Bond Dissociation Energies of Carbonyl Gold Complexes: a New Descriptor of Ligand Effects in Gold(I) Complexes?

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Abstract:

Ligand electronic effects in gold(I) chemistry have been evaluated by means of the experimental determination of M-CO bond dissociation energies for 16 $[L\text{-}Au\text{-}CO]^+$ complexes, bearing L ligands widely used in gold catalysis. Energy-resolved analyzes have been achieved using tandem mass spectrometry with collision induced dissociation. Coupled to DFT calculations, this approach enables the quantification of ligand effects based on the LAu-CO bond strength. Further energy decomposition analysis gives access to detailed insights of this bond's properties. Whereas small differences are observed between phosphine- and phosphite-containing gold complexes, carbene ligands are shown to stabilize much more efficiently the gold-carbonyl bond.

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Experimental Procedures

1. Mass spectrometry

1.1. Experimental procedure

[LAuCl] complexes (L = tBu$_3$P, Cy$_3$P, iPr$_3$P, Et$_3$P, Me$_3$P, Me$_2$PhP, MePh$_2$P, Ph$_3$P) and AgOTf were purchased from Sigma-Aldrich or synthesized by addition of 1 equivalent of L (L = pOMe, pCF$_3$, biPh, OMe, OPh, OtBuPh) to a CH_2Cl_2 solution of (SMe_2)AuCl. IPr-Au-Cl and MIC-Au-Cl were prepared according to the procedures described by Nolan and Bertrand, respectively.[1,2]

Solutions of LAuCl (1 mg/mL, MeOH) and AgOTf (1 mg/mL, CH_2Cl_2) were freshly prepared and mixed before injection (1:1 v:v in MeOH) with a 10 µg/mL concentration.
$[LAu]^+$ ions were formed in the Z-spray ESI source of a homemade modified Quattro II triple quadrupole (Micromass, Manchester, UK) with a flow rate of 200 µL/hr, capillary voltage 3.5 kV, cone voltage 25-40 V, extractor 5 V, source block/drying gas temperature 100/100 °C. Subsequently, $[LAuCO]^+$ complexes were formed in the transfer hexapole H0 by reaction with carbon monoxide that was introduced at a pressure of $1x10^{-4}$ mbar. Complexes of various $[LAuCO]^+$ species were selected in the first quadrupole Q1 and then collided with Argon in the collision hexapole H2 at a pressure of $1x10^{-3}$ mbar. The collision energy was varied from 1 to 30 eV (laboratory frame, E_{lab}) and the product ion spectra were obtained by scanning Q3 between *m/z* 250 and 900. In order to allow for the complete transmission of fragment ions, voltages of 175 V and 50 V were applied to 2 lenses located after H2.

1.2. Threshold Collision Induced Dissociation (Threshold-CID)

As outlined in the manuscript, threshold collision induced dissociation (TCID) experiment is usually the method of choice to measure BDEs. In this work, we were not able to use this technique because of the presence of an isobaric $[LAuN_2]^+$ ion. When no carbon monoxide is added in H0, a small signal corresponding to a $[LAuN_2]^+$ ion is indeed observed. The energy dissociation threshold of this ion is much lower than that of $[LAuCO]^+$ which hinders the TCID analysis for $[LAuCO]^+$.(Figure S1).

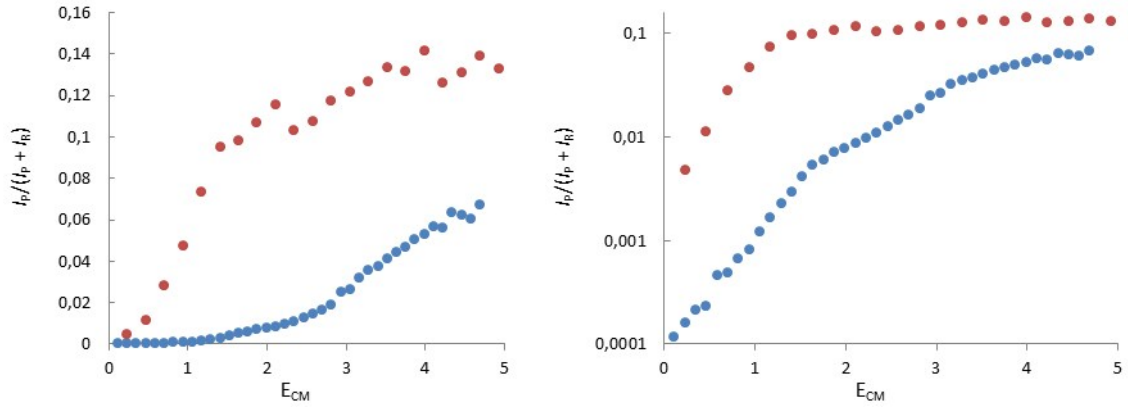

Figure S1. Threshold CID of $[PMe_3AuCO]^+$ and $[PMe_3AuN_2]^+$; Product ion abundance (I_P) of $[Me_3PAu]^+$ relative to the reactant ion abundance (I_R) of $[Me_3PAuCO]^+$ + $[Me_3PAuN_2]^+$ mixture (blue dots) and $[Me_3PAuN_2]^+$ (red dots) after collision with argon (P = $1x10^{-4}$ mbar) as a function of center-of-mass energy E_{CM}. Normal (left) and logarithmic (right) scales are shown.

TCID experiments were also performed on isotope labelled $[LAu\text{-}^{13}CO]^+$ complexes by addition of ^{13}CO in H0. The selected $[LAu\text{-}^{13}CO]^+$ is then subjected to dissociation (Figure S2). The loss of 29 Dalton confirms the dissociation of carbon(13) monoxide. However, from those new TCID experiments we were not able to extract critical energy due to a dissociation of a highly fragile isomass complex in the threshold region. As the dissociation of $[LAuN_2]^+$ (loss of 28 Dalton) cannot be incriminated anymore, the formation of a complex that has coordinated carbon monoxide with oxygen can be considered ($[LAu\text{-}OC]^+$). The fragile nature of this type of complex results in low calculated BDE. For example, the complex $[IPrAu\text{-}OC]^+$ (12.0 kcal/mol, see table XY) is fragile enough to explain the interference of experiments at the threshold region.

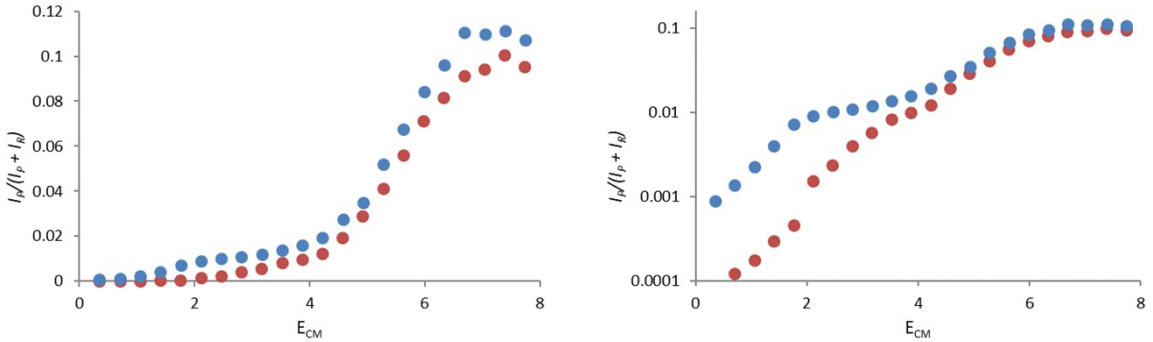

Figure S2. Threshold CID of $[IPrAuCO]^+$ and $[IPrAuN_2]^+$; Product ion abundance (I_P) of $[IPrAu]^+$ relative to the reactant ion abundance (I_R) of $[IPrAuCO]^+$ + $[IPrAuN_2]^+$ mixture (from ion m/z = 613 loss of 28 Dalton; blue dots) and $[IPrAu^{13}CO]^+$ (from ion m/z = 614 loss of 29 Dalton red dots) after collision with xenon (P = $5x10^{-5}$ mbar) as a function of center-of-mass energy E_{CM}. Normal (left) and logarithmic (right) scales are shown.

1.3. RRKM modeling

The Masskinetics software was used to perform the kinetic modelling. All theoretical data used for the simulations (reference BDE and vibrational frequencies) were obtained at the PBE0-D3/def2-TZVP level of theory.

Vibrational frequencies of the transition state were defined as follow: the reaction coordinate corresponding to the Au-C bond at 345 cm^{-1} was removed from vibrational frequencies of the initial state and the 5th frequencies principally impacted by the Au-C dissociation were modified as follows: 40→10, 40→10, 340→68, 340→68, 2305→2240 cm^{-1}.[3]

Mass spectrometer modeling employed an ion population at a temperature, T_{char}. Following previous work, a decomposition time of 2 ms was applied in the mass spectrometer in the modelling.[4]

Table S1: Molecular parameters used for the $[LAuCO]^+$complexes and calibrations values obtained from Figure 1b

	L	DOF[a]	M_R[b]	$S_{<Eint>/ECM}$[c]	$<E_{int\ 0V}>$[d]	$T_{char\ 0V}$[e]	BDE[f]
1-*t*Bu	tBu_3P	123	427	1.9093	1.1409	447	33.5
2-Cy	Cy_3P	159	505	2.6225	1.4380	472	33.4
3-*i*Pr	iPr_3P	96	387	1.6756	1.1858	515	33.7
4-Et	Et_3P	69	345	1.4427	1.0554	573	34.3
5-Me	Me_3P	42	303	1.0234	0.8363	639	35.6
6-Me_2Ph	$(Me_2Ph)P$	62	363	1.4600	0.9986	568	34.7
7-$MePh_2$	$(MePh_2)P$	84	425	1.9833	1.1187	532	34.3
8-Ph	Ph_3P	105	487	2.6657	1.3496	513	33.7
9-*p*OMe	$(p\text{-}OMe\text{-}C_6H_4)_3P$	141	577	3.5792	1.5839	468	31.8
10-*p*CF3	$(p\text{-}CF_3\text{-}C_6H_4)_3P$	132	691	3.8996	1.6842	458	35.1
11-biPh	JohnPhos	147	523	2.5010	1.5705	476	31.9
12-OMe	$(OMe)_3P$	51	351	1.4643	1.0960	640	35.7
13-OPh	$(OPh)_3P$	114	535	2.9963	1.4987	507	35.7
14-O*t*BuPh	$(O\text{-}(2,4\text{-}tBu\text{-}C_6H_3))_3P$	330	871	4.9561	2.9631	434	35.4
15-IPr	IPr	198	613	3.4617	2.3574	510	43.6
16-MIC	MIC	225	690	4.1894	2.6088	500	42.9

[a] DOF = Number of degrees of freedom. [b] M_R = Mass of the reactant (Da). [c] $S_{<Eint>/ECM}$ = slope of the calibration line. [d] $<E_{int\ 0V}>$ = initial mean internal energy prior to decomposition at 0V (eV). [e] $T_{char\ 0V}$ = characteristic temperature at 0 eV (K). [f] BDE = bond dissociation energy at PBE0-D3BJ/def2-TZVP level (kcal/mol)

1.4. Calculation of the uncertainties

Uncertainties on critical energies were estimated by variating the parameters that influence the relative difference between these critical energies. i) The 4th frequencies the most impacted by the Au-C dissociation were varied by a factor of 2.5 that corresponds to an Arrhenius pre-exponential factor varying from 14.7 to 16.5. ii) A shift of E_{lab} = ± 2 eV of the collision energy was estimated in order to take into account an uncertainty on the initial internal energy distribution deposited. iii) The decomposition time was varied from 0.4 ms to 10 ms.

1.5. Truncated Maxwell-Boltzmann internal energy distribution model

Using the model based on a fast activation process and a slower kinetics of dissociation, the calculated Maxwell-Boltzmann initial internal energy distribution prior to fragmentation (Figure S3, blue line, t = 0 ms) is characterized by a characteristic temperature (T_{char})[5] and a corresponding mean internal energy (<E_{int}>). The truncated internal energy distribution corresponds to the dissociation of the population of higher energy after a fixed time of decomposition (Figure S2, orange line, t = 2 ms). If the initial population of the precursor ion is normalized to 1, the surviving ion population corresponds to the survival yield.

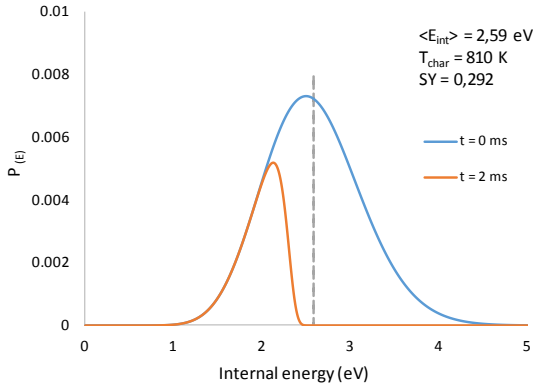

Figure S3: Truncated Maxwell-Boltzmann internal energy distribution model results: initial internal energy distribution of the precursor ions before fragmentation at t = 0 ms (blue curve); internal energy distribution of surviving precursor ions after 2 ms decomposition (orange curve). These curves correspond to the [*i*Pr$_3$PAuCO]$^+$ complex for E_{lab} = 9 eV. The mean internal energy <E_{int}>, characteristic temperature T_{char} and survival yield (SY) are also reported.

2. Computational details

2.1. Choice of the method

The PBE0[6] functionnal coupled to the def2-TZVP[7] basis set was chosen following the benchmark calculations of Yao and collaborators[8] which have shown that the accuracy of this method was similar to that of with B2PLYP but at a lower computer time.

To estimate the efficiency of the theoretical level to describe correctly a phosphine-gold-carbonyl complex, we have optimized the geometry of the $[(PMes_3)AuCO]^+$ complex[9] (a rare example of phosphine-gold-carbonyl complex characterized by X-ray), using PBE0/def2-TZVP, PBE0-D3[10]/def2-TZVP, PBE0-D3BJ[11]/def2-TZVP, and compared results with theoretical data obtained at BP86/def2-TZVP level used by authors in ref 9, for comparison with X-ray data (Table S2). DFT calculations have been performed with Gaussian09 package.[12]

For DLPNO-CCSD(T) calculation the DLPNO settings (TCutPairs = 10^{-4}, TCutPNO = 3.33×10^{-7}, TCutMKN = 10^{-3}) were used as recommended by ORCA manual.[13]

Table S2. Selected bond distances (Å) of $[(PMes_3)AuCO]^+$ ion. Italic numbers indicate deviation from X-ray data (Å)

	P-Au	Au-(CO)	AuC-O
X-ray	2.338	2.008	1.108
BP86/TZVP	2.390 *0.052*	1.970 *-0.038*	1.136 *0.028*
PBE0/def2-TZVP	2.375 *0.037*	1.975 *0.033*	1.119 *0.011*
PBE0-D3/def2-TZVP	2.370 *0.032*	1.973 *-0.035*	1.119 *0.011*
PBE0-D3BJ/def2-TZVP	2.364 *0.026*	1.974 *-0.034*	1.119 *0.011*

All the levels used overestimate the P-Au bond distance, the best value being obtained with PBE0-D3BJ corresponding to a lowest deviation of 0.026 Å. All the levels used underestimate the Au-(CO) bond distance, but the inclusion of the dispersion shorten the phosphorus-gold bond distance and results get closer to the experimental data. Finally, all the tested levels slightly overestimate the C-O bond distance. Thus, the best agreement between X-ray data and computed geometry is clearly obtained at the PBE0-D3BJ/def2-TZVP level. Because the PBE0 method seems to be efficient at modeling geometries such as those of L-Au-CO species, we wanted to test a more sensitive parameter, the computed bond dissociation energy of CO. To do this, we have optimized the geometry of the alkyl $[(PR_3)AuCO]^+$ complexes using the same different levels (Table S3). The same trends were observed between all tested functionals (Table S4). Finally, effect of dispersion was also tested on B2PLYP single-point energy calculations (Table S5).

Table S3 Selected bond distances (in Å) for the alkyl sets of complexes using different functionals with def2-TZVP basis set.

PBE0	Me	Et	*i*Pr	Cy	*t*Bu
P-Au	2.325	2.331	2.340	2.343	2.351
Au-(CO)	1.998	1.998	1.992	1.994	1.990
AuC-O	1.117	1.117	1.118	1.118	1.118
PBE0-D3	Me	Et	*i*Pr	Cy	*t*Bu
P-Au	2.322	2.326	2.340	2.338	2.344
Au-(CO)	1.998	1.998	1.994	1.991	1.990
AuC-O	1.117	1.117	1.118	1.118	1.118
PBE0-D3BJ	Me	Et	*i*Pr	Cy	*t*Bu
P-Au	2.320	2.325	2.332	2.335	2.342
Au-(CO)	1.998	1.997	1.994	1.991	1.990
AuC-O	1.117	1.117	1.118	1.118	1.118

BP86	Me	Et	iPr	Cy	tBu
P-Au	2.337	2.345	2.354	2.358	2.365
Au-(CO)	1.993	1.993	1.990	1.988	1.987
AuC-O	1.133	1.133	1.134	1.135	1.135

Table S4 Computed bond dissociation energy (in kcal/mol) including ZPE correction for the alkyl set of complexes

	Me	Et	*i*Pr	Cy	*t*Bu
BP86/def2-TZVP	34.9	33.2	32.3	31.4	31.8
PBE0/def2-TZVP	34.6	33.2	32.6	32.0	32.1
PBE0-D3/def2-TZVP	35.5	34.1	33.6	33.1	33.3
PBE0-D3BJ/def2-TZVP	35.6	34.3	33.7	33.4	33.5

Table S5 Bond dissociation energy (in kcal/mol) at the B2PLYP/def2-TZVP and B2PLYP-D3BJ level of calculations using the geometry optimized at the **level specified** in the table

B2PLYP	Me_3P	Et_3P	$\Delta(BDE)_{Me-Et}$
BP86/def2-TZVP	33.59	32.11	1.48
PBE0-D3BJ/def2-TZVP	33.63	32.13	1.50
B2PLYP-D3BJ	Me	Et	
BP86/def2-TZVP	34.58	33.13	1.45
PBE0-D3BJ/def2-TZVP	34.64	33.19	1.49

2.2. ETS-NOCV analysis

2.2.1. Orbital Interaction Energy Contributions from each NOCV pair

Table S6 Orbital Interaction Energy Contributions from each NOCV pair (in kcal/mol).

Complex [L-Au-CO]$^+$	ΔE_{orb1} (σ_1)	ΔE_{orb2} (π_1)	ΔE_{orb3}(π_2)	ΔE_{orb4} (σ_2)
1-*t*Bu	-32.0	-12.3	-12.3	-9.0
2-Cy	-31.8	-12.2	-12.3	-9.2
3-*i*Pr	-32.1	-11.9	-11.9	-8.7
4-Et	-32.3	-11.6	-11.6	-8.4
5-Me	-32.9	-11.4	-11.4	-8.1
6-Me_2Ph	-32.9	-11.8	-11.6	-8.6
7-$MePh_2$	-32.9	-12.0	-11.9	-9.0
8-Ph	-33.0	-12.2	-12.2	-9.5
9-*p*OMe	-33.3	-12.5	-12.4	-10.2
10-*p*CF_3	-33.4	-11.8	-11.8	-9.1
11-biPh	-32.4	-12.9	-12.9	-9.4
12-OMe	-32.9	-11.0	-11.0	-8.1
13-OPh	-32.6	-11.7	-11.7	-9.4
14-O*t*BuPh	-33.1	-12.5	-12.1	-10.1
15-IPr	-32.6	-13.6	-12.9	-7.3
16-MIC	-33.6	-15.1	-14.3	-8.1

*2.2.2. Particular case of tBu-JohnPhos (**11-biPh**)*

The first three NOCV components of the *t*Bu-JohnPhos (**11-biPh**) (figure S4) clearly show the participation of the biaryl group on the dissociation of the Au-CO bond; the biaryl substituent accumulates electron density on the σ_1 donation component whereas the two π back-donation components are depleted.

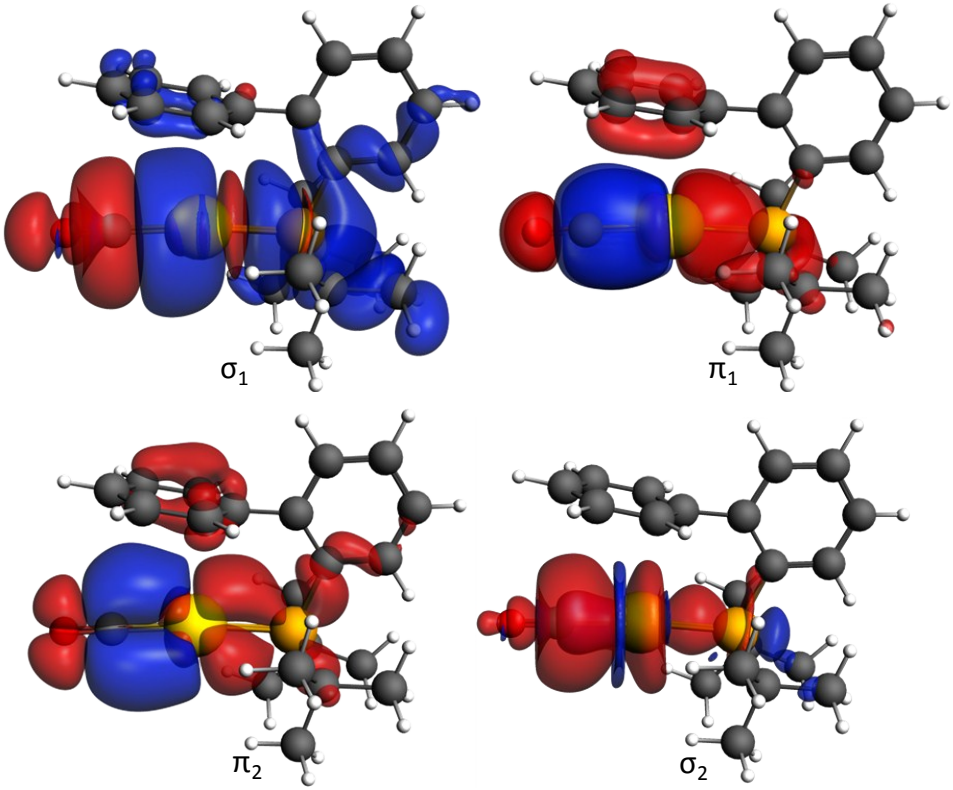

Figure S4 Electron density difference isosurfaces of the σ_1, π_1, π_2 and σ_2 NOCV components upon formation of the Au-CO bond for **11-biPh**: isodensity value ±0.0001 electron a.u.$^{-1}$. Blue isosurfaces identify regions in which the electron density is accumulated and red isosurfaces identify regions in which the electron density is depleted.

2.3. DLPNO-CCSD(T) calculations

Results are in very good agreement with PBE0D3BJ/def2TZVP calculations and confirm the use of the PBE0D3BJ/def2TZVP level of theory (Table S7, Figure S5).

Table S7 Single point energy calculation of the dissociation of CO at the DLPNO-CCSD(T)/CC-PVTZ-PP level on the PBE0D3BJ/def2TZVP optimized geometries

Complex [L-Au-CO]$^+$	ΔE	Complex [L-Au-CO]$^+$	ΔE
1-*t*Bu	32.2	**9-*p*OMe**	31.4
2-Cy	32.1	**10-*p*CF$_3$**	34.7
3-*i*Pr	32.9	**11-biPh**	31.5
4-Et	33.5	**12-OMe**	34.6
5-Me	34.9	**13-OPh**	35.6
6-Me$_2$Ph	34.1	**14-O*t*BuPh**	34.9
7-MePh$_2$	33.7	**15-IPr**	41.9
8-Ph	33.1	**16-MIC**	41.4

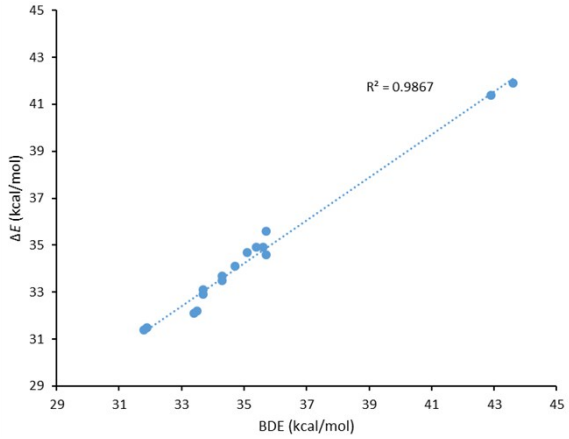

Figure S5. Correlation between ΔE calculated at the DLPNO-CCSD(T)/CC-PVTZ-PP level (Table S7) and BDE calculated at the PBE0D3BJ/def2TZVP level (Table S1).

2.4. Bond dissociation energy calculations on [LAu-N$_2$]$^+$ and [LAu-OC]$^+$

Geometrical optimizations and single point energy calculations were performed on 3 [LAu-N$_2$]$^+$ and 3 [LAu-OC]$^+$ complexes at the PBE0-D3BJ level of calculation with the def2-TZVP basis set. BDE are reported Table S8 and BDE of [LAu-CO]$^+$ were also added for comparison.

Table S8. Bond dissociation energy (in kcal/mol) of [LAu-CO]$^+$, [LAu-N$_2$]$^+$ and [LAu-OC]$^+$ at the PBE0-D3BJ level of calculation with the def2-TZVP basis set

Ligand	[L-Au-CO]$^+$	[L-Au-N$_2$]$^+$	[L-Au-OC]$^+$
PMe$_3$	35.6	18.3	9.8
PPh$_3$	33.7	16.2	7.9
IPr	43.6	23.5	12.0

The BDE of [LAu-N$_2$]$^+$ complexes are approximately the half of BDE obtained for [L-Au-CO]$^+$ complexes suggesting that back donation to N$_2$ is much more difficult than to CO. As expected, the Au-OC bond is even more unstable. The same trend are observed for BDE of [LAu-CO]$^+$, [LAu-N$_2$]$^+$ and [LAu-OC]$^+$ complexes following the same order of stability (IPr > PMe3 > PPh3).

2.5. PBE0D3BJ/def2TZVP optimized geometries

$[Me_3PAuCO]^+$

P	1.726348	0.000442	-0.000036
Au	-0.593682	-0.000699	0.000218
C	-2.591184	0.000262	-0.000403
O	-3.707792	0.002023	-0.000054
C	2.403329	1.652836	-0.260399
H	2.068735	2.321531	0.533664
H	3.494651	1.607362	-0.255791
H	2.064731	2.047370	-1.219196
C	2.407941	-0.599602	1.559325
H	3.499114	-0.577693	1.514562
H	2.069604	0.032182	2.381456
H	2.076698	-1.622658	1.741779
C	2.405995	-1.049963	-1.300400
H	3.497265	-1.020777	-1.262377
H	2.071199	-0.697925	-2.276919

$[Me_3PAu]^+$

P	-1.307841	0.000040	-0.000404
Au	0.930653	0.000025	0.000028
C	-1.950662	-1.486659	-0.781716
H	-3.043469	-1.451156	-0.763000
H	-1.608833	-1.544141	-1.815543
H	-1.609056	-2.370478	-0.242096
C	-1.951035	0.065882	1.677866
H	-3.043823	0.061077	1.637545
H	-1.607013	-0.799594	2.244958
H	-1.612101	0.976170	2.173380
C	-1.951116	1.420522	-0.895940
H	-1.609188	1.397035	-1.931130
H	-3.043928	1.386167	-0.874506
H	-1.609713	2.343863	-0.427056

$[Me_3PAuN_2]^+$

P	-1.434843	0.000195	-0.021776
Au	0.824711	-0.002009	0.153226
C	-2.234252	-0.195896	1.582393
H	-3.318881	-0.190983	1.451317
H	-1.931306	-1.139786	2.036922
H	-1.948504	0.622582	2.244099
C	-2.055832	1.536698	-0.731430
H	-3.145719	1.494019	-0.793915
H	-1.764342	2.380947	-0.105658
H	-1.643689	1.679035	-1.731042
C	-2.031352	-1.339677	-1.070045
H	-1.723563	-2.300936	-0.656989
H	-3.121991	-1.302703	-1.122119
H	-1.619616	-1.238828	-2.074873
N	2.919937	-0.004193	0.318078

$[Me_3PAuOC]^+$

P	0.010708	-0.004778	1.684552
Au	0.002524	0.004012	-0.553786
C	-0.002772	0.014835	-3.951936
O	-0.003676	0.013420	-2.819679
C	1.622626	-0.466364	2.342677
H	2.380317	0.240483	2.002949
H	1.583057	-0.456500	3.434672
H	1.891922	-1.466292	2.000953
C	-0.393747	1.616161	2.358020
H	-0.378668	1.568165	3.449584
H	0.336190	2.352398	2.019871
H	-1.386092	1.921363	2.024456
C	-1.188173	-1.171385	2.353163
H	-1.150025	-1.141642	3.444853
H	-2.192091	-0.905667	2.020496

$[Et_3PAuCO]^+$

P	1.437893	0.140136	-0.185511
Au	-0.878208	0.027934	-0.013242
C	-2.868863	-0.050647	0.129617
O	-3.982435	-0.093087	0.208056
C	2.236362	-0.017823	1.439452
H	1.846771	0.796614	2.055945
C	2.108679	-1.141480	-1.292234
H	3.166400	-1.256841	-1.033362
C	1.377880	-2.475887	-1.261261
H	1.364073	-2.918647	-0.265198
H	0.344465	-2.365677	-1.596375
H	1.868584	-3.182578	-1.931740
C	2.029130	-1.359172	2.126081
H	2.464333	-1.332364	3.125565
H	0.968965	-1.599963	2.232619
H	2.511067	-2.171725	1.581640
C	1.985038	1.732033	-0.872074
H	1.568500	1.793705	-1.881523
C	1.578857	2.938916	-0.040324
H	0.495251	2.990589	0.089683
H	2.040475	2.927843	0.947906
H	1.895666	3.855856	-0.538285
H	2.077850	-0.713763	-2.298776
H	3.073251	1.672817	-0.981005
H	3.301333	0.184351	1.281730

$[Et_3PAu]^+$

P	1.054626	0.223660	-0.228612
Au	-1.158197	-0.071100	0.012966
C	1.876632	0.138404	1.384056
H	1.432250	0.926395	1.997556
C	1.756569	-1.019284	-1.350510
H	2.830125	-1.041543	-1.128565
C	1.143885	-2.409674	-1.274336
H	1.209649	-2.838675	-0.274795
H	0.092591	-2.388927	-1.567038
H	1.667340	-3.077368	-1.959638
C	1.800485	-1.208796	2.084676
H	2.254226	-1.130629	3.073084
H	0.767471	-1.536477	2.218282
H	2.339606	-1.982217	1.537229
C	1.414164	1.850769	-0.938853
H	0.956554	1.863937	-1.931903
C	0.943067	3.026411	-0.097788
H	-0.135730	2.991044	0.068946
H	1.440082	3.060696	0.872390
H	1.168516	3.959598	-0.614650
H	1.650390	-0.605981	-2.357876
H	2.500462	1.876374	-1.088052
H	2.917596	0.429515	1.196653

$[i\text{Pr}_3PAuCO]^+$

P	-1.097188	0.041169	0.043504
Au	1.233803	0.061808	-0.017963
C	3.227725	0.085186	-0.037488
O	4.345320	0.098348	-0.043902
C	-1.826914	-0.377714	-1.598824
H	-1.962197	0.607673	-2.059391
C	-1.665892	-1.164264	1.301156
H	-2.754586	-1.210289	1.194685
C	-1.082270	-2.544581	1.022785
H	-1.326190	-2.914491	0.026461
H	0.006106	-2.537846	1.126364
H	-1.478207	-3.259827	1.746470
C	-1.322010	-0.687771	2.706656
H	-1.635522	-1.444433	3.428740
H	-0.244290	-0.546439	2.829043
H	-1.823104	0.244218	2.969933
C	-0.871056	-1.178157	-2.476444
H	-1.332138	-1.352242	-3.450985
H	0.069120	-0.649014	-2.644649
H	-0.640758	-2.153596	-2.043568
C	-3.190858	-1.052764	-1.495959
H	-3.623366	-1.127811	-2.495792
H	-3.109157	-2.067394	-1.102546
H	-3.895017	-0.500458	-0.874126
C	-1.704100	1.708470	0.519232
H	-1.263205	1.865934	1.509772
C	-1.154204	2.776217	-0.419312
H	-0.063117	2.760384	-0.470113
H	-1.544368	2.668288	-1.433752
H	-1.455646	3.762505	-0.061407
C	-3.221127	1.784605	0.633550
H	-3.698417	1.682254	-0.342714
H	-3.634661	1.027895	1.302473
H	-3.502207	2.762162	1.030703

$[i\text{Pr}_3PAu]^+$

P	-0.753135	0.022206	0.049752
Au	1.495667	0.121598	-0.041907
C	-1.459788	-0.429696	-1.588279
H	-1.636622	0.549769	-2.047428
C	-1.229674	-1.194974	1.326758
H	-2.319579	-1.272040	1.231907
C	-0.610026	-2.558988	1.047523
H	-0.850922	-2.940902	0.055140
H	0.477845	-2.519421	1.143940
H	-0.982432	-3.279063	1.778567
C	-0.883386	-0.694283	2.722803
H	-1.162295	-1.456814	3.452570
H	0.190511	-0.517439	2.826903
H	-1.412688	0.221674	2.986740
C	-0.490377	-1.200812	-2.476407
H	-0.966201	-1.394565	-3.439925
H	0.425871	-0.638644	-2.663641
H	-0.218844	-2.164774	-2.042801
C	-2.798078	-1.155203	-1.456848
H	-3.240660	-1.246563	-2.450743
H	-2.670121	-2.164979	-1.064535
H	-3.513515	-0.627857	-0.826386

C	-1.381052	1.676755	0.524268
H	-0.928418	1.849159	1.506451
C	-0.890046	2.758599	-0.429111
H	0.199165	2.783384	-0.498428
H	-1.295873	2.632526	-1.435073
H	-1.223793	3.732363	-0.065944
C	-2.900871	1.691774	0.664510
H	-3.391140	1.572254	-0.303151
H	-3.274641	0.923397	1.343251
H	-3.206498	2.660186	1.065653

$[Cy_3PAuCO]^+$

P	-0.523367	-0.035819	-0.137126
Au	1.791962	0.129794	-0.388177
C	3.767206	0.281227	-0.588053
O	4.876778	0.368308	-0.697240
C	-3.438109	2.716978	-1.358897
C	-2.793966	1.595350	-0.552752
C	-1.342971	1.375435	-0.986365
C	-0.527822	2.669820	-0.922714
C	-1.197670	3.772732	-1.730686
C	-2.630590	4.001863	-1.277114
H	-2.824328	1.853419	0.510718
H	-3.374553	0.678394	-0.672169
H	-3.520984	2.404820	-2.406566
H	-4.457757	2.877981	-1.000876
H	-0.419207	2.996583	0.115458
H	0.484181	2.490040	-1.300772
H	-0.614085	4.692357	-1.644014
H	-1.191367	3.496782	-2.791823
H	-2.631994	4.369852	-0.243903
H	-3.098296	4.780289	-1.884002
H	-1.348676	1.047413	-2.035511
C	-0.642495	-3.866189	-1.823942
C	-0.104698	-2.666749	-1.054604
C	-1.164748	-1.567812	-0.939610
C	-2.452802	-2.108129	-0.313296
C	-2.974484	-3.302931	-1.102415
C	-1.925921	-4.397785	-1.206519
H	0.209087	-2.984492	-0.054404
H	0.787759	-2.274177	-1.553238
H	-0.834558	-3.567978	-2.861479
H	0.120818	-4.647112	-1.860460
H	-2.254300	-2.424896	0.715389
H	-3.219756	-1.332997	-0.261380
H	3.881487	-3.682156	-0.625626
H	-3.263671	-2.974665	-2.107718
H	-1.713356	-4.794833	-0.206558
H	-2.308863	-5.233282	-1.796703
H	-1.398968	-1.228679	-1.957892
C	-0.571940	-1.268153	3.827452
C	-0.218736	-1.221748	2.346885
C	-0.931952	-0.061557	1.646589
C	-0.595178	1.261940	2.335386
C	-0.940041	1.208291	3.818263
C	-0.250764	0.047831	4.516148
H	0.865383	-1.085067	2.237506
H	-0.462379	-2.175823	1.875713
H	-1.640621	-1.488182	3.934794
H	-0.035588	-2.093371	4.302074
H	0.476706	1.466544	2.215087
H	-1.128523	2.090486	1.867421
H	-0.668161	2.157034	4.287063
H	-2.026311	1.107008	3.927534
H	0.834148	0.208233	4.505079
H	-0.547552	0.007881	5.566514
H	-2.015415	-0.222807	1.703030

$[Cy_3PAu]^+$

P	0.017072	0.286494	0.091149
Au	-0.026875	-0.930745	-1.809006
C	2.967468	2.957668	1.324558
C	1.796649	1.986420	1.425499
C	1.504684	1.355375	0.058824
C	2.745899	0.692323	-0.540935
C	3.896831	1.685173	-0.622376
C	4.201631	2.294646	0.736509
H	2.038423	1.200647	2.148904
H	0.916686	2.510720	1.804234
H	2.674673	3.807589	0.697064
H	3.181247	3.362451	2.316702
H	3.048577	-0.164124	0.067415
H	2.511730	0.302730	-1.536571
H	4.778740	1.182794	-1.026344
H	3.638745	2.481044	-1.331000
H	4.556084	1.511166	1.417145
H	5.012763	3.020987	0.650929
H	1.196159	2.156538	-0.627652
C	-3.736741	1.975375	-0.682708
C	-2.617186	0.943933	-0.698802
C	-1.441532	1.405166	0.166710
C	-1.900433	1.703168	1.599916
C	-3.016797	2.740759	1.591636
C	-4.188336	2.292222	0.733768
H	-2.993988	-0.015039	-0.327554
H	-2.278041	0.773291	-1.725123
H	-3.384209	2.893292	-1.167779
H	-4.573887	1.609028	-1.281390
H	-2.272323	0.784195	2.063092
H	-1.070329	2.054638	2.216154
H	-3.339311	2.925643	2.619141
H	-2.624413	3.691233	1.211666
H	-4.645643	1.400849	1.179596
H	-4.961740	3.063146	0.719269
H	-1.053806	2.336266	-0.268772
C	-1.271180	-2.737683	2.616112
C	-1.218248	-1.798779	1.418944
C	-0.001955	-0.871664	1.501136
C	1.290912	-1.677501	1.628710
C	1.222263	-2.628751	2.817304
C	0.011339	-3.543106	2.741676
H	-1.144977	-2.389567	0.497016
H	-2.145199	-1.226220	1.349347
H	-1.429122	-2.151536	3.529054
H	-2.135020	-3.399123	2.517162
H	1.447399	-2.250751	0.706341
H	2.150078	-1.014584	1.741061
H	2.144608	-3.212542	2.862345
H	1.179835	-2.042142	3.742559
H	0.108868	-4.208032	1.875087
H	-0.030386	-4.186658	3.623059
H	-0.106784	-0.224967	2.383206

$[t\mathrm{Bu}_3PAuCO]^+$

P	0.93196	0.00113	-0.00117
Au	-1.40975	-0.00298	0.00593
C	-3.39982	-0.00806	0.00837
O	-4.51805	-0.01111	0.00740
C	1.49153	1.10062	1.42870
C	1.48715	-1.78825	0.23709
C	1.48964	0.68773	-1.66870
C	0.60771	0.10180	-2.77697
H	0.67380	-0.97736	-2.87250
H	-0.44169	0.37351	-2.63720
H	0.93177	0.53581	-3.72659
C	1.26709	2.20036	-1.71112
H	1.93037	2.75232	-1.04882
H	1.47685	2.53411	-2.73043
H	0.23295	2.47135	-1.48828
C	2.95873	0.39281	-1.96912
H	3.15711	-0.67081	-2.08990
H	3.21608	0.87742	-2.91472
H	3.63138	0.78575	-1.20788
C	0.61053	2.35408	1.47457
H	0.93708	2.96283	2.32197
H	0.67458	2.97340	0.58516
H	-0.43860	2.09907	1.64474
C	2.96020	1.50729	1.32293
H	3.63237	0.65194	1.27277
H	3.15569	2.15037	0.46676
H	3.22129	2.07629	2.21916
C	1.26924	0.37909	2.75911
H	1.93557	-0.46827	2.90582
H	1.47578	1.09455	3.55916
H	0.23617	0.04663	2.88160
C	2.95626	-1.90608	0.63918
H	3.20931	-2.96812	0.69636
H	3.62990	-1.44963	-0.08488
H	3.15852	-1.47562	1.61856
C	1.25726	-2.57698	-1.05244
H	1.45561	-3.62956	-0.83531
H	0.22392	-2.50763	-1.39940
H	1.92427	-2.28384	-1.86031
C	0.60706	-2.45161	1.30206
H	0.92479	-3.49323	1.39747
H	0.68315	-1.99603	2.28427
H	-0.44463	-2.45934	1.00447

$[t\mathrm{Bu}_3PAu]^+$

P	0.00175	-0.00066	-1.13026
Au	-0.00771	-0.00178	1.13489
C	1.63063	-0.78775	-1.6563
C	-1.49499	-1.01652	-1.66197
C	-0.12802	1.80532	-1.65782
C	-1.15589	2.53145	-0.78461
H	-2.16165	2.13048	-0.85841
H	-0.85709	2.53006	0.26591
H	-1.19155	3.57282	-1.11458
C	1.20559	2.51853	-1.43302
H	1.99698	2.17611	-2.09639
H	1.04598	3.57909	-1.6422
H	1.5445	2.44077	-0.3982
C	-0.52319	1.93232	-3.1315

H	-1.53062	1.57055	-3.32996
H	-0.50613	2.99432	-3.38967
H	0.16861	1.42363	-3.80141
C	2.77038	-0.26264	-0.7779
H	3.69246	-0.74618	-1.11057
H	2.92155	0.81004	-0.84225
H	2.61855	-0.52982	0.27013
C	1.94224	-0.50508	-3.12873
H	1.16072	-0.85336	-3.80259
H	2.12706	0.5495	-3.32544
H	2.85776	-1.04516	-3.38358
C	1.58302	-2.30031	-1.4369
H	0.89332	-2.81246	-2.10436
H	2.58253	-2.68939	-1.64598
H	1.34407	-2.55954	-0.40377
C	-1.40332	-1.42129	-3.13497
H	-2.33242	-1.93364	-3.39751
H	-1.30208	-0.56846	-3.8044
H	-0.5881	-2.11577	-3.32897
C	-2.77861	-0.21664	-1.43822
H	-3.61844	-0.88364	-1.64766
H	-2.87977	0.11597	-0.40331
H	-2.87526	0.64011	-2.1014
C	-1.61284	-2.26903	-0.78868
H	-2.49483	-2.82183	-1.12235
H	-0.76247	-2.9399	-0.85639
H	-1.7671	-2.0091	0.26077

$[Ph_3PAuCO]^+$

P	-0.46428	-0.00059	0.00097
Au	1.86021	0.00640	0.00315
C	-1.11285	1.57657	-0.56910
C	-0.54401	2.17297	-1.69431
C	-1.06409	3.35810	-2.18262
C	-2.14537	3.95447	-1.54648
C	-2.70806	3.36539	-0.42431
C	-2.19581	2.17484	0.06850
H	0.29911	1.70696	-2.19437
H	-0.62364	3.82097	-3.05728
H	-2.54786	4.88576	-1.92666
H	-3.54952	3.83329	0.07207
H	-2.63471	1.71529	0.94605
C	-1.10125	-1.28647	-1.08342
C	-2.15684	-1.02854	-1.95322
C	-2.65583	-2.05046	-2.74671
C	-2.10678	-3.32146	-2.67265
C	-1.05249	-3.57919	-1.80553
C	-0.54571	-2.56421	-1.01407
H	-2.58545	-0.03536	-2.01418
H	-3.47626	-1.85051	-3.42514
H	-2.49842	-4.11627	-3.29611
H	-0.62242	-4.57184	-1.75087
H	0.27680	-2.76826	-0.33593
C	-1.10830	-0.30302	1.65238
C	-2.18011	-1.16879	1.85043
C	-2.68617	-1.35081	3.12839
C	-2.12808	-0.67297	4.20159
C	-1.05835	0.19109	4.00457
C	-0.54461	0.37475	2.73339
H	-2.61473	-1.70037	1.01242
H	-3.51876	-2.02592	3.28450
H	-2.52492	-0.82051	5.19889
H	-0.62162	0.71757	4.84444
H	0.29013	1.05143	2.58051
C	3.84991	0.01240	0.00248
O	4.96777	0.01667	0.00119

$[Ph_3PAu]^+$

P	0.001583	0.000917	-0.179239
Au	-0.027558	-0.029955	2.066597
C	0.523581	1.613242	-0.755658
C	1.660187	2.203731	-0.201139
C	2.107106	3.417977	-0.687397
C	1.419805	4.048371	-1.718083
C	0.287337	3.464714	-2.264965
C	-0.167293	2.245252	-1.787500
H	2.192241	1.714040	0.607804
H	2.988280	3.879082	-0.258435
H	1.768569	5.003477	-2.092276
H	-0.247504	3.959158	-3.066612
H	-1.051483	1.789180	-2.215815
C	1.141932	-1.237480	-0.786849
C	2.069438	-0.911977	-1.774111
C	2.907890	-1.896739	-2.273163
C	2.822199	-3.193845	-1.791644
C	1.897537	-3.517370	-0.805249
C	1.059724	-2.542326	-0.297661
H	2.135674	0.100911	-2.151703
H	3.630487	-1.646828	-3.040326
H	3.482415	-3.959079	-2.182006
H	1.836428	-4.530506	-0.427211
H	0.342312	-2.792969	0.476795
C	-1.637307	-0.344933	-0.810811
C	-1.813175	-1.257343	-1.848863
C	-3.083405	-1.466879	-2.363162
C	-4.167178	-0.773357	-1.846658
C	-3.990364	0.136420	-0.810570
C	-2.728924	0.350049	-0.287981
H	-0.965953	-1.797641	-2.253046
H	-3.224526	-2.176007	-3.169633
H	-5.158311	-0.944210	-2.249549
H	-4.839624	0.673537	-0.406418
H	-2.590225	1.055464	0.524663

$[Ph_3PAuN_2]^+$

P	0.440168	0.001702	0.000868
Au	-1.830782	0.003224	0.013831
C	1.074492	-1.456057	-0.837336
C	0.539158	-1.811700	-2.075731
C	1.051837	-2.898564	-2.760171
C	2.091256	-3.638067	-2.209466
C	2.620056	-3.288936	-0.976509
C	2.115900	-2.197046	-0.285969
H	-0.273050	-1.235571	-2.507185
H	0.637485	-3.174207	-3.722271
H	2.486936	-4.492988	-2.744592
H	3.428953	-3.867544	-0.547305
H	2.530820	-1.925806	0.677235
C	1.077870	1.450067	-0.849970
C	2.159722	1.340669	-1.719446
C	2.670718	2.479488	-2.323022
C	2.108243	3.719228	-2.059955
C	1.029120	3.828804	-1.191937
C	0.510242	2.697121	-0.589239
H	2.598822	0.372176	-1.926563
H	3.510651	2.395647	-3.001856
H	2.509040	4.606069	-2.536108
H	0.588965	4.797663	-0.989817
H	-0.332891	2.783228	0.088532
C	1.091209	0.006770	1.675810
C	2.164042	0.825285	2.017768
C	2.684629	0.770738	3.301779
C	2.140968	-0.095607	4.237874
C	1.069905	-0.912107	3.897079
C	0.541130	-0.860136	2.620126
H	2.589658	1.503134	1.287631
H	3.517793	1.408953	3.569856
H	2.549943	-0.133376	5.240440
H	0.643785	-1.585946	4.630334
H	-0.295457	-1.498638	2.355296
N	-5.022519	0.002751	0.034236
N	-3.933329	0.002480	0.026505

$[Ph_3PAuOC]^+$

P	-0.444546	-0.006536	-0.004970
Au	1.798832	-0.007741	0.038136
C	-1.052687	-1.127765	-1.268005
C	-0.497300	-2.402922	-1.374972
C	-0.999681	-3.295308	-2.304324
C	-2.049242	-2.916858	-3.132467
C	-2.598477	-1.647992	-3.030112
C	-2.104269	-0.748319	-2.098030
H	0.324030	-2.697109	-0.729776
H	-0.569278	-4.285711	-2.388576
H	-2.436785	-3.615425	-3.864386
H	-3.414676	-1.353964	-3.678691
H	-2.532887	0.243353	-2.018818
C	-1.109963	-0.523966	1.579785
C	-2.147385	-1.450375	1.643641
C	-2.680082	-1.796559	2.876259
C	-2.183468	-1.221827	4.035907
C	-1.147810	-0.297494	3.971965
C	-0.606723	0.049656	2.747815
H	-2.536558	-1.900568	0.738443
H	-3.485626	-2.518844	2.928095
H	-2.601340	-1.497128	4.996859
H	-0.758607	0.147911	4.879375
H	0.204133	0.769036	2.698498
C	-1.069299	1.637223	-0.367333
C	-2.146927	2.156370	0.345646
C	-2.649932	3.404558	0.011274
C	-2.083491	4.128295	-1.026803
C	-1.008249	3.609977	-1.738060
C	-0.497175	2.368018	-1.408790
H	-2.589317	1.591289	1.157140
H	-3.486582	3.811548	0.565939
H	-2.478098	5.104431	-1.282370
H	-0.565129	4.178753	-2.546370
H	0.343987	1.963848	-1.962365
C	5.225464	-0.000135	0.079452
O	4.094415	-0.005869	0.069974

$[MePh_2PAuCO]^+$

P	0.555972	0.031602	0.747166
Au	-1.654160	-0.056027	0.036671
C	1.396928	1.500555	0.142835
C	0.678839	2.675557	-0.069454
C	1.339809	3.826150	-0.465651
C	2.713887	3.803522	-0.656640
C	3.430470	2.632726	-0.450409
C	2.777318	1.479289	-0.050175
H	-0.396862	2.693743	0.073415
H	0.781280	4.739061	-0.632375
H	3.229048	4.702482	-0.973277
H	4.502557	2.616914	-0.604367
H	3.337774	0.563696	0.100421
C	1.454541	-1.402710	0.143947
C	1.997998	-2.346324	1.010639
C	2.678969	-3.440232	0.497003
C	2.817530	-3.593031	-0.873297
C	2.274257	-2.652700	-1.740259
C	1.591009	-1.561697	-1.236398
H	1.900548	-2.238320	2.083790
H	3.103925	-4.172486	1.172612
H	3.351177	-4.448223	-1.270165
H	2.384148	-2.771991	-2.811215
H	1.175500	-0.824642	-1.915904
C	-3.544000	-0.176851	-0.581680
O	-4.605747	-0.243324	-0.923863
C	0.678333	0.057090	2.549697
H	1.728331	0.073139	2.847331
H	0.195126	0.965625	2.910753
H	0.177112	-0.808379	2.984399

$[MePh_2PAu]^+$

P	0.063639	0.131839	0.683698
Au	-0.655700	-1.784931	-0.236034
C	-0.989012	1.497683	0.200969
C	-2.331376	1.291018	-0.109777
C	-3.147215	2.374535	-0.385667
C	-2.625865	3.660399	-0.354864
C	-1.288000	3.867500	-0.048993
C	-0.463441	2.790731	0.228468
H	-2.736398	0.285237	-0.142441
H	-4.189559	2.214533	-0.632377
H	-3.265076	4.506392	-0.577284
H	-0.882503	4.871702	-0.030461
H	0.582952	2.955703	0.457710
C	1.737874	0.485802	0.174497
C	2.804420	0.365216	1.063366
C	4.090960	0.642960	0.629856
C	4.313713	1.031073	-0.682553
C	3.251239	1.144901	-1.571512
C	1.964526	0.870526	-1.149307
H	2.643011	0.063623	2.090770
H	4.920260	0.556771	1.321079
H	5.321379	1.246397	-1.017189
H	3.428745	1.448019	-2.596028
H	1.135098	0.963080	-1.842078
C	0.006086	-0.016005	2.478923
H	0.378289	0.909901	2.923467
H	-1.032731	-0.162663	2.775624
H	0.598818	-0.864808	2.820011

$[Me_2PhPAuCO]^+$

P	-0.646542	1.146010	0.180905
Au	1.331060	-0.051124	-0.032982
C	-2.065943	0.058393	0.015762
C	-2.148849	-1.049218	0.861147
C	-3.238096	-1.897504	0.784168
C	-4.242773	-1.652783	-0.143122
C	-4.158730	-0.559216	-0.990496
C	-3.073147	0.300220	-0.914249
H	-1.362363	-1.252576	1.581490
H	-3.302412	-2.754018	1.443986
H	-5.093323	-2.320723	-0.206094
H	-4.941545	-0.370168	-1.714806
H	-3.023339	1.151419	-1.581922
C	3.022483	-1.088525	-0.233929
O	3.972480	-1.665205	-0.347524
C	-0.780269	1.959123	1.789841
H	-1.721293	2.510914	1.835333
H	-0.767206	1.212119	2.583699
H	0.057102	2.643953	1.932341
C	-0.768894	2.456248	-1.052563
H	0.076049	3.134552	-0.926768
H	-0.736023	2.037906	-2.058648
H	-1.695817	3.016479	-0.915798

$[Me2PhPAu]^+$

P	-0.080214	0.996156	0.289487
Au	1.549629	-0.472947	-0.165304
C	-1.689047	0.251878	0.081795
C	-2.542396	0.664888	-0.940192
C	-3.790421	0.077335	-1.068909
C	-4.183658	-0.920828	-0.190706
C	-3.330261	-1.339970	0.822833
C	-2.083116	-0.760740	0.959626
H	-2.248683	1.443099	-1.633304
H	-4.456526	0.402032	-1.858713
H	-5.159730	-1.378730	-0.296568
H	-3.638079	-2.122425	1.505403
H	-1.417727	-1.102719	1.745140
C	0.065842	2.434979	-0.780092
H	0.007979	2.143556	-1.828395
H	-0.733680	3.142202	-0.546085
H	1.031386	2.908946	-0.599843
C	0.070900	1.575384	1.988171
H	1.047445	2.038414	2.134793
H	-0.720259	2.305576	2.176291
H	-0.036682	0.742952	2.682870

$[(p\text{-}OMe\text{-}C_6H_4)_3PAuCO]^+$

P	-0.025446	-0.042369	-0.018414
Au	-0.419129	0.282618	2.250654
C	0.690931	1.421651	-0.759738
C	1.703327	2.111035	-0.097749
C	2.308284	3.213074	-0.672902
C	1.891610	3.647936	-1.933525
C	0.870881	2.962543	-2.599277
C	0.279099	1.863279	-2.019874
H	2.035884	1.781941	0.881944
H	3.092150	3.730489	-0.137397
H	0.559966	3.318238	-3.573698
H	-0.513051	1.342375	-2.544745
C	1.101987	-1.410692	-0.269050
C	2.188795	-1.302616	-1.128199
C	3.033068	-2.380150	-1.343166
C	2.790835	-3.589029	-0.692181
C	1.697463	-3.701613	0.176395
C	0.869654	-2.626167	0.386388
H	2.385543	-0.367161	-1.638809
H	3.872440	-2.269620	-2.015496
H	1.528810	-4.648227	0.674498
H	0.024461	-2.731505	1.059330
C	-1.551190	-0.417567	-0.876897
C	-1.596923	-1.404738	-1.865194
C	-2.763054	-1.643862	-2.555882
C	-3.914079	-0.900549	-2.277306
C	-3.877226	0.086178	-1.288817
C	-2.702056	0.314984	-0.597860
H	-0.712723	-1.989801	-2.089344
H	-2.814134	-2.407460	-3.322027
H	-4.756411	0.669369	-1.052828
H	-2.685026	1.086723	0.165547
C	-0.754173	0.550308	4.192390
O	-0.943158	0.701302	5.284603
O	-4.994960	-1.204893	-2.998222
O	3.539971	-4.685096	-0.827002
O	2.402064	4.702487	-2.572897
C	-6.193327	-0.489852	-2.764184
H	-6.545366	-0.634989	-1.738802
H	-6.060762	0.577570	-2.962861
H	-6.924502	-0.897908	-3.457607
C	4.662364	-4.639765	-1.687767
H	5.386973	-3.892690	-1.351373
H	5.114037	-5.627580	-1.641340
H	4.361141	-4.425972	-2.717267
C	3.433301	5.443163	-1.948541
H	3.091342	5.876562	-1.004264
H	4.315346	4.820773	-1.772425
H	3.688027	6.241920	-2.640693

$[(p\text{-}OMe\text{-}C_6H_4)_3PAu]^+$

P	-0.050931	-0.038220	0.219095
Au	-0.218662	0.065017	2.461483
C	0.575636	1.508240	-0.401698
C	1.684891	2.104726	0.195580
C	2.222962	3.269469	-0.313719
C	1.642985	3.864147	-1.439068
C	0.525697	3.271979	-2.037063
C	-0.002939	2.110322	-1.524319
H	2.136663	1.655083	1.073943
H	3.081200	3.714679	0.169970
H	0.090334	3.749765	-2.905796
H	-0.868493	1.661599	-1.996623
C	1.059541	-1.355488	-0.224660
C	2.097030	-1.139441	-1.126835
C	2.928047	-2.178389	-1.508269
C	2.726140	-3.454836	-0.982241
C	1.684528	-3.674371	-0.068940
C	0.867774	-2.638491	0.306508
H	2.257366	-0.152032	-1.542752
H	3.725681	-1.987829	-2.212676
H	1.550669	-4.671360	0.331748
H	0.069334	-2.819721	1.018545

C	-1.656513	-0.353030	-0.480926
C	-1.832332	-1.340571	-1.456319
C	-3.066190	-1.532009	-2.033060
C	-4.155882	-0.743570	-1.649125
C	-3.987354	0.242541	-0.671046
C	-2.746894	0.425586	-0.094706
H	-0.996041	-1.955729	-1.765451
H	-3.218726	-2.290885	-2.790257
H	-4.817902	0.857764	-0.354062
H	-2.627024	1.188447	0.667891
O	-5.309418	-1.003957	-2.261239
O	3.467385	-4.519827	-1.281106
O	2.079628	4.989492	-2.002024
C	-6.454420	-0.244111	-1.917473
H	-6.711697	-0.376198	-0.862926
H	-6.301329	0.816973	-2.133171
H	-7.261706	-0.626197	-2.537068
C	4.540712	-4.370821	-2.193404
H	5.282079	-3.661709	-1.814895
H	4.993676	-5.354881	-2.283115
H	4.180718	-4.044879	-3.173204
C	3.199913	5.647387	-1.437744
H	2.996798	5.956811	-0.408790
H	4.087061	5.008572	-1.465703
H	3.368876	6.527413	-2.053076

[(*p*-CF_3-C_6H_4)$_3$PAuCO]$^+$

P	-0.00502	-0.00581	0.36516
Au	-0.00577	-0.01195	2.68795
C	-0.09614	1.6719	-0.28222
C	0.7205	2.654	0.27821
C	0.71216	3.93514	-0.2387
C	-0.11792	4.23896	-1.31073
C	-0.93676	3.26879	-1.8666
C	-0.92636	1.98094	-1.35467
H	1.37333	2.41802	1.11207
H	1.3504	4.69969	0.18623
H	-1.57762	3.51496	-2.70371
H	-1.56446	1.22349	-1.79317
C	1.49322	-0.75869	-0.29109
C	2.17375	-0.17627	-1.3548
C	3.30271	-0.79369	-1.87045
C	3.74385	-1.98844	-1.32562
C	3.06672	-2.57486	-0.26278
C	1.94513	-1.95941	0.2576
H	1.83035	0.7573	-1.7832
H	3.83581	-0.3469	-2.69981
H	3.41837	-3.51064	0.15382
H	1.41669	-2.42051	1.08544
C	-1.41003	-0.92128	-0.28902
C	-1.25752	-1.79258	-1.36216
C	-2.36427	-2.44988	-1.87663
C	-3.61496	-2.2319	-1.3221
C	-3.77229	-1.36194	-0.24956
C	-2.67082	-0.71032	0.26983
H	-0.28083	-1.96234	-1.79856
H	-2.25321	-3.12722	-2.71365
H	-4.75499	-1.19597	0.17422
H	-2.79642	-0.02919	1.105
C	-0.00903	-0.01447	4.68116
O	-0.0118	-0.01462	5.79815
C	4.99456	-2.6511	-1.84898
F	5.30436	-2.22448	-3.07175
F	6.03294	-2.38762	-1.04906
F	4.85108	-3.97687	-1.89761
C	-4.82061	-2.97127	-1.84866
F	-5.10183	-4.02197	-1.07127
F	-5.89761	-2.18379	-1.86547
F	-4.62034	-3.42257	-3.08543
C	-0.15585	5.65271	-1.83754
F	-1.00237	6.39729	-1.11892
F	1.046	6.22695	-1.76653
F	-0.55778	5.69247	-3.10691

[(*p*-CF_3-C_6H_4)$_3$PAu]$^+$

P	0.00075	-0.00441	0.57491
Au	0.00137	0.00055	2.81911
C	-0.69908	1.52669	-0.04175
C	-0.25125	2.74111	0.48194
C	-0.73787	3.92722	-0.02808
C	-1.67737	3.90329	-1.05393
C	-2.12877	2.70121	-1.57181
C	-1.6395	1.50592	-1.06717
H	0.47767	2.75918	1.28502
H	-0.39255	4.87402	0.36879
H	-2.8582	2.69471	-2.37138
H	-1.9905	0.56661	-1.47599
C	1.67689	-0.16451	-0.03983
C	2.13103	0.66293	-1.06266
C	3.41188	0.49158	-1.56429
C	4.22772	-0.50034	-1.04606
C	3.77716	-1.32806	-0.02309
C	2.50463	-1.15923	0.48381
H	1.49324	1.43659	-1.47143
H	3.77182	1.12814	-2.36228
H	4.42401	-2.10068	0.37378
H	2.15497	-1.80205	1.28448
C	-0.97886	-1.37577	-0.03642
C	-0.49672	-2.18348	-1.06198
C	-1.29199	-3.20383	-1.56049
C	-2.55743	-3.40962	-1.03681
C	-3.04156	-2.60415	-0.01111
C	-2.25278	-1.59027	0.49273
H	0.49074	-2.02034	-1.47537
H	-0.92663	-3.8348	-2.36043
H	-4.03331	-2.7742	0.38952
H	-2.62831	-0.96435	1.29508
C	5.63935	-0.67093	-1.55457
F	5.80244	-0.1115	-2.75141
F	6.50858	-0.1025	-0.71404
F	5.9587	-1.96223	-1.65357
C	-3.42108	-4.53944	-1.54477
F	-3.4052	-5.56138	-0.68439
F	-4.68851	-4.14599	-1.68124
F	-2.99914	-4.99065	-2.72373
C	-2.22187	5.21465	-1.56781
F	-3.06268	5.75047	-0.67864
F	-1.23627	6.09124	-1.77005
F	-2.88035	5.0617	-2.71401

[JohnPhosAuCO]$^+$

P	1.212837	-0.486486	0.018657
Au	-1.089554	-0.878977	-0.029140
C	1.579639	1.292881	0.002264
C	0.583148	2.283321	-0.008375
C	0.968619	3.623034	-0.056275
C	2.299932	3.995335	-0.094033
C	3.283782	3.020233	-0.084357
C	2.921570	1.687705	-0.036631
H	0.195409	4.382296	-0.063000
H	2.566879	5.044627	-0.131095
H	4.331537	3.293266	-0.113637
H	3.703752	0.943211	-0.026517
C	-2.998346	-1.392676	-0.075237
O	-4.076898	-1.691550	-0.102143
C	1.936369	-1.232052	-1.541429
C	3.446599	-1.438362	-1.509531
C	1.261212	-2.580170	-1.803919
C	1.562669	-0.272506	-2.672037
H	3.999431	-0.511140	-1.366699
H	3.748627	-2.155336	-0.745981
H	3.754526	-1.846642	-2.475927
H	0.183107	-2.473389	-1.942562
H	1.673325	-2.996953	-2.726654
H	1.434076	-3.304758	-1.009162
H	1.838429	-0.732918	-3.624206
H	0.486370	-0.078761	-2.698915
H	2.082294	0.682418	-2.591876
C	1.867590	-1.174838	1.627991
C	0.988034	-0.562665	2.720070
C	1.694610	-2.691856	1.625579
C	3.320953	-0.820636	1.928253
H	1.042031	0.528061	2.720159
H	-0.058234	-0.861615	2.618569
H	1.342915	-0.913145	3.692726
H	2.389585	-3.183436	0.944062
H	1.903028	-3.067027	2.630782
H	0.676831	-2.991500	1.363399
H	3.600727	-1.315039	2.862437
H	4.014469	-1.162790	1.160821
H	3.456100	0.250346	2.076165
C	-0.884198	2.039154	0.022591
C	-1.566499	1.951949	1.237336
C	-1.621096	2.039726	-1.163432
C	-2.953585	1.875839	1.264208
H	-1.007725	1.977662	2.165635
C	-3.007987	1.962476	-1.133770
H	-1.102092	2.131888	-2.110939
C	-3.676963	1.888130	0.079867
H	-3.468920	1.830381	2.216459
H	-3.565796	1.983698	-2.062654
H	-4.759615	1.851302	0.103198

[JohnPhosAu]$^+$

P	1.125378	-0.272499	0.134377
Au	-0.940827	-1.153923	-0.260618
C	0.879930	1.519704	-0.180535
C	-0.376437	2.164654	-0.253746
C	-0.414720	3.543187	-0.451190
C	0.740234	4.292384	-0.592023
C	1.972211	3.665620	-0.524745
C	2.031696	2.299561	-0.316389
H	-1.381870	4.029659	-0.502831

H	0.674850	5.361603	-0.753052
H	2.887890	4.234710	-0.628606
H	3.004159	1.832895	-0.250558
C	2.334054	-0.962076	-1.123158
C	3.809260	-0.739118	-0.796750
C	2.086867	-2.470660	-1.218992
C	1.986567	-0.326110	-2.468591
H	4.087085	0.311125	-0.724513
H	4.107667	-1.244268	0.121649
H	4.401404	-1.169450	-1.608603
H	1.067695	-2.688913	-1.544168
H	2.775194	-2.886155	-1.959576
H	2.260810	-2.988567	-0.276214
H	2.566323	-0.827665	-3.247481
H	0.928693	-0.452842	-2.714025
H	2.221255	0.737444	-2.501828
C	1.640596	-0.428244	1.917972
C	0.440053	0.031975	2.744994
C	1.935212	-1.893937	2.222789
C	2.839081	0.448245	2.272765
H	0.182465	1.072195	2.538250
H	-0.441188	-0.588918	2.568218
H	0.698771	-0.043312	3.804277
H	2.845292	-2.245034	1.735533
H	2.078217	-2.004429	3.300618
H	1.107338	-2.542797	1.927206
H	3.071437	0.293018	3.329671
H	3.732206	0.199185	1.702202
H	2.619148	1.507589	2.138974
C	-1.682544	1.473966	-0.091808
C	-2.395175	1.579214	1.092092
C	-2.201116	0.653199	-1.117007
C	-3.547065	0.823187	1.308017
H	-2.026226	2.231440	1.875175
C	-3.339604	-0.133678	-0.888276
H	-1.749497	0.686105	-2.103129
C	-3.999731	-0.056507	0.343404
H	-4.078697	0.916485	2.247118
H	-3.749547	-0.732467	-1.693535
H	-4.882408	-0.658678	0.519478

$[(OMe)_3PAuCO]^+$

P	1.330746	0.047566	-0.056248
Au	-0.976668	-0.017024	-0.066314
C	-2.979402	-0.042799	-0.099932
O	-4.095156	-0.056379	-0.122060
O	1.825174	-0.851839	-1.226203
O	1.973257	1.447712	-0.321278
O	1.999708	-0.388247	1.298811
C	3.214560	-0.952127	-1.622265
H	3.505650	-0.040066	-2.139645
H	3.845888	-1.114068	-0.748778
H	3.270156	-1.805266	-2.292158
C	1.890507	2.536652	0.615846
H	0.848705	2.734986	0.876462
H	2.466834	2.299285	1.508774
H	2.312408	3.400583	0.110131
C	1.645126	-1.602400	1.980854
H	0.561394	-1.675897	2.096040
H	2.022448	-2.464398	1.430774
H	2.113509	-1.549712	2.959792

$[(OMe)_3PAu]^+$

P	0.949797	0.057486	-0.029591
Au	-1.269850	-0.041198	-0.129696
O	1.492897	-0.812457	-1.189942
O	1.554513	1.474115	-0.232991
O	1.521346	-0.400977	1.351104
C	2.898619	-0.877658	-1.553453
H	3.189332	0.062551	-2.017363
H	3.504771	-1.078260	-0.670612
H	2.976200	-1.696334	-2.262553
C	1.386884	2.558242	0.704940
H	0.324699	2.744586	0.872043
H	1.887179	2.313450	1.640349
H	1.846622	3.424994	0.239307
C	1.147362	-1.630231	2.004124
H	0.068619	-1.653170	2.167567
H	1.460403	-2.483852	1.403645
H	1.666148	-1.629176	2.958450

$[(OPh)_3PAuCO]^+$

P	-0.675729	0.084247	-0.227566
Au	1.432460	-0.279258	-1.094740
C	3.258424	-0.574754	-1.834930
O	4.283766	-0.746329	-2.243001
O	-0.760777	-0.404823	1.276193
O	-1.185902	1.572567	-0.167902
O	-1.757667	-0.651755	-1.081801
C	0.145975	-1.354749	1.760481
C	0.972321	-0.976069	2.800979
C	0.191117	-2.622232	1.205622
C	1.870583	-1.904761	3.303985
H	0.902648	0.026438	3.204755
C	1.103116	-3.537938	1.715560
H	-0.486341	-2.897161	0.405190
C	1.939089	-3.181490	2.762047
H	2.520180	-1.627395	4.125218
H	1.146203	-4.536399	1.297797
H	2.641330	-3.901976	3.162724
C	-3.143643	-0.613154	-0.789067
C	-3.919467	0.340360	-1.414480
C	-3.666379	-1.557596	0.070204
C	-5.282807	0.345399	-1.159637
H	-3.466175	1.057896	-2.086232
C	-5.031976	-1.537405	0.314323
H	-3.024668	-2.294793	0.535602
C	-5.837756	-0.588785	-0.297151
H	-5.911714	1.083715	-1.641706
H	-5.464253	-2.270582	0.984121
H	-6.903335	-0.579926	-0.104216
C	-0.407904	2.540005	0.494355
C	0.504439	3.269131	-0.244744
C	-0.605077	2.749369	1.845261
C	1.255767	4.239527	0.403235
H	0.599528	3.099273	-1.310738
C	0.152008	3.725080	2.476919
H	-1.343433	2.166676	2.381164
C	1.082897	4.464530	1.760781
H	1.969042	4.828474	-0.160385
H	0.005946	3.911857	3.533878
H	1.666938	5.227500	2.260379

$[(OPh)_3PAu]^+$

P	-0.449216	0.129016	-0.248717
Au	1.323429	-0.287409	-1.523427
O	-0.286593	-0.558612	1.156599
O	-0.732877	1.633935	0.073442
O	-1.736161	-0.376957	-0.963205
C	0.494995	-1.704374	1.364250
C	1.531765	-1.603888	2.270938
C	0.205427	-2.878534	0.692336
C	2.302142	-2.729998	2.517635
H	1.720474	-0.663043	2.772864
C	0.991937	-3.994302	0.946578
H	-0.624691	-2.928825	-0.002714
C	2.034888	-3.921461	1.857017
H	3.115539	-2.673595	3.230565
H	0.778128	-4.924404	0.434455
H	2.639996	-4.797178	2.056086
C	-3.040454	-0.214373	-0.419252
C	-3.801236	0.843836	-0.868092
C	-3.501790	-1.141065	0.492080
C	-5.089901	0.976576	-0.372596
H	-3.396241	1.541701	-1.589642
C	-4.792904	-0.990797	0.977922
H	-2.874647	-1.962939	0.812945
C	-5.583833	0.064203	0.548483
H	-5.708680	1.797792	-0.712674
H	-5.179128	-1.707270	1.692405
H	-6.591436	0.173574	0.929865
C	0.249261	2.446101	0.678119
C	1.030569	3.238039	-0.140262
C	0.365280	2.448162	2.053819
C	1.978375	4.060944	0.451483
H	0.880033	3.227844	-1.213032
C	1.316093	3.279161	2.627946
H	-0.283355	1.825840	2.656922
C	2.122896	4.079024	1.830818
H	2.596737	4.696560	-0.170348
H	1.418797	3.305852	3.705915
H	2.859786	4.727736	2.287900

$[(O\text{-}(2,4\text{-}t\text{Bu-}C_6H_3))_3PAuCO]^+$

P	0.061568	-0.093060	0.022570
Au	1.226626	1.108485	-1.569476
C	2.197383	2.113206	-2.975521
O	2.746831	2.676747	-3.769372
O	0.980667	-0.983365	0.945636
O	-0.717776	0.769004	1.088386
O	-0.939683	-1.055511	-0.687771
C	-1.894629	-1.952243	-0.172981
C	-2.711766	-2.615060	-1.091146
C	-1.980710	-2.156586	1.187533
C	-3.632034	-3.494559	-0.530831
C	-2.915638	-3.046580	1.691723
H	-1.323978	-1.630603	1.868097
C	-3.763842	-3.733715	0.837228
H	-4.288734	-4.030452	-1.200615
H	-2.965334	-3.192500	2.762067
C	-1.405511	1.951678	0.778868
C	-1.512264	2.933688	1.760448
C	-1.966926	2.096469	-0.478773

C	-2.173792	4.099053	1.368585
C	-2.612273	3.271177	-0.816445
C	-2.717711	4.307270	0.104580
H	-2.270615	4.887122	2.098735
H	-3.048339	3.360435	-1.803947
C	2.380929	-0.867093	0.899661
C	3.161926	-2.004790	0.687631
C	2.929732	0.388548	1.080841
C	4.533232	-1.773235	0.635976
C	4.304893	0.564991	1.013593
H	2.286316	1.225451	1.328779
C	5.134073	-0.521097	0.781582
H	5.178983	-2.624135	0.473339
H	4.712272	1.554908	1.168130
C	2.583330	-3.410647	0.534715
C	1.738937	-3.771146	1.763414
C	1.729123	-3.494147	-0.734281
C	3.688178	-4.458411	0.414025
H	2.339860	-3.717867	2.674006
H	0.876774	-3.117197	1.880807
H	1.368850	-4.794192	1.663767
H	2.309183	-3.209499	-1.615840
H	1.383432	-4.520420	-0.878389
H	0.845244	-2.863039	-0.680869
H	3.230239	-5.445809	0.333401
H	4.301971	-4.309702	-0.477481
H	4.340228	-4.469030	1.290300
C	6.649813	-0.402811	0.696402
C	7.287969	-1.288322	1.771693
C	7.111972	-0.868471	-0.688118
C	7.123471	1.031079	0.908661
H	6.968719	-0.982678	2.770590
H	7.025780	-2.339942	1.641323
H	8.376538	-1.209757	1.723289
H	6.677780	-0.247161	-1.475489
H	8.199622	-0.799098	-0.762979
H	6.831069	-1.905431	-0.882921
H	8.211905	1.070166	0.835298
H	6.720129	1.710137	0.152857
H	6.848337	1.408926	1.896461
C	-2.616119	-2.420046	-2.605050
C	-2.888480	-0.958207	-2.979323
C	-1.229552	-2.840078	-3.107535
C	-3.645248	-3.273379	-3.344325
H	-3.848629	-0.623695	-2.580050
H	-2.109896	-0.291373	-2.612098
H	-2.921681	-0.858481	-4.066918
H	-1.026408	-3.883147	-2.855489
H	-1.188533	-2.743167	-4.195315
H	-0.432932	-2.228971	-2.685841
H	-3.538902	-3.104960	-4.417579
H	-3.498206	-4.340553	-3.164764
H	-4.669563	-3.011120	-3.070335
C	-4.812893	-4.722109	1.328692
C	-4.795394	-4.865271	2.846767
C	-6.200717	-4.232546	0.902205
C	-4.541799	-6.096869	0.709304
H	-3.830121	-5.227256	3.209310
H	-5.022677	-3.920882	3.347457
H	-5.553502	-5.588794	3.152651
H	-6.286065	-4.151349	-0.183339
H	-6.967371	-4.931581	1.244980
H	-6.417426	-3.251764	1.331845
H	-5.286598	-6.817569	1.055288
H	-4.589852	-6.068940	-0.381078
H	-3.553735	-6.465523	0.994566
C	-3.429040	5.598500	-0.278811
C	-4.879456	5.278729	-0.655074
C	-3.438496	6.614352	0.858507
C	-2.716135	6.224996	-1.481437
H	-4.937830	4.589895	-1.500203
H	-5.410224	4.826100	0.185542
H	-5.404805	6.194702	-0.935822
H	-2.427298	6.898457	1.160546
H	-3.949841	7.521462	0.530474
H	-3.970164	6.239175	1.736385
H	-3.217432	7.150540	-1.773959
H	-1.677511	6.463496	-1.239396
H	-2.718544	5.558764	-2.346507
H	-1.947448	1.273966	-1.183785
C	-1.000674	2.750284	3.188981
C	-1.740971	1.575703	3.841672
C	0.509271	2.486369	3.207143
C	-1.258211	3.990924	4.041460
H	-2.816153	1.765300	3.869470
H	-1.573986	0.639508	3.309375
H	-1.393978	1.445593	4.869651
H	1.049269	3.254347	2.646684
H	0.872520	2.508727	4.236997
H	0.755351	1.507976	2.799448
H	-0.890975	3.806417	5.052636
H	-0.736358	4.870568	3.656982
H	-2.322433	4.223315	4.118517

$[(O\text{-}(2,4\text{-}t\text{Bu-}C_6H_3))_3PAu]^+$

P	-0.62049	0.1878	-0.14084
Au	-1.61906	-0.1705	-2.09652
O	-1.68494	0.49058	0.96385
O	0.14866	-1.04598	0.42469
O	0.28147	1.45224	-0.20862
C	1.52905	1.72436	0.39253
C	2.45279	2.48109	-0.32874
C	1.7705	1.24535	1.6596
C	3.68273	2.64625	0.29924
C	3.01071	1.44708	2.24228
H	0.99974	0.70769	2.1966
C	4.00183	2.13325	1.55708
H	4.4419	3.2117	-0.22121
H	3.18702	1.05674	3.23518
C	1.37658	-1.60372	0.02421
C	1.92088	-2.61197	0.81314
C	2.00081	-1.12163	-1.10982
C	3.16911	-3.07894	0.39572
C	3.23082	-1.62224	-1.48243
C	3.84878	-2.61031	-0.72317
H	3.63438	-3.85234	0.98586
H	3.70887	-1.22706	-2.37025
C	-3.03206	0.08924	0.89598
C	-4.03799	1.05615	0.94994
C	-3.29276	-1.26297	0.80853
C	-5.33322	0.55124	0.90103
C	-4.60314	-1.71152	0.75521
H	-2.4694	-1.96721	0.81247
C	-5.65171	-0.80461	0.8007
H	-6.14907	1.25766	0.94503
H	-4.78795	-2.77491	0.69045
C	-3.7668	2.55647	1.05782
C	-2.9284	2.86184	2.30534
C	-3.04334	3.05195	-0.20007
C	-5.06539	3.35204	1.17538
H	-3.44155	2.52037	3.20694
H	-1.94586	2.39425	2.27408
H	-2.78222	3.94112	2.39091
H	-3.61702	2.81176	-1.09881
H	-2.9284	4.13758	-0.15608
H	-2.04386	2.63067	-0.30114
H	-4.82217	4.41153	1.27207
H	-5.69918	3.24172	0.29253
H	-5.64208	3.06574	2.05766
C	-7.1135	-1.2285	0.75439
C	-7.81363	-0.76354	2.03551
C	-7.78738	-0.58023	-0.45957
C	-7.26639	-2.74119	0.64183
H	-7.34949	-1.20852	2.91856
H	-7.77987	0.322	2.14688
H	-8.86423	-1.06265	2.01588
H	-7.30821	-0.8967	-1.38923
H	-8.83896	-0.87271	-0.50356
H	-7.74886	0.50988	-0.41307
H	-8.32681	-2.99847	0.61299
H	-6.80936	-3.12997	-0.27165
H	-6.82753	-3.25922	1.498
C	2.143	3.14644	-1.67046
C	1.80435	2.11636	-2.75334
C	0.96988	4.11889	-1.49242
C	3.336	3.95262	-2.17989
H	2.61378	1.39233	-2.87227
H	0.8783	1.58083	-2.53985
H	1.67001	2.62549	-3.71043
H	1.21101	4.87976	-0.74723
H	0.7647	4.62652	-2.43806
H	0.05761	3.61302	-1.17797
H	3.06611	4.42572	-3.12583
H	3.61875	4.74665	-1.48593
H	4.20963	3.32284	-2.36394
C	5.3997	2.34861	2.11965
C	5.55759	1.73863	3.50814
C	6.41589	1.68854	1.18182
C	5.68823	3.85004	2.21409
H	4.8703	2.18632	4.23009
H	5.39576	0.65776	3.49774
H	6.57262	1.91458	3.86914
H	6.38367	2.12013	0.17927
H	7.4282	1.82273	1.57035
H	6.22268	0.61686	1.09244
H	6.69096	4.01366	2.61584
H	5.63989	4.33792	1.2385
H	4.97227	4.3447	2.87441
C	5.21921	-3.1346	-1.13033
C	6.22068	-1.97505	-1.10771
C	5.72547	-4.2261	-0.19391
C	5.1368	-3.7122	-2.5469
H	5.9279	-1.17145	-1.78634

H	6.30455	-1.55254	-0.10363
H	7.20949	-2.32591	-1.41223
H	5.06556	-5.09709	-0.18831
H	6.70853	-4.56305	-0.52826
H	5.83415	-3.86535	0.83196
H	6.11543	-4.08669	-2.85602
H	4.42636	-4.54096	-2.58959
H	4.82373	-2.96152	-3.27529
H	1.54151	-0.33959	-1.70074
C	1.21728	-3.20419	2.03389
C	0.90615	-2.1249	3.07805
C	-0.07611	-3.89162	1.58194
C	2.08118	-4.25948	2.72225
H	1.80958	-1.57111	3.34398
H	0.15127	-1.41823	2.7371
H	0.52497	-2.59742	3.98602
H	0.14317	-4.71005	0.89299
H	-0.60055	-4.30624	2.44626
H	-0.75044	-3.19926	1.0791
H	1.53685	-4.65483	3.58166
H	2.30727	-5.10059	2.06377
H	3.02088	-3.84168	3.09082

$[IPrAuCO]^+$

C	0.000352	0.034339	-0.637174
C	0.677224	0.107289	-2.760871
C	-0.678290	0.107730	-2.760287
H	1.389078	0.134161	-3.567983
H	-1.390824	0.135068	-3.566784
N	-1.070731	0.062742	-1.445663
N	1.070759	0.061904	-1.446592
Au	0.001325	-0.029471	1.385720
C	0.002336	-0.090058	3.333189
O	0.002927	-0.124393	4.452404
C	2.424799	0.046485	-0.972383
C	3.042442	-1.191405	-0.782985
C	4.341106	-1.177639	-0.287005
C	4.981170	0.015316	0.000169
C	4.338531	1.224055	-0.203610
C	3.040108	1.269677	-0.697829
H	4.858848	-2.115457	-0.124145
H	5.994077	0.003102	0.384991
H	4.854194	2.149176	0.025293
C	-2.424378	0.048049	-0.970310
C	-3.041987	-1.189562	-0.779022
C	-4.340224	-1.175113	-0.281932
C	-4.979892	0.018220	0.004500
C	-4.337306	1.226675	-0.201189
C	-3.039333	1.271621	-0.696632
H	-4.857954	-2.112700	-0.117668
H	-5.992464	0.006545	0.390219
H	-4.852683	2.152079	0.027182
C	2.341976	2.595337	-0.896215
H	1.376723	2.407304	-1.373565
C	2.347948	-2.501938	-1.074187
H	1.381054	-2.283610	-1.535207
C	-2.340984	2.596924	-0.896737
H	-1.377524	2.408450	-1.377531
C	2.348103	-2.500510	-1.069806
H	-1.380866	-2.282762	-1.530371
C	2.065625	3.268413	0.445655
H	1.527388	4.207367	0.299737
H	1.461856	2.628282	1.094794
H	2.995986	3.492975	0.972080
C	3.132943	3.514785	-1.821444
H	3.321122	3.042778	-2.787787
H	2.581277	4.440896	-1.995493
H	4.098589	3.783488	-1.388156
C	3.140757	-3.349451	-2.064352
H	2.590518	-4.260842	-2.307127
H	3.329424	-2.806945	-2.992826
H	4.106320	-3.648058	-1.650939
C	2.077300	-3.270875	0.216339
H	3.009928	-3.527578	0.723656
H	1.471642	-2.682557	0.910977
H	1.543675	-4.199832	0.004324
C	-2.059644	3.268855	0.444698
H	-1.453719	2.628066	1.091182
H	-1.521740	4.207830	0.297675
H	-2.988158	3.493073	0.974523
C	-3.134272	3.517671	-1.818651
H	-4.097806	3.787805	-1.381577
H	-2.581922	4.443006	-1.994637
H	-3.326878	3.046163	-2.784360
C	-3.141067	-3.347402	-2.060399
H	-2.591562	-4.259358	-2.302723
H	-4.107197	-3.644959	-1.647550
H	-3.328614	-2.804813	-2.989055
C	-2.078475	-3.269707	0.220754
H	-1.545194	-4.198889	0.008877
H	-1.472849	-2.681748	0.915722
H	-3.011416	-3.526061	0.727661

$[IPrAu]^+$

C	0.036760	-0.644321	0.000549
C	0.106911	-2.756293	0.676539
C	0.107530	-2.755621	-0.677465
H	0.132779	-3.562398	1.389505
H	0.134006	-3.561021	-1.391206
N	0.063810	-1.439513	-1.075856
N	0.063025	-1.440574	1.076188
Au	-0.024609	1.319220	0.001529
C	0.049295	-0.972567	2.433060
C	-1.188419	-0.787912	3.051964
C	-1.172161	-0.304311	4.355175
C	0.022092	-0.025220	4.996458
C	1.230164	-0.225088	4.351289
C	1.274273	-0.706975	3.048267
H	-2.109096	-0.144222	4.875264
H	0.011402	0.350605	6.012727
H	2.156012	-0.002431	4.868293
C	0.050843	-0.970184	-2.432282
C	-1.186555	-0.784194	-3.051415
C	-1.169582	-0.299395	-4.354172
C	0.025049	-0.020438	-4.994799
C	1.232794	-0.221651	-4.349425
C	1.276193	-0.704796	-3.046847
H	-2.106250	-0.138299	-4.874438
H	0.014923	0.356326	-6.010725
H	2.158929	0.000922	-4.865941
C	2.598787	-0.901300	2.347019
H	2.409785	-1.370518	1.377751
C	-2.499821	-1.069756	2.355441
H	-2.283567	-1.523917	1.384628
C	2.600337	-0.900470	-2.345255
H	2.410842	-1.372063	-1.377235
C	-2.498367	-1.066053	-2.355672
H	-2.282689	-1.520325	-1.384785
C	3.273539	0.441845	2.081202
H	4.212165	0.298715	1.541696
H	2.633800	1.096053	1.482418
H	3.498904	0.960880	3.015417
C	3.517480	-1.834893	3.129147
H	3.044575	-2.802400	3.309008
H	4.443121	-2.004803	2.575495
H	3.787045	-1.410470	4.098417
C	-3.349974	-2.064202	3.140153
H	-4.262595	-2.298779	2.588479
H	-2.810656	-2.996234	3.320330
H	-3.646506	-1.658199	4.109433
C	-3.264964	0.225205	2.095475
H	-3.519498	0.726086	3.032065
H	-2.674438	0.922452	1.494852
H	-4.194796	0.020068	1.560749
C	3.274451	0.442302	-2.075901
H	2.634210	1.094806	-1.475789
H	4.212943	0.298286	-1.536395
H	3.499883	0.963624	-3.008826
C	3.519890	-1.831915	-3.128911
H	3.790487	-1.404952	-4.096773
H	4.444970	-2.003184	-2.574739
H	3.047263	-2.798992	-3.311775
C	-3.348001	-2.060414	-3.141062
H	-4.261060	-2.294965	-2.590100
H	-3.643730	-1.654333	-4.110555
H	-2.808597	-2.992469	-3.320872
C	-3.263664	0.228856	-2.095960
H	-4.193748	0.023635	-1.561707
H	-2.673437	0.926037	-1.494969
H	-3.517779	0.729867	-3.032591

$[IPrAuN_2]^+$

C	0.026583	-0.444514	0.000336
C	0.099852	-2.566672	0.676621
C	0.100259	-2.566031	-0.677919
H	0.127619	-3.373435	1.388736
H	0.128485	-3.372121	-1.390778
N	0.054836	-1.250767	-1.071961
N	0.054102	-1.251783	1.071881
Au	-0.041986	1.539098	0.001224
N	-0.112325	3.568247	0.001629
N	-0.150069	4.657681	0.001899
C	0.037176	-0.781742	2.427192
C	-1.201525	-0.596085	3.044286
C	-1.189430	-0.106285	4.345183
C	0.002712	0.178335	4.988050
C	1.212249	-0.022063	4.345936
C	1.259431	-0.509855	3.045073
H	-2.127889	0.054194	4.862589
H	-0.010922	0.558204	6.002814
H	2.136846	0.203754	4.863916
C	0.038786	-0.779434	-2.426834
C	-1.199545	-0.592259	-3.044202

C	-1.186611	-0.101232	-4.344631
C	0.005974	0.183088	-4.986797
C	1.215131	-0.018831	-4.344432
C	1.261476	-0.507876	-3.044014
H	-2.124768	0.060429	-4.862221
H	-0.007001	0.563929	-6.001206
H	2.140080	0.206797	-4.861865
C	2.586218	-0.705521	2.348086
H	2.399138	-1.176210	1.379343
C	-2.510915	-0.883767	2.346315
H	-2.290784	-1.341108	1.378128
C	2.587839	-0.704989	-2.346619
H	2.400121	-1.177243	-1.378761
C	-2.509422	-0.879788	-2.347092
H	-2.289989	-1.337251	-1.378804
C	3.262777	0.636658	2.082222
H	4.203364	0.491942	1.546441
H	2.625958	1.290282	1.480085
H	3.485244	1.156562	3.016734
C	3.501966	-1.637895	3.134995
H	3.027239	-2.604131	3.316741
H	4.428655	-1.811001	2.583983
H	3.769805	-1.210920	4.103686
C	-3.360783	-1.876654	3.133088
H	-4.272634	-2.113932	2.581218
H	-2.820541	-2.807574	3.316213
H	-3.658697	-1.468474	4.101099
C	-3.278460	0.408229	2.078834
H	-3.537133	0.912070	3.012826
H	-2.687873	1.103963	1.476765
H	-4.206323	0.198436	1.542400
C	3.264442	0.636668	-2.078184
H	2.627448	1.289357	-1.475219
H	4.204794	0.490956	-1.542258
H	3.487331	1.158089	-3.011752
C	3.503920	-1.636203	-3.134491
H	3.772695	-1.207577	-4.102193
H	4.430118	-1.810560	-2.583048
H	3.029064	-2.601975	-3.318345
C	-3.358831	-1.872511	-3.134583
H	-4.271272	-2.109508	-2.583569
H	-3.655668	-1.464310	-4.102916
H	-2.818661	-2.803589	-3.317130
C	-3.277008	0.412238	-2.079947
H	-4.205137	0.202477	-1.543965
H	-2.686650	1.107885	-1.477550
H	-3.535223	0.916187	-3.014005

$[IPrAuOC]^+$

C	0.053982	-0.615509	0.000640
C	0.237746	-2.729307	-0.673799
C	0.213538	-2.729796	0.679693
H	0.315766	-3.532927	-1.385674
H	0.266082	-3.533928	1.393323
N	0.099918	-1.417551	1.074570
N	0.138241	-1.416782	-1.071540
Au	-0.104778	1.340835	-0.001495
C	-0.373569	4.648601	-0.005092
O	-0.281756	3.520790	-0.003920
C	0.124583	-0.949648	-2.427812
C	1.344248	-0.623326	-3.023882
C	1.298747	-0.141973	-4.327186
C	0.093352	0.000420	-4.992190
C	-1.096101	-0.337306	-4.370380
C	-1.109696	-0.823466	-3.068142
H	2.221406	0.124867	-4.828857
H	0.081024	0.376300	-6.008465
H	-2.031222	-0.221940	-4.905555
C	0.037799	-0.951388	2.429822
C	1.235450	-0.626323	3.069623
C	1.143406	-0.145875	4.370799
C	-0.085042	-0.003137	4.992120
C	-1.251574	-0.339606	4.327678
C	-1.218629	-0.824824	3.025430
H	2.047586	0.120002	4.905535
H	-0.133670	0.372026	6.007571
H	-2.205270	-0.224013	4.828952
C	-2.417036	-1.169111	-2.393095
H	-2.193877	-1.614334	-1.419957
C	2.665320	-0.754847	-2.301557
H	2.482383	-1.232226	-1.335294
C	-2.501075	-1.169246	2.303634
H	-2.243385	-1.613096	1.338433
C	2.581536	-0.758081	2.395095
H	2.433242	-1.235443	1.422903
C	-3.246782	0.087354	-2.142463
H	-4.173761	-0.163429	-1.622299
H	-2.698568	0.809373	-1.531353
H	-3.511047	0.577444	-3.082211
C	-3.206852	-2.200883	-3.192293
H	-2.621972	-3.106856	-3.363051
H	-4.116937	-2.477971	-2.656282
H	-3.505302	-1.808519	-4.166660
C	3.639109	-1.644071	-3.068450
H	4.562475	-1.771564	-2.499695
H	3.214562	-2.632279	-3.256166
H	3.904490	-1.206848	-4.033242
C	3.272128	0.618459	-2.026275
H	3.487379	1.146719	-2.957807
H	2.593169	1.241357	-1.437782
H	4.208204	0.519371	-1.472477
C	-3.321249	0.087667	2.025337
H	-2.751438	0.810531	1.435346
H	-4.228992	-0.162252	1.471900
H	-3.619032	0.576411	2.955713
C	-3.318954	-2.202065	3.072701
H	-3.651581	-1.811148	4.036525
H	-4.209558	-2.478042	2.504368
H	-2.740694	-3.108476	3.262617
C	3.527156	-1.647421	3.196320
H	4.470125	-1.775287	2.660784
H	3.758224	-1.210090	4.169851
H	3.095918	-2.635473	3.369003
C	3.197984	0.615164	2.141750
H	4.153369	0.515974	1.621987
H	2.540703	1.238123	1.529206
H	3.379624	1.143394	3.080434

$[MICAuCO]^+$

N	-0.682414	-1.490860	0.371562
C	-0.891843	0.633205	-0.245185
C	0.462014	0.363450	-0.135295
N	0.494003	-0.943354	0.242689
N	-1.522171	-0.534816	0.069757
C	-2.933011	-0.795124	0.141331
C	-3.627782	-0.321759	1.252412
C	-4.992063	-0.588060	1.292574
C	-5.611159	-1.291042	0.275397
C	-4.883843	-1.743108	-0.813126
C	-3.519647	-1.501736	-0.910148
H	-5.575173	-0.242867	2.137721
H	-6.674970	-1.489867	0.329692
H	-5.385988	-2.289497	-1.601459
C	1.673163	-1.708293	0.535893
C	2.152480	-1.672651	1.845488
C	3.314316	-2.390375	2.103536
C	3.952789	-3.095844	1.098288
C	3.442452	-3.106697	-0.188083
C	2.280191	-2.411965	-0.503195
H	3.722115	-2.400776	3.107072
H	4.857568	-3.648808	1.321573
H	3.952747	-3.668263	-0.961227
C	-2.719253	-2.006866	-2.088437
H	-1.781643	-1.442148	-2.129246
C	-2.964510	0.424894	2.385328
H	-1.914548	0.588119	2.128541
C	1.734773	-2.425777	-1.911553
H	0.774036	-1.903986	-1.915303
C	1.448252	-0.922244	2.951156
H	0.631573	-0.343989	2.510597
C	-2.366153	-3.480874	-1.894921
H	-1.767562	-3.843141	-2.733553
H	-1.803692	-3.638150	-0.973219
H	-3.274027	-4.086494	-1.842558
C	-3.430940	-1.786961	-3.418395
H	-3.722446	-0.743553	-3.557388
H	-2.772293	-2.067178	-4.242730
H	-4.330078	-2.400476	-3.501232
C	-3.597999	1.797000	2.593995
H	-3.060991	2.345369	3.370920
H	-3.575131	2.389645	1.677633
H	-4.638483	1.708836	2.913936
C	-2.991070	-0.406253	3.665843
H	-4.016511	-0.591224	3.993296
H	-2.506260	-1.374017	3.522251
H	-2.474890	0.121896	4.470734
C	1.477924	-3.849153	-2.396206
H	.808306	-4.384147	-1.720842
H	1.023167	-3.832230	-3.388992
H	2.406486	-4.419143	-2.470669
C	2.667665	-1.678314	-2.860705
H	3.645774	-2.161975	-2.912147
H	2.250591	-1.656431	-3.869688
H	2.822721	-0.646442	-2.534224
C	2.378822	0.069696	3.640850
H	1.832530	0.637460	4.396998
H	3.204891	-0.437048	4.144118
H	2.807711	0.776774	2.926548
C	0.829191	-1.896426	3.950423
H	0.274017	-1.353048	4.718051
H	0.144591	-2.588391	3.455968
H	1.600268	-2.487507	4.449976
C	-1.575106	1.882553	-0.559175

C	-2.675163	1.924779	-1.413890
C	-3.298142	3.131528	-1.681357
C	-2.831827	4.303042	-1.102270
C	-1.735147	4.267652	-0.253231
C	-1.109167	3.063777	0.018408
H	-3.040479	1.016843	-1.875522
H	-4.151079	3.157200	-2.348494
H	-3.325392	5.244496	-1.311213
H	-1.374295	5.178709	0.208441
H	-0.273846	3.028850	0.708452
Au	2.114368	1.484659	-0.450154
C	3.707088	2.559648	-0.761348
O	4.626988	3.173937	-0.939386

[MICAu]$^+$

N	-0.207129	-1.360357	0.544038
C	-0.846409	0.577018	-0.345980
C	0.534374	0.567579	-0.280430
N	0.843011	-0.634471	0.269695
N	-1.223332	-0.629463	0.167250
C	-2.555312	-1.131287	0.361459
C	-3.284743	-0.638786	1.441741
C	-4.570193	-1.143207	1.604153
C	-5.081431	-2.085561	0.730525
C	-4.322921	-2.547280	-0.332327
C	-3.034181	-2.076643	-0.547354
H	-5.176546	-0.794035	2.431055
H	-6.085114	-2.466258	0.878289
H	-4.741110	-3.284000	-1.006521
C	2.155773	-1.119675	0.593078
C	2.655464	-0.822942	1.860742
C	3.939915	-1.272495	2.143207
C	4.671857	-1.973427	1.200509
C	4.135813	-2.248979	-0.045455
C	2.854056	-1.829735	-0.382122
H	4.370771	-1.072569	3.116723
H	5.672040	-2.313527	1.441581
H	4.720475	-2.803752	-0.769292
C	-2.195453	-2.591704	-1.694374
H	-1.385517	-1.875974	-1.871997
C	-2.730512	0.369040	2.420254
H	-1.750392	0.697832	2.064515
C	2.279014	-2.132330	-1.745544
H	1.237966	-1.798480	-1.764039
C	1.857570	-0.071200	2.899757
H	0.919060	0.258823	2.446042
C	-1.559027	-3.930695	-1.323898
H	-0.932697	-4.294341	-2.141366
H	-0.944066	-3.845067	-0.426617
H	-2.330910	-4.679712	-1.131898
C	-2.983852	-2.703899	-2.994009
H	-3.476820	-1.764831	-3.254935
H	-2.313578	-2.972682	-3.812663
H	-3.749455	-3.479920	-2.936455
C	-3.615633	1.608497	2.509778
H	-3.160489	2.347691	3.172361
H	-3.757848	2.068099	1.529906
H	-4.599862	1.366158	2.915976
C	-2.522573	-0.272464	3.790210
H	-3.472109	-0.606173	4.214606
H	-1.860967	-1.138895	3.728476
H	-2.083071	0.448555	4.483157
C	2.277440	-3.631423	-2.028339
H	1.741455	-4.181686	-1.253245
H	1.796737	-3.832705	-2.988086
H	3.293476	-4.028212	-2.081203
C	3.026416	-1.364536	-2.832426
H	4.076758	-1.661457	-2.871981
H	2.584925	-1.559779	-3.811906
H	2.990418	-0.286680	-2.651863
C	2.591551	1.179556	3.372190
H	1.974337	1.735215	4.081242
H	3.527041	0.928500	3.876410
H	2.830720	1.840581	2.535582
C	1.500414	-0.985505	4.068881
H	0.884659	-0.450903	4.795273
H	0.948295	-1.864224	3.729876
H	2.399318	-1.332602	4.583374
C	-1.768994	1.618216	-0.781875
C	-2.875674	1.328720	-1.577936
C	-3.736164	2.343344	-1.959618
C	-3.501639	3.649099	-1.553178
C	-2.399571	3.942756	-0.763234
C	-1.535828	2.932672	-0.377990
H	-3.061411	0.313870	-1.904548
H	-4.593041	2.113220	-2.580901
H	-4.180294	4.439035	-1.851565
H	-2.218451	4.959652	-0.437113
H	-0.691302	3.154145	0.264231
Au	1.880398	1.883934	-0.837844

PMe3AuCl

P	1.64711	0.00126	-0.00065
Au	-0.58274	-0.00008	-0.00039
C	2.40223	1.63087	-0.25734
H	2.0735	2.30886	0.53125
H	3.49253	1.56255	-0.24824
H	2.07094	2.03564	-1.2144
C	2.40348	-0.59085	1.53883
H	3.49379	-0.56552	1.47399
H	2.07363	0.03656	2.3678
H	2.07428	-1.61238	1.73308
C	2.4031	-1.03609	-1.28322
H	3.4934	-0.99192	-1.22969
H	2.07396	-2.06777	-1.15327
H	2.073	-0.69454	-2.26506
Cl	-2.85444	-0.00197	0.0005

PEt3AuCl

P	1.36707	0.13001	-0.17923
Au	-0.8585	0.02684	0.00962
C	2.25368	-0.03997	1.40768
H	1.94297	0.81534	2.01385
C	2.09973	-1.11033	-1.30783
H	3.16844	-1.18395	-1.07959
C	1.4267	-2.47409	-1.2823
H	1.49302	-2.94709	-0.30215
H	0.36786	-2.38647	-1.53139
H	1.89534	-3.14182	-2.00816
C	1.96817	-1.33411	2.15332
H	2.4305	-1.31249	3.14189
H	0.89407	-1.48111	2.28489
H	2.36553	-2.20152	1.62422
C	1.99143	1.70918	-0.85201
H	1.59842	1.77611	-1.87057
C	1.56938	2.92526	-0.0428
H	0.48298	2.96785	0.05955
H	2.0008	2.9147	0.95985
H	1.90021	3.84294	-0.53253
H	2.02029	-0.67694	-2.30969
H	3.08201	1.64189	-0.93032
H	3.32449	0.07679	1.20854
Cl	-3.1224	-0.07587	0.20827

P*i*Pr3AuCl

P	-1.02203	0.04294	0.0365
Au	1.22284	0.08235	-0.0008
C	-1.80629	-0.37977	-1.58883
H	-1.92225	0.60193	-2.06317
C	-1.66531	-1.14735	1.28389
H	-2.75428	-1.17614	1.1756
C	-1.10075	-2.53761	1.01683
H	-1.36897	-2.91603	0.02942
H	-0.01035	-2.52903	1.08593
H	-1.48457	-3.24197	1.75928
C	-1.3148	-0.68306	2.69178
H	-1.63144	-1.43779	3.41607
H	-0.23539	-0.54741	2.80039
H	-1.80511	0.25514	2.95609
C	-0.87559	-1.20785	-2.46737
H	-1.33438	-1.36362	-3.4476
H	0.08684	-0.71519	-2.60942
H	-0.68043	-2.18982	-2.03125
C	-3.18257	-1.02651	-1.48446
H	-3.62172	-1.10701	-2.4822
H	-3.11746	-2.03822	-1.07904
H	-3.87498	-0.45932	-0.86272
C	-1.6989	1.6929	0.50906
H	-1.25298	1.85797	1.49611
C	-1.16382	2.77441	-0.42157
H	-0.07413	2.75326	-0.47807
H	-1.55837	2.66613	-1.43525
H	-1.46973	3.75856	-0.05819
C	-3.21354	1.7644	0.63353
H	-3.69532	1.66756	-0.3417
H	-3.61983	0.99602	1.29433
H	-3.50297	2.73641	1.04146
Cl	3.49934	0.12736	-0.01141

PCy3AuCl

P	0.01873	-0.17663	-0.42334
Au	0.08859	-0.13997	1.82336
C	3.06168	-1.219	-3.14931
C	1.78469	-0.56434	-2.6358
C	1.60062	-0.80747	-1.13918
C	2.83079	-0.36774	-0.34342
C	4.09038	-1.0377	-0.87303
C	4.2806	-0.77172	-2.35843
H	1.83022	0.51294	-2.82984
H	0.92939	-0.94826	-3.19562
H	2.96078	-2.30838	-3.0698
H	3.18787	-0.99436	-4.21232
H	2.94964	0.71804	-0.40326

H	2.6849	-0.60146	0.7141
H	4.95765	-0.68963	-0.30559
H	4.02086	-2.11951	-0.70472
H	4.44138	0.30218	-2.51615
H	5.17715	-1.27843	-2.72604
H	1.49762	-1.89152	-0.98469
C	-3.30856	-2.70897	-0.60924
C	-2.37097	-1.62709	-0.09399
C	-1.26096	-1.33426	-1.10518
C	-1.85863	-0.95197	-2.46018
C	-2.789	-2.04539	-2.9703
C	-3.89119	-2.34931	-1.96728
H	-2.93828	-0.7106	0.1028
H	-1.93324	-1.92278	0.86228
H	-2.75349	-3.65169	-0.69211
H	-4.10686	-2.88126	0.11762
H	-2.42947	-0.02327	-2.35921
H	-1.07733	-0.75645	-3.19738
H	-3.21634	-1.74566	-3.93151
H	-2.20599	-2.95571	-3.15705
H	-4.53445	-1.46685	-1.86203
H	-4.52833	-3.15783	-2.33616
H	-0.69523	-2.26669	-1.24164
C	-1.97812	3.40204	-1.08674
C	-1.64816	2.02122	-0.53766
C	-0.33808	1.48498	-1.121
C	0.79504	2.4735	-0.84789
C	0.46411	3.86012	-1.38451
C	-0.84787	4.38382	-0.82358
H	-1.5449	2.07356	0.55254
H	-2.47432	1.3346	-0.73512
H	-2.15603	3.33085	-2.16724
H	-2.90935	3.76056	-0.63947
H	0.9664	2.5241	0.23409
H	1.72637	2.12514	-1.29752
H	1.28252	4.54664	-1.15047
H	0.39743	3.81441	-2.47885
H	-0.74501	4.53203	0.25794
H	-1.08263	5.36142	-1.25361
H	-0.4506	1.36985	-2.20612
Cl	0.16874	-0.07883	4.10065

P*t*Bu3AuCl

P	-0.87011	-0.00012	-0.00047
Au	1.38769	-0.00437	-0.00437
C	-1.48902	1.57361	0.85266
C	-1.49356	-0.04756	-1.78777
C	-1.49577	-1.52224	0.93773
C	-0.63759	-2.73338	0.55289
H	-0.73061	-3.02175	-0.48991
H	0.41812	-2.55151	0.76158
H	-0.96279	-3.58287	1.16148
C	-1.2638	-1.31722	2.43577
H	-1.928	-0.57306	2.87133
H	-1.46354	-2.26722	2.93976
H	-0.22927	-1.04173	2.64978
C	-2.96831	-1.85492	0.70923
H	-3.17194	-2.15829	-0.31704
H	-3.23685	-2.69819	1.35303
H	-3.63176	-1.02797	0.95956
C	-0.62538	1.83977	2.09181
H	-0.94435	2.79226	2.52616
H	-0.71882	1.07936	2.86132
H	0.42971	1.92448	1.82544
C	-2.96057	1.54591	1.25965
H	-3.62679	1.34639	0.42107
H	-3.16315	0.81307	2.04
H	-3.22652	2.52737	1.66433
C	-1.25449	2.77027	-0.07077
H	-1.92209	2.78537	-0.93057
H	-1.44559	3.68037	0.50505
H	-0.22103	2.81348	-0.42005
C	-2.96524	0.31981	-1.96801
H	-3.22678	0.1903	-3.02292
H	-3.63374	-0.31395	-1.38608
H	-3.16902	1.35913	-1.71277
C	-1.26061	-1.44738	-2.35913
H	-1.45263	-1.40689	-3.4352
H	-0.2275	-1.77141	-2.2197
H	-1.92865	-2.19688	-1.93851
C	-0.6305	0.89081	-2.63979
H	-0.95525	0.79487	-3.6805
H	-0.71855	1.93729	-2.36334
H	0.42395	0.61393	-2.58719
Cl	3.66694	-0.00866	-0.00848

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