705	6.4793598386				
H50	-1.7049778231	4.3614463383	7.4483846783				
H51	1.7795362396	6.6496560092	6.3760284576				
H52	-0.4752435228	6.5331159649	7.3976033669				
Au53	0.0232077717	0.5337401787	3.9553023335				
H54	-2.1649350631	-0.7089939329	4.1583057329				
H55	-2.0971884199	0.0752232917	2.5355371274				
H56	-0.1092177830	-2.1119106905	2.6806940800				
F57	-0.7636843857	0.3865997349	5.8143612524				
Ci58	0.8501222426	0.6278455797	1.7662341944				
B59	-3.2274801504	0.5603629542	6.1904075864				
O60	-2.8839972237	1.4216325470	7.2012003495				
H61	-2.3944714200	0.9966097378	7.9098076110				
O62	-3.2624215260	-0.8058575575	6.2967919862				
H63	-2.7386355219	-1.1671842503	7.0156599876				
C64	-3.7665229675	1.1713697388	4.8536049339				
C65	-4.6171431092	2.2376390990	2.3946651978				
C66	-3.3413040568	2.4354922800	4.4301241404				
C67	-4.6326948198	0.4555705601	4.0185971465				
C68	-5.0636423088	0.9833117155	2.8062445015				
C69	-3.7485882514	2.9607977174	3.2067961838				
H70	-2.6666429287	3.0089476104	5.0676126608				
H71	-4.9616606160	-0.5376277054	4.3259238116				
H72	-5.7484636421	0.4165763912	2.1769745063				
H73	-3.3950150763	3.9400102967	2.8894866215				
H74	-4.9453049725	2.6495757876	1.4423203192				

Theoretical Method Validation

Calculation of redox potentials at the M06/LACV3P**++(2f)

REDOX POTENTIAL VALIDATION	E _{SCF} (Ha)	V _{solv} (Kcal)	H _{tot} (Kcal)	ZPE (Kcal)	Stot (Kcal)	G (Kcal)	ΔG _{red}	E absolute - ΔG/nF	E (vs FeCp ₂)	ΔE (V)
19 Au(I)	- 2400.53 3307	- 19.7795	17.8 72	236. 732	200. 843	- 150618 2.75				
20 Au(I)	- 4298.73 9951	- 24.9591	29.7 24	341. 403	301. 535	- 269724 4.32				
19 Au(III)	- 2399.83 3381	- 140.234 9	18.3 07	235. 832	198. 761	- 150586 3.84	- 318. 91	6.91	2.07	
20 Au(III)	- 4298.09 6754	- 123.938 3	28.7 57	340. 375	287. 338	- 269693 7.45	- 306. 87	6.65	1.81	- 0.26
FeCp ₂	- 510.337 016	-3.742	6.19 2	105. 979	93.3 63	- 320160. 78	- 111. 62	4.84		
FeCp ₂ ⁺	- 510.091 2334	- 45.1975	6.19 2	104. 826	93.3 63	- 320049. 16				

The redox potentials were calculated using an explicit molecule of CH₂Cl₂ for the Au complexes for the first layer of solvation and implicit CH₂Cl₂ solvation beyond that. The redox potentials correlate well with the experimental values of 1.96 V (2.07 V predicted) for **19**, and 1.64 V (1.81 V predicted) for **20**.