Supplementary Information:

Coordination and Insertion of Alkenes and Alkynes in Au^{III} Complexes: Nature of the Intermediates from a Computational Perspective

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DFT Functional Benchmarking

The geometry of the Zeise's salt anion, $[PtCl_3(ethylene)]^-$, was fully optimized using Gaussian09[1] at the DFT(PBE0)[2] (already used by us in a previous study[3]), DFT(PBE0-GD3)[4] and B2PLYPD[5] levels (see Table S1). The optimized distances and their root-mean square deviations from the X-ray structure are given in Table S3.

Table S1. Optimized bond distances in $[PtCl_3(ethylene)]^-$ and their root-mean square deviations, in Å, from the X-Ray structure for different DFT functionals.

	Exp	**PBE0**	**PBE0-D3**	**B2PLYPD**
Pt-Cl_{cis1}	2.297	2.335	2.337	2.350
Pt-Cl_{cis2}	2.297	2.335	2.337	2.350
Pt-Cl_{trans}	2.335	2.331	2.33	2.346
PtC_1	2.140	2.097	2.100	2.109
PtC_2	2.165	2.097	2.100	2.109
C_1-C_2	1.375	1.404	1.403	1.411
RMSD		0.041	0.040	0.043

[1] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[2] C. Adamo, V. Barone, *J. Chem. Phys.* **1999**, *110*, 6158-6170.

[3] E. Langseth, M. L. Scheuermann, D. Balcells, W. Kaminsky, K. I. Goldberg, O. Eisenstein, R. H. Heyn, M. Tilset, *Angew. Chem., Int. Ed.* **2013**, *52*, 1660-1663.

[4] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, **2010**, *132,* 154104.

[5] T. Schwabe and S. Grimme, *Phys. Chem. Chem. Phys.*, **2007**, *9*, 3397.

Complete energy profiles for AuX_3(ethylene) with X = Cl and Me.

The energy profile for the rotation of ethylene in AuX_3(ethylene) with X = Cl and Me, its insertion into the Au-X bond and the cis-trans isomerization of **Au-D-en-Cl** show that the insertion process has the highest energy barrier.

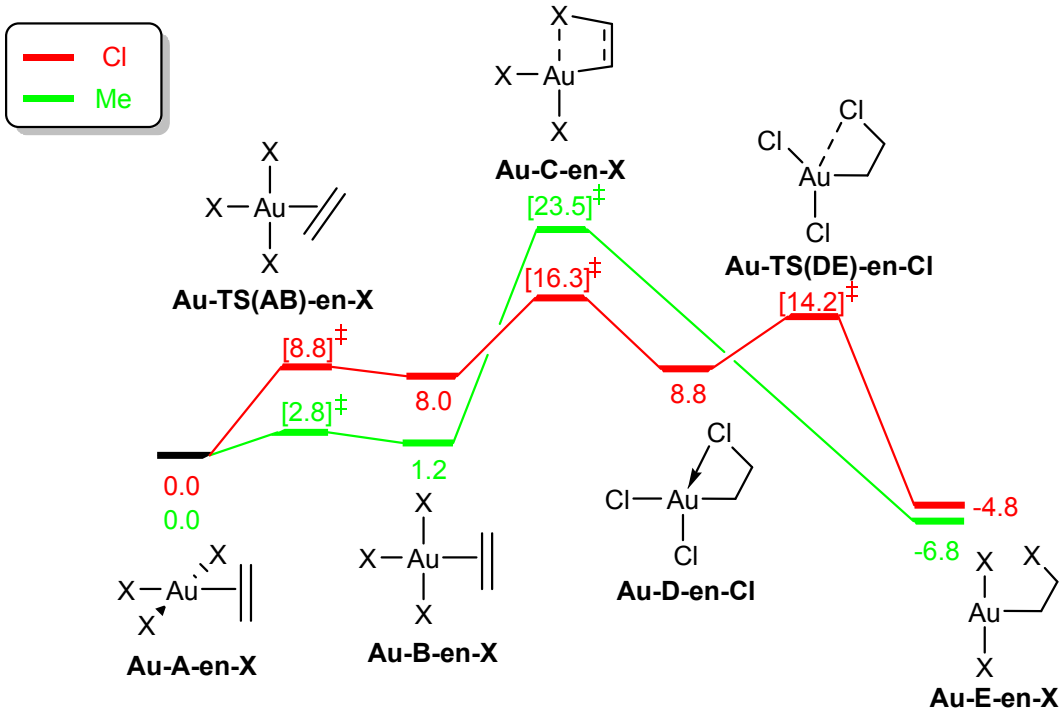

Figure S1. Free Gibbs energy profiles, in kcal mol^{-1}, for the rotation and insertion into the Au-X bond of ethylene in AuX_3L (X = Cl (red) and Me (green)). The *cis-trans* isomerization profile is also given for X = Cl. Square bracketed energies are for TS.

Energy profiles for $AuCl_3$(ethylene) in toluene and TFE

Solvent effects in the energy profile for the rotation and insertion of ethylene into the Au-Cl bond of $AuCl_3$(ethylene) were evaluated (Figure S2). This was done by performing SCRF(SMD) single point calculations in toluene (ε=2.7) and TFE (ε=26.7) on the gas-phase optimized geometries. The Gibbs free energies in solvent were obtained by adding the thermochemistry parameters (zero-point, thermal and entropy energies at the PBE0+GD3 level) calculated in gas phase for the standard conditions (T = 298 K and p = 1 atm) to the potential energies calculated in solvent. The main energy difference found upon comparing the gas-phase results with those in solvent are within a range of 1-2 kcal/mol for each stationary point. The barriers and reaction energies become lower and more exoergic, respectively, by increasing the polarity of the solvent thus favoring the overall process.

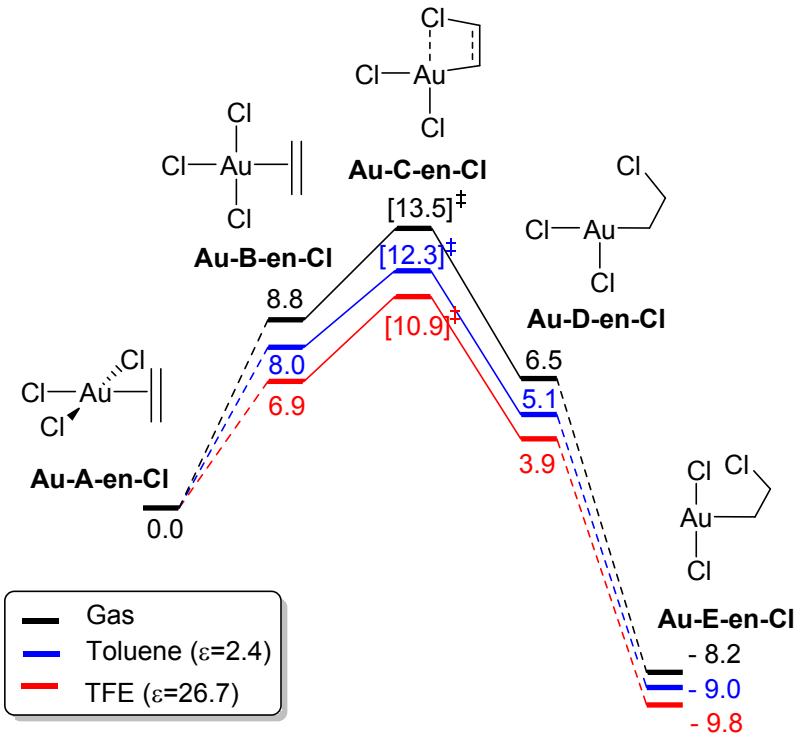

Figure S2. Free Gibbs energy profiles, in kcal mol^{-1}, for the rotation and insertion of ethylene into the Au-Cl bond of $AuCl_3L$ in gas phase (black), toluene (blue) and TFE (red). Transition state energies are given within brackets.

NBO analysis with acetylene

The relative stabilities of the in- and out-of-plane coordination isomers of acetylene to MX_3 (M = Pt and Au; X = Cl, Me and H) are supported by the gold-acetylene donor-acceptor stabilization energies and the X-acetylene steric exchange energies shown in Figures S2a and S2b, respectively.

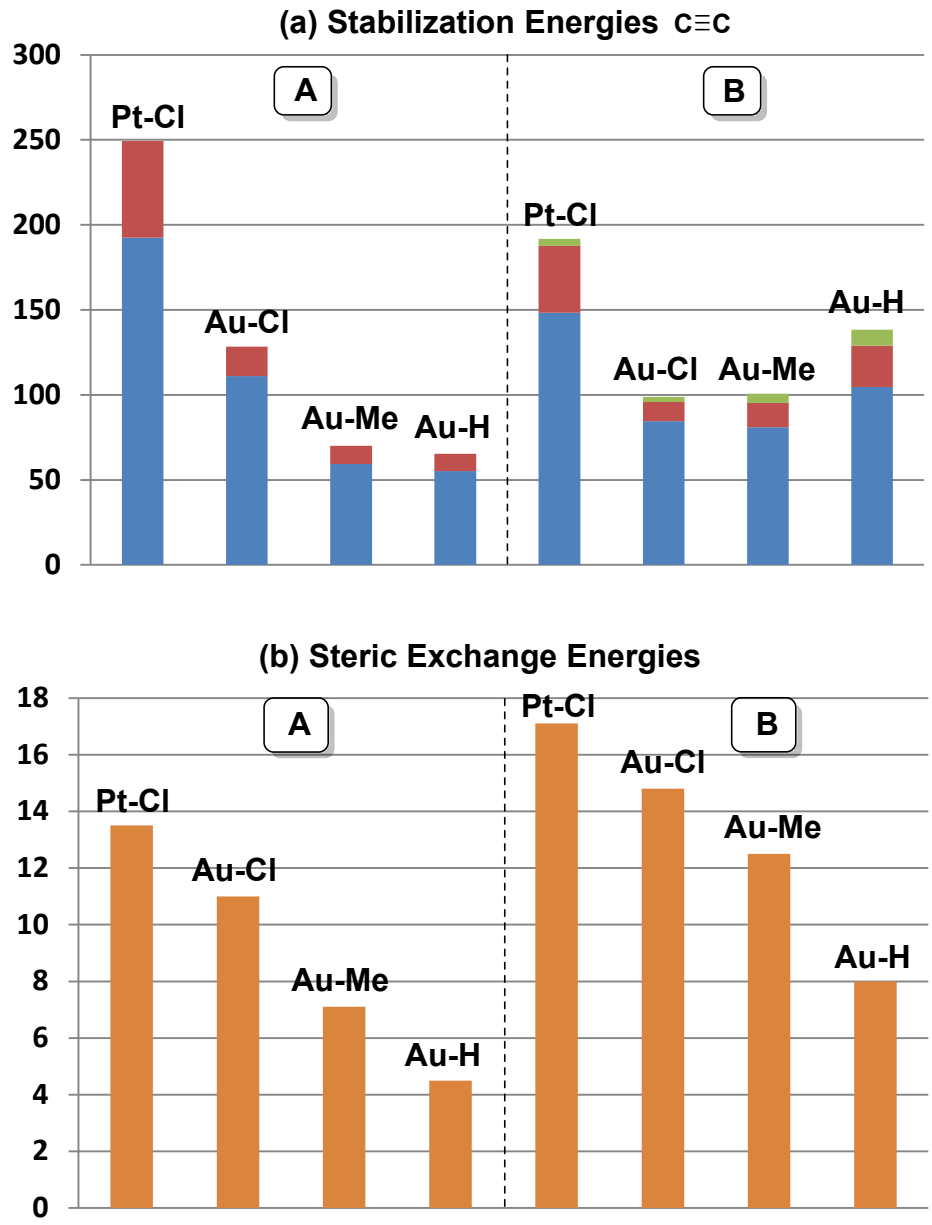

Figure S3. (a) Stabilization energies for $\pi_{CC} \rightarrow \sigma^*_{M\text{-}Xt}$ donation (blue bars), M(d) $\rightarrow \pi^*_{CC}$ back donation (red bars) and X(*p/sp/s*) $\rightarrow \pi^*_{CC}$ back donation (green bars). (b) Steric exchange energies between ethylene and X^c fragments (orange bars) in **Au-A-yn-X** and **Au-B-yn-X** for X = Cl, Me and H, and in **Pt-A-yn-Cl** and **Pt-B-yn-Cl**. Energies are given in kcal mol^{-1}.

<u>Optimized coordinates and energies</u>

MX_3(ethylene)

Au-A-en-Cl
$G_{CCSD(T)}$: -1593.12536
Au 0.216573 0.118056 0.009787

C	1.797372	-1.331425	0.679816
C	1.763303	-1.350922	-0.696296
Cl	-1.449749	1.672985	0.029005
Cl	1.820091	1.779529	-0.053474
Cl	-1.329375	-1.597137	0.072386
H	2.509203	-0.701795	1.204326
H	2.447874	-0.736896	-1.272996
H	1.177868	-2.098502	-1.222262
H	1.239197	-2.063400	1.255058

Au-A-en-Me

$G_{CCSD(T)}$: -333.2425939

Au	-0.006423	-0.017013	-0.004632
C	-0.001897	-2.287634	-0.658618
C	0.004709	-2.270339	0.696758
C	0.002663	2.024783	-0.043015
C	-2.115118	0.036889	-0.039820
C	2.102786	0.049329	0.055964
H	-0.930041	-2.365865	-1.214560
H	-0.919231	-2.333683	1.262036
H	0.934072	-2.329175	1.253560
H	0.921950	-2.359728	-1.222633
H	-2.471400	0.631771	-0.887180
H	-2.565000	-0.961125	-0.113327
H	-2.490100	0.508448	0.875127
H	0.803732	2.394880	0.597626
H	0.202341	2.318447	-1.076619
H	-0.963493	2.416723	0.273313
H	2.432743	0.366253	1.051972
H	2.560556	-0.924714	-0.156529
H	2.495025	0.771490	-0.666516

Au-A-en-H

$G_{CCSD(T)}$: -215.5995972

Au	-0.149861	-0.000176	0.000527
C	2.141497	0.001680	0.682812
C	2.144658	-0.025557	-0.670573
H	-1.696780	0.007784	-0.003246
H	-0.228568	1.631538	-0.032493
H	-0.245494	-1.630994	0.033122
H	2.208388	0.939568	1.224020
H	2.214164	0.889804	-1.248760
H	2.204569	-0.964095	-1.211472
H	2.198795	-0.914332	1.261307

Au-TS(AB)-en-Cl

$G_{CCSD(T)}$: -1593.111386

Au	-0.114501	-0.000670	0.003010
C	2.095443	-0.736610	-0.287528
H	2.130031	-1.643251	0.304003

C	2.160973	0.494446	0.297945
H	2.236906	0.603890	1.375006
H	2.293544	1.392107	-0.293440
H	2.161254	-0.853654	-1.364458
Cl	-0.346007	-2.275847	-0.458384
Cl	-2.394864	0.121763	0.000764
Cl	-0.102032	2.286260	0.464196

Au-TS(AB)-en-Me

$G_{CCSD(T)}$: -333.2381042

Au	-0.129491	0.013526	-0.001342
C	2.112202	-0.642702	-0.425487
H	2.145187	-1.667923	-0.079941
C	2.172516	0.401869	0.440869
H	2.231287	0.234332	1.512351
H	2.330671	1.416077	0.097992
H	2.198334	-0.485837	-1.496744
C	-0.354447	-2.097946	0.089199
H	0.003608	-2.575976	-0.829260
H	0.220850	-2.501532	0.930762
H	-1.400236	-2.378394	0.230006
C	-2.174964	0.073227	0.009421
H	-2.516128	-0.406324	0.928753
H	-2.543583	1.095766	-0.043820
H	-2.528769	-0.502263	-0.848238
C	-0.094572	2.131946	-0.102115
H	-1.085403	2.538588	-0.312374
H	0.257771	2.568668	0.839164
H	0.578723	2.460939	-0.902703

Au-B-en-Cl

$G_{CCSD(T)}$: -1593.112556

Au	-0.000115	0.023031	0.000074
C	0.679114	-2.221967	0.059065
C	-0.681664	-2.221588	-0.044974
Cl	0.001065	2.306593	-0.007019
Cl	2.324888	0.129594	0.177530
Cl	-2.325007	0.130891	-0.178049
H	1.311962	-2.301357	-0.817712
H	-1.173910	-2.300664	-1.007771
H	-1.314590	-2.294875	0.832278
H	1.171282	-2.295570	1.022337

Au-B-en-Me

$G_{CCSD(T)}$: -333.2407295

Au	-0.111459	0.011767	-0.006139
C	2.134075	0.589739	0.100245
C	2.073680	-0.773607	0.110074
C	-2.162558	0.070406	-0.109118
C	-0.255996	2.139397	-0.033458

C	-0.377858	-2.106843	0.000666
H	2.305810	1.138208	-0.819066
H	2.196773	-1.348010	-0.800766
H	2.105258	-1.330655	1.039275
H	2.214242	1.155506	1.021615
H	-0.871336	2.439874	0.819526
H	0.683730	2.692976	0.008795
H	-0.781993	2.423213	-0.949590
H	-2.470719	-0.463110	-1.010308
H	-2.559413	-0.444751	0.767739
H	-2.524807	1.097272	-0.137778
H	-1.440632	-2.347735	-0.049141
H	0.117609	-2.568935	-0.858672
H	0.030853	-2.552508	0.912699

Au-B-en-H

$G_{CCSD(T)}$: -215.6111384

Au	-0.080685	-0.002619	0.002405
C	2.073366	0.697861	0.020358
C	2.080648	-0.680518	0.006644
H	-1.637914	-0.010767	-0.005603
H	-0.280979	1.609398	0.017467
H	-0.263936	-1.616642	-0.014630
H	2.203231	1.266503	-0.893645
H	2.216417	-1.229458	-0.918479
H	2.207048	-1.247820	0.921965
H	2.193862	1.248142	0.946799

Au-C-en-Cl

$G_{CCSD(T)}$: -1593.099323

Au	-0.037903	-0.150862	-0.000025
C	2.135238	-1.757664	0.005771
C	0.793952	-2.149512	-0.001174
Cl	-0.944571	1.970752	0.001038
Cl	2.171175	0.692899	0.011553
Cl	-2.105241	-1.119711	-0.011318
H	0.375140	-2.548902	0.918721
H	2.697166	-1.712972	0.930969
H	0.383408	-2.544479	-0.926688
H	2.705439	-1.708606	-0.914127

Au-C-en-Me

$G_{CCSD(T)}$: -333.2051344

C	2.181453	-1.001007	0.215859
C	1.089067	-1.919096	0.052052
H	0.791876	-2.501236	0.920279
H	2.647533	-0.957988	1.194846
Au	-0.065794	-0.145219	-0.041286
H	1.018577	-2.451491	-0.892818
H	2.883018	-0.911605	-0.607322

C	-1.075987	1.675254	-0.101642
H	-1.593580	1.834433	0.850465
H	-0.373271	2.501271	-0.260077
H	-1.824131	1.687312	-0.898983
C	-1.863948	-1.094954	-0.297904
H	-2.147701	-0.987642	-1.347405
H	-1.787552	-2.152365	-0.043190
H	-2.613147	-0.608224	0.328048
C	1.947685	1.041312	0.215589
H	1.501983	1.596406	1.043262
H	1.795479	1.561895	-0.731377
H	3.016524	0.987518	0.398978

Au-C-en-H

$G_{CCSD(T)}$: -215.5981122

Au	0.049390	0.116149	0.001852
C	-2.197432	-0.293482	-0.008455
C	-1.431661	-1.488551	-0.004836
H	-1.334508	-2.056438	-0.923353
H	-2.692088	0.017881	-0.923558
H	-1.342966	-2.056291	0.914626
H	-2.700488	0.018027	0.902007
H	1.347636	-0.798595	0.007898
H	1.047599	1.343519	0.006349
H	-1.318728	1.089237	-0.004522

Au-D-en-Cl

$G_{CCSD(T)}$: -1593.111322

Au	0.114787	-0.061492	-0.129541
C	-2.493103	-1.065055	-0.006853
C	-1.128512	-1.689438	0.071216
Cl	1.241021	1.977567	-0.381264
Cl	-2.173451	0.774955	-0.234475
Cl	1.953266	-1.367724	0.033278
H	-0.910730	-2.146148	1.035364
H	-3.082743	-1.340028	-0.878290
H	-3.083738	-1.119285	0.904683
H	-0.909688	-2.367383	-0.752253

Au-D-en-H

$G_{CCSD(T)}$: -215.6056524

C	-1.793238	-0.749436	0.000027
C	-1.568589	0.734724	-0.000043
H	-1.888846	1.251962	0.901015
H	-2.267954	-1.142952	0.899927
Au	0.438441	0.119292	0.000046
H	-1.888797	1.251870	-0.901171
H	-2.267895	-1.143045	-0.899864
H	1.233772	1.436476	-0.000003
H	1.856681	-0.651169	0.000130

H	-0.790759	-1.380984	0.000093

Au-E-en-Cl

$G_{CCSD(T)}$: -1593.132942

C	1.874752	-1.307552	0.591142
C	0.841815	-0.486267	1.290879
Cl	-1.467417	-1.914525	-0.240927
Cl	2.858184	-0.375853	-0.563665
Cl	0.082546	2.343662	0.034839
H	0.245985	-1.074186	1.989912
H	2.556107	-1.678433	1.367665
Au	-0.592492	0.181357	-0.042420
H	1.443194	-2.158877	0.067356
H	1.215866	0.441378	1.719931

Au-E-en-Me

$G_{CCSD(T)}$: -333.2533655

C	-1.860286	0.094906	-0.549449
C	-0.665398	-0.777088	-0.830082
H	-0.774549	-1.790166	-0.442423
H	-1.705282	1.090944	-0.972470
Au	1.033862	-0.057579	0.073207
H	-2.688076	-0.357791	-1.119506
H	-0.379248	-0.790378	-1.882538
C	-2.254038	0.187989	0.916932
H	-3.191415	0.736894	1.037208
H	-2.383975	-0.806032	1.355710
C	1.045963	1.677631	-1.099183
H	2.070108	2.074534	-1.142459
H	0.723914	1.507786	-2.132386
H	0.406136	2.458810	-0.672158
C	1.135158	-1.735937	1.309624
H	0.241513	-1.846915	1.933568
H	1.272448	-2.663075	0.742053
H	1.998533	-1.625638	1.981772
H	-1.480972	0.705693	1.492767

Au-E-en-H

$G_{CCSD(T)}$: -215.6042664

Au	0.541463	-0.087039	-0.032563
C	-2.320144	-0.549150	0.494339
C	-1.188713	0.289877	1.012814
H	-1.333008	1.362633	0.882525
H	-2.121841	-1.616222	0.601238
H	-3.214427	-0.306154	1.088042
H	-0.911063	0.075276	2.045024
H	-2.540689	-0.338334	-0.552707
H	1.111853	1.031602	0.999138
H	-0.008731	-1.222901	-1.090658

Au-TSre-en-Cl

$G_{CCSD(T)}$:-1593.095828

C	2.125879	-1.294281	0.086282
C	1.306999	-0.508627	1.040289
Cl	-2.636618	-1.097724	-0.126837
Cl	3.687336	-0.569634	-0.332025
Cl	1.065277	1.579281	0.008252
H	0.484779	-1.078143	1.475018
H	2.335345	-2.243430	0.599546
Au	-0.795057	0.216120	-0.026762
H	1.589135	-1.528079	-0.832505
H	1.831041	0.090886	1.773116

Au-TSre-en-Me

$G_{CCSD(T)}$:-333.241826

C	2.319655	-0.843491	0.491342
C	1.349465	0.173930	1.054676
H	0.767363	-0.245924	1.889102
Au	-0.593010	0.039989	0.047950
H	1.773451	-1.713374	0.113558
H	1.858631	1.049945	1.453813
C	0.855837	1.580425	-0.413984
H	0.275288	1.677319	-1.342923
H	0.700371	2.454615	0.215530
H	1.902756	1.478269	-0.688698
C	-2.400962	-0.913186	-0.204300
H	-2.971400	-0.939600	0.729540
H	-3.007201	-0.389422	-0.951361
H	-2.262255	-1.942192	-0.551390
C	3.317233	-1.285228	1.559886
H	4.019063	-2.020041	1.156371
H	3.898390	-0.436862	1.934812
H	2.807357	-1.744117	2.412231
H	2.858637	-0.421583	-0.363560

Au(I)-enCl_2

$G_{CCSD(T)}$:-1593.142754

C	2.487775	-0.719682	0.897129
C	2.205933	0.749127	1.041466
Cl	-2.779941	-1.015245	0.171996
Cl	3.485950	-1.083467	-0.531555
Cl	1.150657	1.381336	-0.297735
H	1.661107	0.950419	1.964105
H	3.042073	-1.047531	1.779384
Au	-0.874708	0.152609	-0.076031
H	1.564011	-1.295934	0.818942
H	3.109174	1.355701	0.986467

Au(I)-en-Me_2

$G_{CCSD(T)}$: -333.3076761

C	-3.256978	-0.369337	0.570309
C	-2.406989	0.386758	-0.442860
H	-1.988887	-0.319692	-1.169107
Au	1.094364	0.133512	0.055495
H	-2.614408	-1.058994	1.132559
H	-3.041801	1.075853	-1.013333
C	-1.277062	1.176241	0.198116
H	-0.674050	0.489773	0.858193
H	-0.665221	1.698328	-0.548239
H	-1.629650	1.934576	0.903393
C	2.935832	-0.631733	-0.258155
H	3.298138	-0.313410	-1.239038
H	3.615476	-0.269711	0.517320
H	2.888728	-1.722881	-0.222438
C	-4.396098	-1.143676	-0.076470
H	-4.988116	-1.682556	0.667912
H	-5.071766	-0.473299	-0.617592
H	-4.014609	-1.877508	-0.793629
H	-3.659796	0.339764	1.304641

Pt-A-en-Cl

$G_{CCSD(T)}$: -1577.06085

Pt	0.000002	0.051589	0.000005
C	0.000001	2.030677	-0.701602
C	-0.000008	2.030677	0.701609
Cl	0.000008	-2.279052	0.000007
Cl	2.337167	0.086904	0.000019
Cl	-2.337164	0.086892	-0.000009
H	0.924885	2.202505	-1.243765
H	0.924870	2.202505	1.243783
H	-0.924893	2.202501	1.243772
H	-0.924878	2.202500	-1.243776

Pt-B-en-Cl

$G_{CCSD(T)}$: -1577.034038

Pt	0.000000	0.098605	0.000000
C	0.689222	2.156277	0.000000
C	-0.689222	2.156277	0.000000
Cl	0.000000	-2.228447	0.000000
Cl	2.362450	-0.100854	0.000000
Cl	-2.362450	-0.100854	0.000000
H	1.250711	2.292609	0.917373
H	-1.250711	2.292609	0.917372
H	-1.250711	2.292609	-0.917373
H	1.250712	2.292609	-0.917373

Pt-C-en-Cl

$G_{CCSD(T)}$: -1576.994209

Pt	-0.085449	-0.051926	-0.000073
C	2.427534	-1.110973	0.000651

C	1.154905	-1.745063	-0.000146
Cl	-1.330396	1.962446	-0.000049
Cl	2.045114	1.051457	0.000536
Cl	-1.953796	-1.395062	-0.000634
H	0.887879	-2.269993	0.916836
H	3.011707	-1.076781	0.914460
H	0.888760	-2.269537	-0.917642
H	3.012821	-1.076608	-0.912441

Pt-D-en-Cl

$G_{CCSD(T)}$: -1576.999942

Pt	-0.119426	-0.054462	0.008644
C	2.525691	-0.880489	-0.094044
C	1.216778	-1.592536	0.015520
Cl	-1.403787	1.987764	-0.003294
Cl	2.074363	0.971120	-0.058330
Cl	-1.914704	-1.474112	0.069409
H	1.033063	-2.246095	-0.841905
H	3.214542	-0.981639	0.744697
H	3.049396	-0.982692	-1.043902
H	1.129568	-2.155278	0.949446

Pt-E-en-Cl

$G_{CCSD(T)}$: -1577.018594

Pt	-0.611225	0.176843	-0.014238
C	1.852087	-1.327345	0.607096
C	0.819744	-0.418862	1.228347
Cl	-1.421048	-1.986873	-0.286196
Cl	2.971572	-0.475112	-0.530961
Cl	-0.047428	2.409388	0.108611
H	0.311089	-0.992225	2.015527
H	2.504977	-1.749072	1.379038
H	1.389771	-2.132118	0.038148
H	1.289001	0.466079	1.669340

MX_3(acetylene)

Au-A-yn-Cl

$G_{CCSD(T)}$: -1591.88444

Au	0.049410	0.057462	-0.005095
C	1.664960	1.529506	-0.585221
C	1.563131	1.613356	0.628390
Cl	-1.580707	-1.519862	-0.032886
Cl	1.664783	-1.572795	0.245013
Cl	-1.522408	1.729864	-0.254459
H	1.598126	1.805042	1.681292
H	1.876202	1.576083	-1.633924

Au-A-yn-Me

$G_{CCSD(T)}$: -332.0064574

Au	0.104972	-0.002252	-0.002413
C	-2.242863	0.013751	-0.598223
C	-2.241307	-0.007515	0.612028
C	2.137752	0.007581	-0.004680
C	0.155965	-2.108578	-0.063240
C	0.158442	2.106058	0.036834
H	-2.339623	-0.026127	1.674724
H	-2.348342	0.031956	-1.660290
H	-0.838742	-2.540264	0.093244
H	0.525420	-2.446319	-1.038512
H	0.830381	-2.508120	0.701392
H	2.488238	0.848893	-0.602318
H	2.448406	0.139849	1.034119
H	2.514095	-0.938262	-0.391837
H	0.370891	2.488445	-0.968824
H	-0.800694	2.524219	0.361716
H	0.942225	2.477813	0.704118

Au-A-yn-H

$G_{CCSD(T)}$: -214.3635579

Au	0.109680	-0.000976	0.000500
C	-2.245436	-0.001686	0.603405
C	-2.244376	-0.005038	-0.606520
H	1.645762	0.000581	0.001841
H	0.195663	1.631513	-0.003947
H	0.198963	-1.633287	0.005100
H	-2.343117	-0.008084	-1.669958
H	-2.346042	0.001158	1.666670

Au-B-yn-Cl

$G_{CCSD(T)}$: -1591.878884

Au	0.000150	0.016057	0.000047
C	0.609840	2.281107	0.000181
C	-0.608253	2.281453	0.000078
Cl	-0.000496	-2.258516	-0.000043
Cl	2.331792	-0.089597	0.000217
Cl	-2.331551	-0.088273	-0.000127
H	-1.667368	2.433333	-0.000005
H	1.669041	2.432385	0.000274

Au-B-yn-Me

$G_{CCSD(T)}$: -332.0104635

Au	-0.018939	-0.088642	-0.003524
C	0.606899	-2.325225	0.056318
C	-0.605380	-2.335775	-0.082119
C	0.025475	1.956046	0.012099
C	2.094107	0.060083	0.238200
C	-2.133453	0.008827	-0.244107
H	-1.643719	-2.554347	-0.201774
H	1.649658	-2.522680	0.174317
H	-2.641930	-0.486581	0.590429
H	-2.478126	1.042844	-0.277904
H	-2.440413	-0.477177	-1.176848
H	0.462781	2.273800	0.960350
H	0.664782	2.282944	-0.809975
H	-0.972763	2.373994	-0.099645
H	2.412350	-0.424318	1.167613
H	2.613984	-0.415219	-0.600578
H	2.404273	1.105055	0.278949

Au-B-yn-H

$G_{CCSD(T)}$: -214.3789855

Au	-0.039136	0.001099	0.001286
C	2.011200	-0.865892	-0.010310
C	2.158244	0.357306	0.019339
H	-1.580527	0.186449	-0.001057
H	-0.441096	-1.571993	-0.037761
H	-0.056821	1.624652	0.039694
H	2.585821	1.335878	0.044407
H	2.194672	-1.917942	-0.034449

Au-C-yn-Cl

$G_{CCSD(T)}$: -1591.868685

Au	0.021971	0.116445	0.001676
C	1.265185	2.468632	-0.001072
C	0.046279	2.240787	-0.004051
Cl	-0.034845	-2.173794	0.007757
Cl	2.382770	0.139068	0.008595
Cl	-2.266293	0.220996	-0.005370
H	-0.930493	2.696436	-0.008181
H	2.286253	2.783710	0.001087

Au-C-yn-Me

$G_{CCSD(T)}$: -331.9799775

C	1.963145	-1.181660	-0.583423
C	0.907212	-1.871269	-0.667891

H	0.582354	-2.863630	-0.930177
H	3.030603	-1.120607	-0.690686
Au	-0.070563	-0.131065	-0.025656
C	2.057511	0.845252	0.019348
H	1.548131	1.749607	0.353264
H	2.562382	1.069678	-0.918324
H	2.764022	0.551290	0.793247
C	-1.974131	-0.907225	-0.036485
H	-1.974325	-1.950774	-0.352512
H	-2.384312	-0.825753	0.972011
H	-2.583662	-0.313224	-0.720288
C	-0.882987	1.661860	0.613067
H	-0.434801	1.928116	1.576868
H	-0.634232	2.440911	-0.116231
H	-1.967540	1.622125	0.728783

Au-C-yn-H

$G_{CCSD(T)}$: -214.3670682

Au	0.010034	0.084783	-0.000010
C	2.161742	-0.506292	-0.000085
C	1.423135	-1.524442	-0.000008
H	1.346215	-2.594139	0.000042
H	3.113370	-0.011277	-0.000151
H	1.370382	1.046657	-0.000111
H	-0.964422	1.318315	-0.000016
H	-1.347088	-0.740765	0.000088

Au-D-yn-Cl

$G_{CCSD(T)}$: -1591.891568

C	1.483474	2.145311	0.000183
C	0.178058	1.998648	0.000075
Cl	-0.180176	-2.296952	-0.000106
Cl	2.300777	0.535804	0.000191
Cl	-2.422823	0.301428	-0.000187
H	-0.560153	2.791093	0.000043
H	2.157830	2.990520	0.000266
Au	-0.186159	0.026432	-0.000023

Au-D-yn-Me

$G_{CCSD(T)}$: -332.0460242

C	-2.319538	-0.860699	0.602815
C	-1.114450	-0.897131	1.190668
H	-1.018892	-1.591953	2.030740
H	-3.126286	-1.480157	1.005356

Au	0.517976	0.260835	0.726660
C	-2.702666	-0.041370	-0.588128
H	-3.514589	0.653711	-0.342924
H	-1.858211	0.541841	-0.966097
H	-3.074722	-0.677842	-1.400011
C	1.230879	-0.921952	-0.765434
H	1.635602	-0.270938	-1.536542
H	2.005908	-1.528308	-0.297935
H	0.390639	-1.521117	-1.106271
C	2.132863	1.538555	0.395830
H	3.097440	1.021247	0.388230
H	2.029023	2.083678	-0.548402
H	2.152102	2.275220	1.211742

Au-E-yn-Cl

$G_{CCSD(T)}$: -1591.914228

Au	-0.578511	0.049119	-0.033930
C	2.150480	-0.205236	0.958195
C	0.886042	-0.110469	1.308483
H	0.495971	-0.107598	2.318851
H	2.906700	-0.289203	1.734505
Cl	-0.908631	-2.192333	-0.133754
Cl	2.770416	-0.212239	-0.636270
Cl	-0.445279	2.311082	-0.110737

Au-E-yn-Me

$G_{CCSD(T)}$: -332.0442976

C	-2.342784	0.318619	0.579694
C	-1.116598	0.240007	1.062166
H	-0.837408	0.341780	2.105298
H	-3.114482	0.506625	1.329485
Au	0.506376	-0.058032	-0.038910
C	-2.798133	0.193202	-0.833979
H	-3.270380	1.121928	-1.171474
H	-1.963145	-0.030978	-1.501099
H	-3.544558	-0.601843	-0.931607
C	0.171766	-2.120482	-0.021579
H	0.916663	-2.586723	-0.683567
H	0.288561	-2.549338	0.978156
H	-0.823640	-2.383921	-0.390545
C	0.951294	1.981877	-0.150822
H	1.231224	2.399965	0.821194
H	1.803493	2.114502	-0.833959
H	0.112880	2.564910	-0.543149

Au(I)-yn-H_2

$G_{CCSD(T)}$: -214.4388469

Au	-0.472233	0.526308	-0.020355
C	2.107182	-0.959379	0.047136
C	1.505307	0.227863	-0.056898
H	2.138711	1.108321	-0.171801
H	3.192871	-1.048061	0.018348
H	1.557275	-1.888609	0.164326
H	-2.203806	0.759392	-0.397005
H	-2.175647	0.847063	0.416464

Au-TSre-yn-Cl

$G_{CCSD(T)}$: -1591.895388

Au	-0.563902	0.212354	-0.030496
C	2.086512	-0.734469	0.960850
C	1.167804	0.206044	1.147746
H	0.989515	0.695933	2.095882
H	2.623841	-1.123997	1.819864
Cl	-2.328095	-1.190781	-0.001883
Cl	2.518284	-1.429316	-0.537846
Cl	1.069165	1.844960	-0.293104

Au-TSre-yn-Me

$G_{CCSD(T)}$: -332,0437854

C	2.149319	-0.716191	0.572200
C	1.015252	-0.203836	1.012905
H	0.753021	-0.047012	2.053708
H	2.851569	-1.007277	1.356466
Au	-0.498257	0.346931	-0.145948
C	2.579278	-0.953983	-0.834946
H	2.737105	-2.022672	-1.015280
H	1.832260	-0.591464	-1.544237
H	3.528668	-0.448980	-1.040862
C	0.472790	2.178572	-0.410056
H	-0.124131	2.753643	-1.133404
H	0.535527	2.752798	0.518672
H	1.483547	2.063425	-0.810791
C	-1.580314	-1.435480	0.006750
H	-1.959625	-1.607321	1.019046
H	-2.445505	-1.387053	-0.671380
H	-0.979888	-2.303339	-0.282613

Au(I)-ynCl_2

$G_{CCSD(T)}$: -1591.925282

Au	-0.719906	0.198199	-0.040157
C	2.922376	-0.424617	0.725404
C	2.479939	0.823709	0.758837
H	2.820753	1.553602	1.479640
H	3.659487	-0.746376	1.451540
Cl	-2.648582	-0.928858	0.238968
Cl	2.414621	-1.632685	-0.364917
Cl	1.297413	1.463385	-0.354552

Au(I)-ynMe$_2$

$G_{CCSD(T)}$: -332.125162

C	1.794916	-0.612184	0.565735
C	1.575026	0.743283	0.516726
H	1.342573	1.236758	1.459266
H	1.719339	-1.086190	1.543248
Au	-0.402996	-0.287244	0.104162
C	2.429385	-1.448831	-0.503176
H	1.959820	-2.434225	-0.551972
H	2.362991	-0.991759	-1.491132
H	3.490032	-1.600960	-0.269176
C	1.925685	1.660188	-0.615346
H	1.170028	2.441329	-0.728017
H	2.881560	2.154767	-0.404337
H	2.018196	1.137333	-1.567968
C	-2.370680	-0.616775	-0.338981
H	-3.012711	-0.370350	0.512530
H	-2.684461	-0.013603	-1.197038
H	-2.529603	-1.670403	-0.592929

Pt-A-yn-Cl

$G_{CCSD(T)}$: -1575.81716

Pt	-0.000003	0.075462	0.000000
C	0.000077	2.065685	0.622015
C	-0.000055	2.065686	-0.622013
Cl	-0.000019	-2.245936	0.000001
Cl	-2.339872	0.095376	0.000181
Cl	2.339866	0.095344	-0.000183
H	0.000235	2.430059	1.628756
H	-0.000209	2.430062	-1.628754

Pt-B-yn-Cl

$G_{CCSD(T)}$: -1575.80158

Pt	0.000001	0.119935	0.000006

C	0.616357	2.180374	0.000120
C	-0.616348	2.180376	0.000022
Cl	-0.000003	-2.202374	-0.000071
Cl	2.367266	-0.061828	0.000177
Cl	-2.367265	-0.061819	-0.000174
H	-1.648097	2.460286	-0.000050
H	1.648107	2.460280	0.000209

Pt-C-yn-Cl

$G_{CCSD(T)}$: -1575.773788

Pt	-0.037017	-0.064746	-0.000033
C	2.111989	-1.563220	-0.000068
C	0.892316	-1.863419	-0.000037
Cl	-1.080928	2.032581	-0.000030
Cl	2.186556	0.870605	-0.000067
Cl	-2.065130	-1.179885	0.000000
H	0.289931	-2.760776	-0.000019
H	3.177489	-1.537672	-0.000097

Pt-D-yn-Cl

$G_{CCSD(T)}$: -1575.793879

Pt	0.119724	-0.052198	-0.000011
C	-2.398784	-1.043099	0.000196
C	-1.163392	-1.523505	0.000085
Cl	1.319382	2.025153	-0.000097
Cl	-2.313561	0.774425	0.000206
Cl	1.933117	-1.427368	-0.000176
H	-0.970813	-2.595458	0.000058
H	-3.405933	-1.436623	0.000278

Pt-E-yn-Cl

$G_{CCSD(T)}$: -1575.814487

Pt	-0.601897	0.047054	0.009725
C	2.173685	-0.199156	0.982696
C	0.870946	-0.118346	1.224941
H	0.573291	-0.151337	2.275420
H	2.911649	-0.291530	1.771658
Cl	-1.042649	-2.217515	-0.112721
Cl	2.905763	-0.173800	-0.602251
Cl	-0.513600	2.347753	-0.144125

$[MX_2(ethylene)_2]^+$

Au-F'-en-Me

$G_{CCSD(T)}$: -371.6234841

Au	-0.000026	-0.186788	-0.000002
C	1.378004	-1.710400	0.096062
H	0.985430	-2.543088	0.675868
H	2.272567	-1.303499	0.569337
H	1.585795	-2.026267	-0.927859
C	-1.378082	-1.710386	-0.095908
H	-0.985519	-2.543146	-0.675617
H	-2.272634	-1.303521	-0.569237
H	-1.585888	-2.026133	0.928047
C	1.845671	1.305581	-0.641382
H	2.597814	0.578988	-0.932608
C	1.584333	1.568590	0.659970
H	2.118124	1.063597	1.460049
C	-1.845697	1.305677	0.641226
H	-2.597853	0.579127	0.932524
C	-1.584350	1.568547	-0.660153
H	-2.118147	1.063480	-1.460180
H	-1.419682	1.906764	1.439578
H	0.947955	2.399471	0.949526
H	1.419664	1.906593	-1.439795
H	-0.947957	2.399388	-0.949793

Au-G-en-Me

$G_{CCSD(T)}$: -371.6172478

Au	-0.026099	-0.175034	0.028303
C	1.354800	-1.724839	0.116552
H	0.865938	-2.694468	0.109235
H	1.918635	-1.595065	1.040727
H	2.001651	-1.623366	-0.755307
C	-1.371394	-1.735094	-0.009294
H	-1.170342	-2.346219	-0.888186
H	-2.370824	-1.303299	-0.062294
H	-1.253142	-2.317988	0.903175
C	2.159037	1.050568	0.109989
H	2.560052	0.714169	1.060676
C	1.217380	2.015536	0.051261
H	0.847535	2.488692	0.955522
C	-1.886044	1.345271	0.596409
H	-2.508562	0.648022	1.148946
C	-1.823515	1.323955	-0.756424
H	-2.393436	0.608776	-1.341822
H	-1.444221	2.153287	1.169966
H	0.933190	2.459492	-0.897680
H	2.645526	0.685030	-0.788617

H	-1.329506	2.114181	-1.311909

Au-I'-en-Me

$G_{CCSD(T)}$: -371.6102331

Au	-0.137706	0.274829	0.024690
C	-1.732013	1.619400	-0.061503
H	-1.555773	2.435989	0.632673
H	-2.638608	1.088215	0.217189
H	-1.784020	1.984061	-1.087690
C	0.855746	2.075377	0.382663
H	1.884150	1.967235	0.047341
H	0.804378	2.257735	1.456374
H	0.370301	2.873968	-0.170810
C	-2.045228	-1.165448	-0.665680
H	-2.679756	-1.169697	0.215281
C	-1.007970	-2.024004	-0.771553
H	-0.799464	-2.738248	0.016714
C	2.185528	-0.460095	0.527111
H	2.749330	-0.086091	-0.321998
C	1.538456	-1.643561	0.456875
H	1.581021	-2.243714	-0.444786
H	2.307536	0.057361	1.473096
H	-0.464496	-2.133291	-1.705384
H	-2.377942	-0.579851	-1.516515
H	1.102553	-2.096932	1.342196

Au-J-en-Me

$G_{CCSD(T)}$: -371.5605683

Au	0.153622	0.039355	0.052407
C	-1.861132	1.198583	-0.264345
H	-1.694909	1.663603	0.706053
H	-2.935841	1.171850	-0.411428
H	-1.429773	1.761315	-1.089719
C	0.842093	1.998848	0.494521
H	1.921102	2.139953	0.502720
H	0.448346	2.246363	1.484675
H	0.406511	2.664846	-0.253237
C	-2.099346	-0.735738	-0.511503
H	-2.842442	-0.808479	0.275841
C	-1.020394	-1.690252	-0.427945
H	-1.041861	-2.376974	0.412912
C	2.244635	-0.393200	0.438976
H	2.814631	0.105035	-0.338413
C	1.638426	-1.623187	0.185369

H	1.719252	-2.083525	-0.793387
H	2.443263	-0.077966	1.458167
H	-0.679068	-2.125621	-1.362589
H	-2.507128	-0.584603	-1.505834
H	1.342036	-2.268968	1.005043

Au-K-en-Me

$G_{CCSD(T)}$: -371.5808957

Au	0.279975	0.233338	0.120792
C	-2.113415	0.801713	-0.625459
H	-1.317851	1.331667	0.003032
H	-2.963798	1.409973	-0.301169
H	-1.901629	1.012280	-1.675043
C	1.014521	2.135978	0.676416
H	2.089116	2.203469	0.834926
H	0.500162	2.421786	1.598255
H	0.738335	2.811654	-0.139035
C	-2.294418	-0.692522	-0.329874
H	-2.596962	-0.829346	0.711711
C	-0.979735	-1.399320	-0.596076
H	-0.888357	-2.368660	-0.113873
C	2.240410	-0.406381	0.565898
H	2.911295	0.038303	-0.162713
C	1.503057	-1.571407	0.232589
H	1.597653	-2.015696	-0.752116
H	2.446821	-0.175203	1.606033
H	-0.729392	-1.471453	-1.657316
H	-3.098677	-1.105458	-0.948413
H	1.130911	-2.215474	1.021717

Au-F-en-Cl

Au	0.000000	-0.045810	0.000001
C	1.648401	-1.510148	0.687278
H	2.307157	-0.848191	1.242441
C	1.648420	-1.510138	-0.687258
H	2.307191	-0.848172	-1.242393
C	-1.648402	-1.510145	-0.687279
H	-2.307158	-0.848187	-1.242441
C	-1.648421	-1.510139	0.687256
H	-2.307191	-0.848174	1.242393
H	-1.146044	-2.293219	-1.247271
H	1.146076	-2.293203	-1.247273
H	1.146043	-2.293223	1.247267
H	-1.146077	-2.293206	1.247269

Cl	-1.604315	1.570022	-0.000014
Cl	1.604316	1.570022	0.000021

Au(I)-en-H_2

Au	0.000000	0.044031	0.000002
C	2.197893	0.390988	0.000712
H	2.386570	0.927550	-0.926617
C	2.044290	-0.972001	-0.001022
H	2.070976	-1.539589	-0.927730
C	-2.197893	0.390987	-0.000747
H	-2.386583	0.927564	0.926571
C	-2.044289	-0.972002	0.001023
H	-2.070986	-1.539577	0.927739
H	-2.386322	0.925206	-0.929473
H	2.070686	-1.542017	0.924203
H	2.386334	0.925223	0.929427
H	-2.070675	-1.542031	-0.924194
H	-0.374916	2.975690	0.001423
H	0.374906	2.975686	-0.001283

Pt-F-en-Cl

Pt	-0.000020	-0.071643	0.000146
C	-1.520752	-1.441859	-0.695124
H	-2.231074	-0.830795	-1.241701
C	-1.520766	-1.442020	0.695073
H	-2.231099	-0.831083	1.241777
C	1.520415	-1.442347	0.695093
H	2.230872	-0.831568	1.241811
C	1.520425	-1.442183	-0.695104
H	2.230890	-0.831273	-1.241667
H	1.066204	-2.257688	1.247676
H	-1.066737	-2.257455	1.247666
H	-1.066711	-2.257166	-1.247898
H	1.066221	-2.257391	-1.247889
Cl	1.627083	1.559990	0.000342
Cl	-1.626767	1.560344	0.000319

Pt-F-en-Me

Pt	-0.000034	0.140155	-0.000037
C	1.391917	1.652170	-0.084061
H	1.031583	2.496380	-0.678547
H	2.349002	1.315094	-0.499985
H	1.572598	2.022625	0.933161
C	-1.393619	1.650658	0.083914

H	-1.034276	2.495192	0.678544
H	-2.350402	1.312513	0.499669
H	-1.574549	2.021030	-0.933293
C	1.682852	-1.169730	0.655684
H	2.467850	-0.488717	0.966126
C	1.450906	-1.421851	-0.676713
H	2.043852	-0.942916	-1.449176
C	-1.681437	-1.171648	-0.655709
H	-2.467101	-0.491523	-0.966420
C	-1.449426	-1.423226	0.676781
H	-2.043003	-0.944733	1.449036
H	-1.305531	-1.838075	-1.425495
H	0.895722	-2.302900	-0.984572
H	1.307739	-1.836368	1.425671
H	-0.893371	-2.303620	0.984937

Pt-G-en-H

Pt	0.037292	-0.348470	0.000472
C	-1.779370	0.763533	0.688258
H	-2.360378	0.037440	1.245648
C	-1.780329	0.760746	-0.688772
H	-2.362223	0.032519	-1.242427
C	2.046376	0.537090	-0.001202
H	2.541768	0.232591	0.915062
C	1.129914	1.578220	-0.001521
H	0.905543	2.108175	0.919527
H	2.540854	0.231148	-0.917479
H	-1.449084	1.630065	-1.246936
H	-1.447427	1.635129	1.242436
H	0.904546	2.106831	-0.923105
H	1.003068	-1.606703	0.001241
H	-0.866807	-1.643466	0.002045

Au-F-yn-Cl

Au	-0.000001	0.074208	0.000001
C	1.657661	1.610684	-0.502020
C	1.577285	1.610649	0.715625
C	-1.657689	1.610662	0.502004
H	-1.875836	1.706536	1.549420
C	-1.577313	1.610614	-0.715640
H	-1.655893	1.706407	-1.782650
H	1.655863	1.706456	1.782633
H	1.875806	1.706549	-1.549436
Cl	-1.591947	-1.527346	-0.105119

Cl	1.591972	-1.527318	0.105141

Au-F'-yn-Me

Au	-0.152528	-0.000076	-0.000027
C	-1.666725	-1.375703	0.134318
H	-2.479288	-0.982174	0.741365
H	-1.224287	-2.259538	0.593816
H	-2.011294	-1.581087	-0.880374
C	-1.668051	1.374086	-0.134419
H	-2.480243	0.979753	-0.741441
H	-1.226466	2.258326	-0.593956
H	-2.012808	1.579181	0.880269
C	1.367762	-1.882927	-0.496648
C	1.719679	-1.514702	0.602410
C	1.365919	1.884254	0.496628
C	1.718230	1.516358	-0.602414
H	1.126241	2.308249	1.450290
H	2.115296	1.275916	-1.566941
H	1.128526	-2.307143	-1.450323
H	2.116480	-1.273886	1.566953

Au-I'-yn-H

Au	-0.000012	-0.379749	0.000078
C	1.431221	1.507285	-0.469504
C	2.091394	0.762434	0.229004
C	-1.430983	1.507552	0.469378
C	-2.091260	0.762688	-0.229019
H	-0.989906	2.257288	1.095465
H	-2.799728	0.200892	-0.805538
H	0.990248	2.256987	-1.095704
H	2.799785	0.200627	0.805609
H	-0.886508	-1.651735	0.104373
H	0.886309	-1.651873	-0.104028

Pt-F-ac-Cl

Pt	0.000017	-0.096907	-0.000004
C	-1.482442	-1.530670	-0.616858
H	-1.731970	-1.717959	-1.641504
C	-1.482391	-1.530658	0.617004
H	-1.731833	-1.717927	1.641674
C	1.482792	-1.530329	0.616879
H	1.732362	-1.717542	1.641529
C	1.482741	-1.530342	-0.616983
H	1.732225	-1.717577	-1.641649

Cl	1.626458	1.513304	-0.000089
Cl	-1.626780	1.512944	0.000048

Pt-F'-ac-Me

Pt	0.115873	0.000288	-0.000040
C	1.613227	-1.390056	-0.016549
H	2.419168	-1.105125	-0.699738
H	1.242775	-2.383176	-0.289742
H	2.045867	-1.448084	0.990317
C	1.604416	1.400062	0.018296
H	2.412946	1.119039	0.700019
H	1.227791	2.390212	0.293826
H	2.035543	1.463036	-0.988940
C	-1.369287	-1.577141	0.583531
H	-1.495081	-1.842063	1.611562
C	-1.419442	-1.514518	-0.639521
H	-1.630132	-1.663596	-1.676681
C	-1.378289	1.568568	-0.585539
H	-1.504260	1.832739	-1.613741
C	-1.429778	1.505529	0.637428
H	-1.642831	1.653149	1.674312

Pt-I'-ac-H

Pt	-0.000001	0.285218	-0.018632
C	1.439867	-1.389077	-0.029962
C	2.052262	-0.327932	0.167363
C	-1.439849	-1.389093	-0.029989
C	-2.052260	-0.327955	0.167326
H	-1.295009	-2.440232	-0.161431
H	-2.895073	0.310244	0.330195
H	1.295040	-2.440218	-0.161407
H	2.895065	0.310276	0.330247
H	-0.834229	1.619393	-0.107589
H	0.834215	1.619403	-0.107574