

SUPPORTING INFORMATION

Theoretical study on intramolecular allene-diene cycloadditions catalyzed by PtCl₂ and Au(I) complexes

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1. Tables of electronic NBO and Bader analysis of the seven membered intermediates **3** and **3'**. Some structural parameters are also presented.

Complex (3)	NBO analysis									Structural parameters			
	Occupancy Bond Orbital (e ⁻)				Mayer	Electron donor orbital to LP* C ₂ (kcal/mol)				Distances (Å)			
	σ(C ₂ -M)	π(C ₂ -M)	LP (M)	LP* C ₂	Bond Order	LP (M)	σ (C ₃ -C ₇)	σ(C ₁ -C ₄)	σ(C ₁ -H)	C-M	C ₃ -C ₇	C ₁ -C ₄	C ₁ -H
PtCl ₂	1.814	1.947	1.974	-	1.3041	-	-	-	-	1.848	1.590	1.601	1.097
AuCl	1.967	-	1.814	0.459	0.8675	30.46	11.36	12.96	1.25	1.972	1.600	1.608	1.095
[AuPH ₃] ⁺	1.963	-	1.911	0.451	0.7537	15.17	16.39	20.35	0.96	2.052	1.631	1.655	1.093
[AuP(OMe) ₃] ⁺	1.961	-	1.911	0.428	0.7176	15.14	16.52	20.16	1.03	2.061	1.630	1.648	1.093
[AuNHC] ⁺	1.952	-	1.884	0.415	0.8053	18.21	12.50	21.86	0.88	2.047	1.614	1.654	1.091
Different conformation (3') required for the 1,2-H migration due to it allows overlap between σ(C ₁ -H) bond and C ₂ LP bond													
[AuP(OMe) ₃] ⁺	1.958	-	1.907	0.358	0.7156	15.74	0.60	0.54	27.40	2.071	1.562	1.564	1.119
[AuNHC] ⁺	1.961	-	1.867	0.369	0.8236	20.37	0.62	0.98	23.23	2.043	1.565	1.571	1.115

Complex (3)	Bader analysis		Hyperbonding NBO analysis (L: Au-L)			
	C ₂ -M BCP		Occupancy Bond Orbital (e ⁻)		Donation (kcal/mol)	
	Density (a.u)	Ellipticity	Hyperbond	LP (L)	σ*(C ₂ -Au)	LP (L) to σ*(C ₂ -Au)
PtCl ₂	0.2056	0.1283	-	-	-	-
AuCl	0.1556	0.0773	3.976	1.695	0.314	131.68
[AuPH ₃] ⁺	0.1335	0.0504	3.992	1.689	0.341	120.82
[AuP(OMe) ₃] ⁺	0.1310	0.0499	3.871	1.469	0.442	194.28
[AuNHC] ⁺	0.1345	0.0552	3.950	1.604	0.383	178.13

2. Absolute energies (in hartrees) and cartesian coordinates of the optimized structures.

4a

E(Gas Phase) = -468.083983

6	1.821887	-0.333561	-0.013497
6	0.512830	-1.100840	0.094081
6	1.652495	1.110080	-0.563094
6	-1.255719	0.675292	-0.551586
6	0.717385	1.986244	0.235305
6	-0.603018	1.786241	0.247154
6	-0.747600	-0.718574	-0.140582
1	1.145991	2.794666	0.825265
1	-1.017248	0.845962	-1.613096
6	-1.955827	-1.613490	0.076301
1	-1.765183	-2.418231	0.794290
1	1.291253	1.038530	-1.599954
1	2.646710	1.570522	-0.616811
6	2.471121	-0.286867	1.389242
1	2.616439	-1.298012	1.788142
1	3.454069	0.200374	1.347512
1	1.841973	0.265845	2.094377
6	2.758377	-1.107522	-0.969198
1	2.336250	-1.160356	-1.979445
1	3.739516	-0.619994	-1.033753
1	2.917875	-2.134673	-0.619242
1	-1.251724	2.429294	0.841640
6	-2.801591	0.590497	-0.390540
6	-3.052321	-0.628546	0.516366
1	-4.065855	-1.032647	0.420073
1	-2.901088	-0.355058	1.568731
1	-3.267764	0.419656	-1.368604
1	-3.227774	1.517779	0.007980
1	0.654625	-2.129920	0.435140
1	-2.256176	-2.087459	-0.871948

PtCl₂

Substrate 1a:

PtCl₂: 1

E(Gas Phase) = -1507.643801

G(Solv.=Toluene) = -1507.627083

6	-0.713215	-0.870945	1.510833
6	-0.121957	0.337351	1.034935
6	3.995412	-2.401077	0.018379
6	3.399102	0.610873	-0.348027
6	0.710770	1.339848	1.234798
6	0.951745	2.529414	0.339912
1	0.405321	3.378146	0.776589
1	0.503540	2.349937	-0.644336
1	4.154492	-3.415893	0.372254
6	0.057424	-2.172525	1.471142
1	-0.600208	-3.014118	1.231844

1	0.451251	-2.341791	2.484577
1	0.887266	-2.152311	0.767238
6	-1.824626	-0.827788	2.537514
1	-1.364536	-1.013436	3.519760
1	-2.552889	-1.626382	2.363413
1	-2.341065	0.130221	2.556171
6	3.292243	2.059007	-0.741300
6	2.432274	2.935483	0.199291
1	2.896773	2.958079	1.194921
1	2.463416	3.965073	-0.179564
1	4.295252	2.502371	-0.790373
1	2.869668	2.125363	-1.754714
78	-1.364107	-0.156345	-0.463884
1	1.261774	1.315914	2.178782
17	-3.114679	1.230703	0.208707
17	0.100460	-1.418029	-1.774363
6	4.486981	0.051681	0.207488
6	4.630977	-1.361846	0.580295
1	2.522118	-0.006802	-0.531762
1	3.314196	-2.276261	-0.819736
1	5.345763	-1.564288	1.379267
1	5.347126	0.688775	0.423184

PtCl₂: ts1

E(Gas Phase) = -1507.631010

G(Solv.=Toluene) = -1507.625074

1 Imaginary Frequency = -93.4 cm⁻¹

6	-0.341305	-1.208273	1.587341
6	-0.080636	0.009964	0.903818
6	3.750082	-2.432415	-0.307786
6	3.300879	0.620419	-0.370774
6	0.738947	1.009783	1.300188
6	0.916384	2.347281	0.651214
1	0.368463	3.066780	1.283200
1	0.427516	2.358711	-0.327756
1	3.887479	-3.489339	-0.096975
6	-0.260071	-2.555892	0.953133
1	-1.225004	-3.075953	1.023828
1	0.450352	-3.151255	1.548176
1	0.054952	-2.516147	-0.089193
6	-0.721369	-1.145011	3.026634
1	-0.144083	-0.371744	3.548613
1	-0.639707	-2.109571	3.534464
1	-1.769058	-0.809132	3.067182
6	3.234988	2.115892	-0.523475
6	2.378193	2.827197	0.550945
1	2.863051	2.709777	1.530218
1	2.372023	3.902479	0.333350
1	4.245406	2.543017	-0.483606
1	2.824942	2.358554	-1.513270
78	-1.396237	0.000601	-0.546648
1	1.359831	0.820231	2.179197
17	-3.101829	0.804325	0.852367

17	0.057167	-0.756373	-2.213264
6	4.310140	-0.040877	0.224142
6	4.408801	-1.496056	0.392941
1	2.459096	0.059429	-0.772212
1	3.073512	-2.180805	-1.120775
1	5.109030	-1.827211	1.160846
1	5.137703	0.538067	0.638553

PtCl₂: 2

E(Gas Phase) = -1507.641270
G(Solv.=Toluene) = -1507.630405

6	-0.341305	-1.208273	1.587341
6	-0.080636	0.009964	0.903818
6	3.750082	-2.432415	-0.307786
6	3.300879	0.620419	-0.370774
6	0.738947	1.009783	1.300188
6	0.916384	2.347281	0.651214
1	0.368463	3.066780	1.283200
1	0.427516	2.358711	-0.327756
1	3.887479	-3.489339	-0.096975
6	-0.260071	-2.555892	0.953133
1	-1.225004	-3.075953	1.023828
1	0.450352	-3.151255	1.548176
1	0.054952	-2.516147	-0.089193
6	-0.721369	-1.145011	3.026634
1	-0.144083	-0.371744	3.548613
1	-0.639707	-2.109571	3.534464
1	-1.769058	-0.809132	3.067182
6	3.234988	2.115892	-0.523475
6	2.378193	2.827197	0.550945
1	2.863051	2.709777	1.530218
1	2.372023	3.902479	0.333350
1	4.245406	2.543017	-0.483606
1	2.824942	2.358554	-1.513270
78	-1.396237	0.000601	-0.546648
1	1.359831	0.820231	2.179197
17	-3.101829	0.804325	0.852367
17	0.057167	-0.756373	-2.213264
6	4.310140	-0.040877	0.224142
6	4.408801	-1.496056	0.392941
1	2.459096	0.059429	-0.772212
1	3.073512	-2.180805	-1.120775
1	5.109030	-1.827211	1.160846
1	5.137703	0.538067	0.638553

PtCl₂: ts2

E(Gas Phase) = -1507.639542
G(Solv.=Toluene) = -1507.622381
1 Imaginary Frequency = -176.7 cm⁻¹

6	0.360816	1.944409	-0.585261
6	0.231433	0.526536	-0.602154
6	1.888367	2.003461	1.287341
6	2.732354	-0.744597	0.441417
6	1.153674	-0.267399	-1.289006

6	1.081321	-1.742555	-1.545423
1	0.648930	-1.891045	-2.546964
1	0.402796	-2.220938	-0.833045
1	1.671842	3.038462	1.534718
6	-0.713638	2.781483	0.062733
1	-1.591198	2.774711	-0.599982
1	-0.390600	3.819424	0.192953
1	-1.041837	2.365817	1.017562
6	1.171669	2.696557	-1.621676
1	2.075846	2.183052	-1.949720
1	1.454325	3.684841	-1.248401
1	0.534047	2.852039	-2.503935
6	3.116933	-2.100826	-0.089505
6	2.490794	-2.350101	-1.488621
1	3.121200	-1.873910	-2.251731
1	2.467985	-3.421210	-1.716080
1	4.207623	-2.198402	-0.152932
1	2.755437	-2.863612	0.608802
78	-1.289865	-0.321194	0.289770
1	1.885034	0.245624	-1.908465
17	-2.611155	-0.069173	-1.628291
17	-0.312589	-0.740035	2.394152
6	3.507561	0.390198	0.313735
6	3.103657	1.689475	0.721358
1	1.881763	-0.725236	1.117962
1	1.260771	1.259136	1.766138
1	3.767443	2.508397	0.447676
1	4.452045	0.312696	-0.225895

PtCl₂: 3

E(Gas Phase) = -1507.687033
G(Solv.=Toluene) = -1507.650399

6	0.638892	1.898416	-0.498964
6	0.372807	0.408259	-0.421798
6	1.677004	2.243389	0.654544
6	2.505519	-0.675895	0.400703
6	1.428472	-0.577365	-0.779122
6	1.049373	-2.047131	-1.038598
1	0.515955	-2.172242	-1.985574
1	0.396523	-2.414654	-0.239724
1	1.671437	3.336470	0.721963
6	-0.623337	2.752444	-0.247179
1	-1.405201	2.527142	-0.977861
1	-0.359982	3.812399	-0.340881
1	-1.031238	2.589141	0.754158
6	1.215925	2.279016	-1.887669
1	2.199425	1.840063	-2.068778
1	1.321582	3.368311	-1.934828
1	0.536048	1.974004	-2.690458
6	3.143773	-2.086386	0.201104
6	2.411725	-2.752825	-0.985794
1	2.960435	-2.573953	-1.919484
1	2.317802	-3.836915	-0.870090
1	4.221443	-2.008046	0.021134
1	3.014015	-2.674551	1.115120
78	-1.240430	-0.217775	0.226889
1	1.964910	-0.198793	-1.657742

17	-2.479368	-0.430553	-1.733073
17	-0.781247	-0.315067	2.509459
6	3.465757	0.480500	0.386216
6	3.094385	1.763672	0.478418
1	1.940644	-0.672426	1.340552
1	1.254308	1.872866	1.597438
1	3.863406	2.531355	0.416791
1	4.520709	0.245268	0.251164

PtCl₂: ts3

E(Gas Phase) = -1507.646245
G(Solv.=Toluene) = -1507.630600
l Imaginary Frequency = -481.2 cm⁻¹

6	-0.746840	1.899514	-0.214008
6	-0.482173	0.365571	-0.084959
6	-2.257861	2.282720	-0.380415
6	-2.925321	-0.498334	-0.590825
6	-1.422362	-0.660281	-0.343804
6	-1.102537	-2.128193	-0.268534
1	-0.278308	-2.335377	0.419543
1	-0.732747	-2.398107	-1.271410
1	-2.306318	3.374016	-0.308759
6	-0.017189	2.429306	-1.467753
1	1.065467	2.328171	-1.375920
1	-0.261291	3.490680	-1.597046
1	-0.320859	1.891919	-2.372219
6	-0.198090	2.614909	1.039835
1	-0.719273	2.298497	1.949978
1	-0.329860	3.697218	0.925254
1	0.864862	2.407166	1.181015
6	-3.473140	-1.945412	-0.685088
6	-2.439865	-2.816607	0.049256
1	-2.614692	-2.797843	1.131997
1	-2.458722	-3.862398	-0.268866
1	-4.481117	-2.022177	-0.266068
1	-3.535060	-2.245546	-1.737190
78	1.402652	-0.212699	0.115677
1	-0.940081	-0.019216	0.971086
17	1.077375	-0.438224	2.443411
17	1.994297	-0.316328	-2.136966
6	-3.553194	0.365710	0.489807
6	-3.224666	1.656523	0.589653
1	-3.036097	0.022955	-1.553033
1	-2.567471	2.036215	-1.406101
1	-3.661877	2.270533	1.373618
1	-4.252445	-0.111376	1.172768

PtCl₂: 4

E(Gas Phase) = -1507.697014
G(Solv.=Toluene) = -1507.661674

6	-1.302298	-1.766859	-0.716000
6	-0.515075	-0.471377	-0.949270
6	-2.299250	-1.693779	0.471598
6	-1.699028	1.199479	0.760764

6	-0.724141	0.850184	-0.384174
6	-0.521507	2.124138	-1.224897
1	-0.648786	1.915831	-2.292612
1	0.498697	2.495036	-1.103819
1	-2.771949	-2.677848	0.567718
6	-0.334679	-2.951504	-0.507869
1	0.427884	-2.982939	-1.294229
1	-0.892891	-3.894722	-0.538157
1	0.173187	-2.880232	0.458239
6	-2.086294	-2.005783	-2.035763
1	-2.750181	-1.168101	-2.272483
1	-2.700153	-2.908738	-1.939029
1	-1.402474	-2.153369	-2.879038
6	-1.652664	2.737186	0.817686
6	-1.523293	3.149614	-0.656328
1	-2.492768	3.060759	-1.162153
1	-1.177280	4.178963	-0.789206
1	-2.533459	3.156336	1.315199
1	-0.767860	3.059221	1.380108
78	1.168824	-0.032537	0.241087
1	-0.104331	-0.443393	-1.958991
17	2.382446	0.456118	-1.700565
17	0.670636	-0.647007	2.441068
6	-3.082797	0.678137	0.400479
6	-3.354234	-0.627621	0.306299
1	-1.386131	0.749861	1.703978
1	-1.731723	-1.527713	1.396146
1	-4.370877	-0.942817	0.077841
1	-3.867966	1.416018	0.241993

PtCl₂: 2'

E(Gas Phase) = -1507.636921
G(Solv.=Toluene) = -1507.633083

6	0.268888	1.217691	1.740165
6	0.175816	0.070038	0.939387
6	-3.827762	2.647285	-0.129314
6	-3.368997	-0.407034	-0.361339
6	-2.803987	2.014014	-0.722135
6	-2.736841	0.581609	-1.027519
6	-0.879140	-0.821632	1.118082
1	-1.937793	2.588314	-1.048161
1	-3.988800	-0.155214	0.501824
6	-1.018218	-2.151945	0.479911
1	-0.435126	-2.836569	1.124171
1	-0.485659	-2.161871	-0.477835
1	-4.740060	2.129395	0.157579
1	-3.796796	3.716424	0.060308
6	1.481691	2.084362	1.670194
1	2.392637	1.475140	1.687272
1	1.503728	2.833031	2.467432
1	1.488381	2.592853	0.694050
6	-0.791355	1.701800	2.685650
1	-1.725723	1.143260	2.670235
1	-1.019038	2.748429	2.446173
1	-0.387715	1.703793	3.707989
1	-2.076939	0.315871	-1.852736
6	-3.262172	-1.864231	-0.704635

6	-2.461244	-2.661502	0.350832
1	-2.968675	-2.606905	1.324511
1	-2.440633	-3.720236	0.068842
1	-4.265847	-2.304901	-0.784975
1	-2.781537	-1.981941	-1.683493
78	1.566384	-0.325763	-0.387765
1	-1.606145	-0.604863	1.898491
17	2.564809	-2.004243	0.920217
17	0.817844	1.329709	-1.896705

PtCl₂: ts2'

E(Gas Phase) = -1507.630519
G(Solv.=Toluene) = -1507.609114
1 Imaginary Frequency = -256.8 cm⁻¹

6	-0.387631	1.464758	1.482662
6	-0.267094	0.163575	0.870109
6	-2.234458	2.311920	0.496422
6	-3.095669	-0.378967	-0.459906
6	-2.222706	1.901979	-0.824722
6	-2.562660	0.597363	-1.263671
6	-1.168743	-0.844009	1.163243
1	-1.746222	2.546808	-1.557315
1	-3.583370	-0.090951	0.469860
6	-1.170148	-2.254578	0.659647
1	-0.776866	-2.904161	1.456182
1	-0.485961	-2.351302	-0.187837
1	-2.851054	1.796467	1.224507
1	-1.998942	3.344358	0.734461
6	0.615207	2.540763	1.132415
1	1.581386	2.266511	1.577997
1	0.315985	3.508941	1.548052
1	0.772104	2.625970	0.055980
6	-0.909465	1.590691	2.904633
1	-1.709444	0.892904	3.157862
1	-1.251812	2.609028	3.112034
1	-0.069357	1.383508	3.581814
1	-2.221199	0.320806	-2.257778
6	-3.190042	-1.825209	-0.829424
6	-2.591317	-2.715548	0.285341
1	-3.240489	-2.670014	1.171447
1	-2.578891	-3.761255	-0.041482
1	-4.243562	-2.106947	-0.975903
1	-2.667439	-2.001919	-1.776213
78	1.202822	-0.164538	-0.370483
1	-1.896715	-0.651278	1.950962
17	2.305162	-1.402086	1.290415
17	0.632493	0.976208	-2.352032

PtCl₂: 3'

E(Gas Phase) = -1507.684014
G(Solv.=Toluene) = -1507.648474

6	0.367600	2.103228	-0.167925
6	0.340278	0.598121	-0.400693
6	1.842449	2.544604	0.118879

6	2.774563	-0.255244	-0.317859
6	2.482985	1.721581	1.210263
6	2.859275	0.454079	1.012183
6	1.443900	-0.035749	-1.194712
1	2.588079	2.166340	2.196877
1	3.587894	0.126802	-0.954262
6	1.167195	-1.419103	-1.857089
1	0.902850	-1.303217	-2.912762
1	0.319562	-1.905181	-1.366868
1	2.430433	2.476075	-0.805380
1	1.815603	3.605707	0.388441
6	-0.534529	2.558948	0.999077
1	-1.587285	2.341149	0.801675
1	-0.429966	3.642867	1.126295
1	-0.252398	2.070169	1.935639
6	-0.137231	2.769690	-1.480258
1	0.503158	2.536093	-2.337113
1	-0.127611	3.856216	-1.337510
1	-1.159549	2.458967	-1.713972
1	3.279212	-0.119051	1.836484
6	2.922415	-1.786212	-0.253162
6	2.439126	-2.256003	-1.628325
1	3.197038	-2.031476	-2.391069
1	2.237593	-3.330815	-1.672512
1	3.955580	-2.076325	-0.029385
1	2.278174	-2.189486	0.537717
78	-1.067311	-0.407291	0.239109
1	1.696799	0.696818	-1.972112
17	-2.695133	0.001453	-1.372587
17	-0.233869	-1.368547	2.183000

PtCl₂: ts_exo_endo

E(Gas Phase) = -1507.630000
G(Solv.=Toluene) = -1507.624864
1 Imaginary Frequency = -107.9 cm⁻¹

6	-0.168054	-1.654038	1.421881
6	-0.214687	-0.385362	0.806622
6	5.531595	-1.615967	0.395633
6	3.777732	0.854777	-0.245250
6	5.408018	-0.964108	-0.768739
6	4.806910	0.362861	-0.952229
6	0.750138	0.563823	1.111684
1	5.800595	-1.432893	-1.671657
1	3.327910	0.208890	0.508799
6	0.814067	1.939652	0.572169
1	0.056566	2.498261	1.155847
1	0.402654	1.948770	-0.446246
1	5.219668	-1.170007	1.337340
1	5.968310	-2.609100	0.446026
6	-1.291657	-2.612670	1.244727
1	-2.255845	-2.104146	1.363202
1	-1.215685	-3.474524	1.913269
1	-1.279023	-2.957552	0.197625
6	0.987158	-2.182917	2.215271
1	1.837714	-1.511189	2.320358
1	1.342028	-3.101155	1.725870
1	0.636418	-2.488057	3.210169

1	5.231161	0.973357	-1.751629
6	3.185180	2.234162	-0.426877
6	2.174356	2.656184	0.655535
1	2.612848	2.520459	1.654605
1	1.985861	3.730140	0.549706
1	3.994373	2.976034	-0.455268
1	2.689620	2.298618	-1.407221
78	-1.675671	0.066540	-0.406344
1	1.481829	0.324908	1.882468
17	-2.669705	1.571661	1.091641
17	-0.959661	-1.395150	-2.092876

PtCl₂: ts3'

E(Gas Phase) = -1507.642617

G(Solv.=Toluene) = -1507.642129

1 Imaginary Frequency = -332.8 cm⁻¹

6	0.810399	-1.521491	1.094938
6	0.369422	-0.224822	0.725196
6	2.270513	-1.767174	1.459637
6	2.346940	0.592036	-0.663111
6	1.451776	0.847895	0.572602
6	1.022519	2.313797	0.382621
1	0.625778	2.766654	1.296611
1	0.226739	2.360908	-0.366349
1	2.616353	-1.058980	2.219479
6	-0.034159	-2.752993	0.967696
1	-1.083372	-2.520641	0.783043
1	0.081315	-3.402214	1.843344
1	0.338104	-3.296843	0.090122
6	-0.073112	-0.351664	2.443479
1	0.722103	-0.538312	3.167225
1	-0.959103	-0.956204	2.611707
1	-0.366302	0.700499	2.483875
6	3.200224	1.888648	-0.737337
6	2.306370	3.012137	-0.134334
1	2.832070	3.519724	0.681819
1	2.060839	3.779646	-0.874409
1	4.114274	1.763666	-0.144623
1	3.512376	2.100478	-1.764932
78	-1.265448	0.002361	-0.366825
1	2.098734	0.812078	1.462552
17	-2.516579	1.348807	1.092432
17	-0.399365	-1.277592	-2.130050
6	3.157328	-0.673372	-0.671975
6	3.138491	-1.680325	0.210274
1	1.690133	0.560478	-1.544925
1	2.360751	-2.763600	1.901637
1	3.779449	-2.541032	0.034639
1	3.825505	-0.777136	-1.527105

PtCl₂: ts3''

E(Gas Phase) = -1507.644289

G(Solv.=Toluene) = -1507.622786

1 Imaginary Frequency = -92.9 cm⁻¹

6	-0.148132	2.106542	-0.204141
6	-0.415622	0.689702	-0.192738
6	-0.926835	0.806133	-1.859403
6	-2.633694	-0.672582	-0.201480
6	-1.613937	0.159105	0.631478
6	-1.357351	-0.761528	1.840107
1	-0.867205	-0.246401	2.669695
1	-0.700753	-1.583835	1.537626
1	-0.362668	1.541537	-2.434648
6	1.119930	2.688203	-0.737956
1	1.677398	3.084775	0.120812
1	0.906315	3.529562	-1.409242
1	1.755095	1.939928	-1.214268
6	-1.181263	3.100137	0.225534
1	-2.161371	2.860607	-0.205944
1	-0.900453	4.121993	-0.039054
1	-1.293756	3.036564	1.316064
6	-3.593402	-1.243011	0.864505
6	-2.769988	-1.292838	2.188114
1	-3.240647	-0.661546	2.950445
1	-2.720011	-2.303201	2.604985
1	-4.465184	-0.586646	0.977841
1	-3.973957	-2.226604	0.571896
78	1.234388	-0.445151	0.005735
1	-2.175708	1.021920	1.010903
17	1.809743	0.859092	1.887319
17	0.944546	-1.992095	-1.736118
6	-3.225112	0.186115	-1.279419
6	-2.399682	0.943279	-2.019194
1	-2.070649	-1.498558	-0.662299
1	-0.560737	-0.177637	-2.169144
1	-2.775617	1.637164	-2.767850
1	-4.304753	0.237668	-1.407978

Substrate 1b:

PtCl₂: 1-1b

E(Gas Phase) = -1468.328934

G(Solv.=Toluene) = --1468.335152

6	-0.573323	-0.337874	2.473787
6	-0.624580	0.206941	1.276356
6	6.237204	-1.683107	-0.592890
6	4.295476	0.711606	-0.306421
6	-0.184878	1.139092	0.299725
6	1.158715	1.067514	-0.385706
1	1.054548	1.418270	-1.420095
1	1.507386	0.033422	-0.417546
1	6.818331	-2.594100	-0.484152
6	-1.367467	-1.509655	2.974118
1	-1.996883	-1.929246	2.185936
1	-2.007302	-1.208905	3.812922
1	-0.696043	-2.295856	3.339516
6	3.555125	2.020391	-0.318894
6	2.165411	1.974152	0.358837
1	2.281142	1.624289	1.392639
1	1.765481	2.995802	0.408970
1	4.158557	2.785472	0.185306

1	3.420751	2.361403	-1.357093
78	-1.692087	-0.181690	-0.398320
1	-0.648102	2.127926	0.324310
17	-3.317344	1.458748	-0.087083
17	-0.447111	-2.050400	-1.022245
6	5.449352	0.501929	0.347693
6	6.216308	-0.750539	0.369309
1	3.849285	-0.114145	-0.860899
1	5.685173	-1.565395	-1.522066
1	6.834575	-0.904912	1.254171
1	5.864484	1.321316	0.937527
1	0.123116	0.131882	3.172561

PtCl₂: ts1'-1b

E(Gas Phase) = -1468.308548

G(Solv.=Toluene) = -1468.321734

1 Imaginary Frequency = -66.4 cm⁻¹

6	6	-0.057738	1.200384	1.462085
6	0.371515	0.202678	0.633970	
6	-6.996993	1.788420	-0.005308	
6	-4.912021	-0.442005	-0.512241	
6	-0.425421	-0.796676	0.057295	
6	-1.787792	-0.585400	-0.490850	
1	-1.656105	-0.442397	-1.579328	
1	-2.197654	0.363085	-0.122789	
1	-7.620200	2.582058	0.396121	
6	0.764698	2.307124	2.015765	
1	1.647866	2.490737	1.398420	
1	1.103215	2.052993	3.031884	
1	0.165301	3.221069	2.103035	
6	-4.101397	-1.625762	-0.965283	
6	-2.737498	-1.777459	-0.253974	
1	-2.903483	-1.898738	0.823392	
1	-2.252585	-2.696240	-0.608117	
1	-4.674213	-2.546501	-0.801980	
1	-3.920939	-1.556820	-2.049111	
78	2.132796	-0.031551	-0.162691	
1	0.004198	-1.793009	-0.036874	
17	2.570245	-2.057154	0.929971	
17	2.072993	1.939192	-1.421784	
6	-6.060575	-0.526614	0.177933	
6	-6.889256	0.605095	0.614229	
1	-4.525447	0.546374	-0.763278	
1	-6.481622	1.998654	-0.939327	
1	-7.478298	0.435032	1.515844	
1	-6.420052	-1.516700	0.464050	
1	-1.088257	1.128038	1.817052	

PtCl₂: 3-1b

E(Gas Phase) = -1468.377787

G(Solv.=Toluene) = -1468.358736

6	0.520244	1.716747	-1.200286
6	0.358024	0.326914	-0.658849
6	1.483575	2.512704	-0.226100

6	2.601825	-0.303576	0.300620
6	1.482758	-0.633173	-0.794952
6	1.234261	-2.138834	-0.602162
1	0.679099	-2.574291	-1.438340
1	0.647138	-2.306251	0.307279
1	1.374384	3.565448	-0.505065
6	-0.780582	2.504461	-1.419070
1	-1.488800	1.938749	-2.030328
1	-0.548055	3.444128	-1.932897
1	-1.266498	2.742631	-0.468059
6	3.390431	-1.644540	0.430661
6	2.656823	-2.694221	-0.437348
1	3.139051	-2.777320	-1.419475
1	2.664905	-3.692936	0.009739
1	4.431033	-1.517822	0.113006
1	3.412342	-1.951076	1.481256
78	-1.166286	-0.144248	0.270767
1	1.947701	-0.465837	-1.776799
17	-2.503398	-1.010270	-1.424592
17	-0.569912	0.494393	2.429154
6	3.429150	0.901235	-0.053190
6	2.938132	2.125089	-0.287889
1	2.066148	-0.116626	1.239093
1	1.085599	2.415505	0.791952
1	3.634707	2.913767	-0.566516
1	4.502582	0.744018	-0.150846
1	1.047370	1.622296	-2.160016

PtCl₂: ts3-1b

E(Gas Phase) = -1468.337047

G(Solv.=Toluene) = -1468.338144

1 Imaginary Frequency = - 505.2 cm⁻¹

6	-0.680029	1.844248	-0.653391
6	-0.471691	0.398221	-0.157695
6	-2.152314	2.347558	-0.770435
6	-2.960790	-0.404098	-0.361217
6	-1.460732	-0.607748	-0.129898
6	-1.217605	-2.029166	0.291088
1	-0.376860	-2.116685	0.985198
1	-0.900171	-2.552448	-0.625120
1	-2.101009	3.436318	-0.871341
6	0.024504	2.057261	-2.007479
1	1.096710	1.865433	-1.935182
1	-0.127612	3.092193	-2.334572
1	-0.381509	1.388976	-2.775013
6	-3.587456	-1.799072	-0.107616
6	-2.580049	-2.534390	0.794807
1	-2.717725	-2.246660	1.844495
1	-2.671017	-3.622338	0.737612
1	-4.586052	-1.718745	0.332709
1	-3.692953	-2.331403	-1.059606
78	1.403539	-0.111547	0.151275
1	-0.921815	0.311133	0.964761
17	1.325909	0.879338	2.284742
17	1.688142	-1.235342	-1.880234
6	-3.479171	0.708777	0.537036
6	-3.084368	1.972152	0.353566

1 -3.094088 -0.095317 -1.408219
1 -2.568464 1.976822 -1.719271
1 -3.444671 2.753098 1.019334
1 -4.156765 0.427655 1.340219
1 -0.172675 2.462238 0.095336

PtCl₂: 4-1b

E(Gas Phase) = -1468.386005
G(Solv.=Toluene) = -1468.368501

6 -0.889428 -1.739173 -1.418808
6 -0.369185 -0.321547 -1.219400
6 -1.983676 -2.206108 -0.436077
6 -2.045449 0.565107 0.648419
6 -0.898215 0.730726 -0.371936
6 -0.871372 2.206332 -0.806045
1 -0.805032 2.299357 -1.895130
1 0.015268 2.699172 -0.400154
1 -2.240516 -3.241191 -0.686638
6 0.261077 -2.756162 -1.531504
1 1.039186 -2.404820 -2.217971
1 -0.119197 -3.713012 -1.905787
1 0.721399 -2.925373 -0.552770
6 -2.345644 2.009075 1.092351
6 -2.140131 2.829228 -0.189635
1 -2.996563 2.702396 -0.863599
1 -2.023097 3.901249 -0.005114
1 -3.348963 2.106317 1.519915
1 -1.625687 2.318846 1.859588
78 1.061079 0.029055 0.286439
1 0.124843 0.049092 -2.118092
17 2.342379 1.265747 -1.233224
17 0.468766 -1.285092 2.125417
6 -3.234473 -0.075053 -0.055412
6 -3.213451 -1.334109 -0.504719
1 -1.745999 -0.064347 1.487379
1 -1.570279 -2.221666 0.580807
1 -4.105575 -1.745973 -0.973919
1 -4.131396 0.532529 -0.166830
1 -1.362372 -1.679859 -2.414605

PtCl₂: ts3-Hb-1b

E(Gas Phase) = -1468.331458
G(Solv.=Toluene) = -1468.335006
1 Imaginary Frequency = - 431.1 cm⁻¹

6 6 -0.708625 1.759295 -0.565172
6 -0.466364 0.481064 0.016088
6 -2.088015 2.364016 -0.769678
6 -2.998223 -0.302900 -0.081977
6 -1.523635 -0.597575 0.306099
6 -1.273015 -1.963516 -0.383384
1 -0.449337 -2.504718 0.087537
1 -0.988625 -1.804578 -1.428140
1 -1.966699 3.435726 -0.942434
6 0.443632 2.620091 -0.972171
1 1.325522 2.423247 -0.354082

1 0.189957 3.682957 -0.980718
1 0.732530 2.301896 -1.984744
6 -3.675347 -1.656209 0.185320
6 -2.633414 -2.711597 -0.274474
1 -2.577622 -3.540881 0.437233
1 -2.909806 -3.143935 -1.241382
1 -3.875051 -1.754182 1.260298
1 -4.636958 -1.748008 -0.330447
78 1.388401 -0.192750 0.117274
1 -1.485684 -0.760792 1.391079
17 1.416605 0.189499 2.438354
17 1.623063 -0.572316 -2.183301
6 -3.558101 0.900842 0.616026
6 -3.122535 2.125736 0.313275
1 -3.016918 -0.125352 -1.169722
1 -2.439516 1.939263 -1.726990
1 -3.496401 3.006478 0.828473
1 -4.296104 0.760548 1.403995
1 -0.457045 1.259276 0.927086

PtCl₂: 4-Hb-1b

E(Gas Phase) = -1468.382202
G(Solv.=Toluene) = -1468.365588

6 -0.120478 1.549375 -0.156447
6 0.327625 0.470012 -1.025240
6 0.711927 2.054757 1.026429
6 2.732556 0.197980 0.028112
6 1.713294 -0.135596 -1.086124
6 1.810804 -1.671933 -1.226850
1 1.480068 -2.020474 -2.210604
1 1.164319 -2.139690 -0.477829
1 0.158861 2.861623 1.515691
6 -1.047454 2.604785 -0.718904
1 -1.571579 2.280977 -1.617572
1 -0.431090 3.485076 -0.956045
1 -1.785739 2.917612 0.026074
6 3.928531 -0.694684 -0.355697
6 3.304409 -1.995299 -0.934959
1 3.831886 -2.310612 -1.840940
1 3.380599 -2.822128 -0.222177
1 4.529656 -0.187000 -1.121852
1 4.590387 -0.885199 0.495111
78 -1.151337 -0.341593 0.233636
1 2.123921 0.301655 -2.014707
17 -2.761064 -0.169795 -1.451753
17 -0.034093 -1.104128 2.143496
6 3.002508 1.678473 0.125089
6 2.069883 2.540970 0.546477
1 2.318490 -0.163934 0.979818
1 0.849290 1.270371 1.770846
1 2.266777 3.610667 0.561254
1 3.974788 2.046637 -0.201293
1 -0.160332 0.462360 -2.000364

PtCl₂: ts-metal-allyl-cation-1b

E(Gas Phase) = -1468.300859

G(Solv.=Toluene) = -1468.310772
1 Imaginary Frequency = - 224.6 cm⁻¹

6	-1.702573	1.753511	1.607515
6	-1.079986	1.102468	0.589415
6	5.781901	-1.959908	0.478165
6	4.123227	0.395912	-0.648248
6	-0.214348	1.621668	-0.387507
6	1.030509	1.043024	-0.951359
1	0.881519	0.849315	-2.024970
1	1.261317	0.089128	-0.472353
1	6.291351	-2.704612	1.082462
6	-1.302034	3.096978	2.123890
1	-0.644735	3.631021	1.428340
1	-0.757522	2.998172	3.074153
1	-2.190589	3.704731	2.332175
6	3.514349	1.541478	-1.407728
6	2.187095	2.069191	-0.811358
1	2.339567	2.312035	0.247192
1	1.912400	3.001048	-1.323836
1	4.227391	2.374428	-1.443727
1	3.325464	1.244226	-2.451158
78	-1.550777	-0.673479	-0.075471
1	-0.466489	2.616379	-0.774223
17	-3.488272	0.112465	-1.125244
17	0.205813	-1.864283	0.908519
6	5.326548	0.445738	-0.053647
6	5.977999	-0.649163	0.676582
1	3.536839	-0.519975	-0.575954
1	5.114131	-2.333672	-0.293902
1	6.698719	-0.341201	1.434512
1	5.882545	1.384385	-0.092847
1	-2.505638	1.241506	2.130861

Substrate 1c:

PtCl₂: 1-1c

E(Gas Phase) = -1429.007817
G(Solv.=Toluene) = -1429.031965

6	-0.735904	-0.667943	1.728572
6	-0.106223	0.437863	1.111896
6	4.151782	-2.345670	0.793027
6	3.378025	0.393894	-0.411835
6	0.736135	1.441911	1.034119
6	0.896442	2.420221	-0.102464
1	0.392438	3.349916	0.198866
1	0.362042	2.050312	-0.985354
1	4.409052	-3.199900	1.412842
6	3.152558	1.657486	-1.197309
6	2.357666	2.758257	-0.456292
1	2.897596	3.037315	0.458958
1	2.343292	3.652369	-1.092643
1	4.120906	2.083876	-1.489125
1	2.621778	1.415947	-2.130021
78	-1.504452	-0.331183	-0.172390
1	1.367818	1.591609	1.913476
17	-3.216754	1.074877	0.535663

17	-0.049076	-1.815166	-1.225542
6	4.551890	0.043861	0.139989
6	4.816005	-1.185688	0.899377
1	2.519387	-0.263632	-0.290151
1	3.343310	-2.485890	0.079632
1	5.650947	-1.131122	1.599091
1	5.396981	0.727846	0.039731
1	-0.231379	-1.633283	1.755608
1	-1.518081	-0.503324	2.469016

PtCl₂: ts1'-1c

E(Gas Phase) = -1428.982321
G(Solv.=Toluene) = -1429.002610
1 Imaginary Frequency = -347.5 cm⁻¹

6	-0.202632	1.295747	-1.602366
6	-0.025508	0.012266	-1.097221
6	2.897970	2.864571	0.025474
6	3.217478	-0.182950	0.320743
6	0.966661	-0.899658	-1.300414
6	1.179964	-2.188680	-0.581368
1	0.675256	-2.981119	-1.157988
1	0.683019	-2.156379	0.395735
1	2.809083	3.919918	-0.215833
6	3.467568	-1.653921	0.517375
6	2.672081	-2.554139	-0.462053
1	3.132208	-2.491206	-1.457690
1	2.760492	-3.598960	-0.142072
1	4.534599	-1.881358	0.399051
1	3.192229	-1.923298	1.544623
78	-1.408374	0.065252	0.292526
1	1.610111	-0.714113	-2.161624
17	-3.184319	-0.103027	-1.215816
17	0.004258	0.177176	2.159955
6	3.964250	0.634861	-0.450380
6	3.735659	2.068433	-0.662550
1	2.364955	0.225412	0.860235
1	2.299587	2.504634	0.858545
1	4.330009	2.517621	-1.458225
1	4.820932	0.212944	-0.978406
1	0.645639	1.972387	-1.719577
1	-1.184858	1.664163	-1.877592

PtCl₂: 3-1c

E(Gas Phase) = -1429.065148
G(Solv.=Toluene) = -1429.064047

6	-0.566889	-1.405367	-1.628755
6	-0.356963	-0.197026	-0.777595
6	-1.508932	-2.437969	-0.912000
6	-2.584615	0.223385	0.315632
6	-1.444638	0.799074	-0.642580
6	-1.141101	2.173620	-0.024184
1	-0.556270	2.807264	-0.697508
1	-0.557286	2.041925	0.893058
1	-1.433451	-3.366574	-1.485981

6	-3.385544	1.499859	0.713351
6	-2.538245	2.730399	0.298015
1	-2.968290	3.200919	-0.594221
1	-2.502151	3.498318	1.076420
1	-4.359512	1.508615	0.211886
1	-3.582497	1.487856	1.790045
78	1.214180	-0.060979	0.173018
1	-1.902435	0.927620	-1.634829
17	2.600727	1.053736	-1.321255
17	0.604951	-1.116533	2.157312
6	-3.415265	-0.876330	-0.290628
6	-2.953875	-2.019028	-0.816676
1	-2.063545	-0.157045	1.203000
1	-1.088412	-2.646661	0.079817
1	-3.680195	-2.716008	-1.231095
1	-4.491131	-0.706420	-0.306467
1	0.386068	-1.894786	-1.840712
1	-1.027030	-1.104791	-2.579230

PtCl₂: ts3-1c

E(Gas Phase) = -1429.26397

G(Solv.=Toluene) = -1429.045319

1 Imaginary Frequency = -430.0 cm⁻¹

6	6	-0.627656	1.946528	0.599160
6		-0.464640	0.491632	0.144976
6		-2.047494	2.569954	0.614912
6		-2.942788	0.079806	-0.594733
6		-1.463669	-0.287769	-0.476166
6		-1.258287	-1.682222	-0.986519
1		-0.439039	-2.192600	-0.472078
1		-0.938682	-1.568407	-2.035798
1		-1.971560	3.541312	1.113690
6		-3.617854	-1.187890	-1.184307
6		-2.643943	-2.343972	-0.889412
1		-2.794144	-2.728628	0.126688
1		-2.757461	-3.184282	-1.579430
1		-4.614744	-1.347530	-0.762345
1		-3.739599	-1.067642	-2.266529
78		1.410774	-0.089852	0.058456
1		-0.893932	-0.255700	0.987552
17		1.073438	-1.478253	1.938644
17		1.948209	1.150726	-1.842803
6		-3.506422	0.564650	0.731872
6		-3.092382	1.710292	1.281380
1		-2.993388	0.914786	-1.310689
1		-2.353806	2.782503	-0.419201
1		-3.504563	2.029329	2.236204
1		-4.250794	-0.065544	1.213492
1		0.013645	2.538148	-0.062890
1		-0.179526	2.014621	1.595507

PtCl₂: 4-1c

E(Gas Phase) = -1429.072243

G(Solv.=Toluene) = -1429.072466

6	0.934873	-1.345227	1.890114
6	0.373848	-0.043617	1.344046
6	2.049508	-2.040007	1.088306
6	2.018134	0.328225	-0.710966
6	0.862260	0.741278	0.227017
6	0.775564	2.275532	0.215002
1	0.684633	2.678640	1.229032
1	-0.119954	2.593516	-0.324576
1	2.331946	-2.953989	1.621088
6	2.274594	1.596415	-1.546733
6	2.030657	2.740035	-0.549902
1	2.883715	2.837348	0.133203
1	1.882244	3.711184	-1.031300
1	3.277710	1.602921	-1.985529
1	1.551133	1.651033	-2.369224
78	-1.078409	-0.189379	-0.162245
1	-0.115683	0.546948	2.118531
17	-2.389796	1.377429	0.978909
17	-0.437613	-1.937617	-1.574328
6	3.223152	-0.048090	0.141256
6	3.247348	-1.137690	0.916983
1	1.740381	-0.522713	-1.334164
1	1.654387	-2.352074	0.113331
1	4.150275	-1.370954	1.479010
1	4.094752	0.602238	0.082605
1	0.102125	-2.036977	2.065630
1	1.324554	-1.093506	2.888878

PtCl₂: ts3-Hb-1c

E(Gas Phase) = -1429.011447

G(Solv.=Toluene) = -1429.030026

1 Imaginary Frequency = -560.9 cm⁻¹

6	-0.446723	2.068992	-0.233544
6	-0.310894	0.790172	0.338377
6	-1.730954	2.840222	-0.261849
6	-2.542381	-0.270773	-0.267923
6	-1.580757	0.135705	0.869270
6	-1.455120	-1.148736	1.707147
1	-1.125429	-0.943059	2.730520
1	-0.712002	-1.806931	1.248832
1	-2.125617	2.943660	0.758846
6	-3.633136	-1.059854	0.500556
6	-2.869846	-1.792760	1.640624
1	-3.403706	-1.689297	2.590792
1	-2.790477	-2.864826	1.437706
1	-4.367516	-0.358604	0.916224
1	-4.177379	-1.745680	-0.156454
1	-2.097854	0.887401	1.487197
6	-3.062985	0.827180	-1.150756
6	-2.734596	2.126805	-1.169557
1	-2.006176	-0.984111	-0.912330
1	-1.543290	3.852046	-0.629252
1	-3.190624	2.769143	-1.919033
1	-3.790365	0.500942	-1.894742
17	0.409302	-1.922907	-1.503059
1	0.234798	1.483620	1.143408
78	1.299039	-0.260544	-0.141814

17 2.621351 1.254937 1.094752
1 0.453869 2.531889 -0.633037

PtCl₂: 4-Hb-1c

E(Gas Phase) = -1429.065955

G(Solv.=Toluene) = -1429.068010

6 0.287407 0.496313 1.593667
6 -0.306112 -0.722330 1.108987
6 -0.382225 1.831407 1.818828
6 -2.464802 0.164186 -0.123055
6 -1.735856 -0.912333 0.700420
6 -2.012822 -2.217419 -0.080342
1 -1.952111 -3.101439 0.563039
1 -1.252654 -2.335577 -0.861777
1 -0.429203 1.924432 2.919429
6 -3.803204 -0.539258 -0.436043
6 -3.421772 -2.017617 -0.709232
1 -4.158377 -2.703631 -0.279241
1 -3.391378 -2.221471 -1.784204
1 -4.466992 -0.467406 0.435971
1 -4.325922 -0.072645 -1.277410
1 -2.261971 -0.978069 1.672652
6 -2.604609 1.524840 0.499833
6 -1.741327 2.190132 1.273608
1 -1.919634 0.281707 -1.070287
1 0.329837 2.616255 1.524959
1 -2.038352 3.191475 1.586062
1 -3.523636 2.051273 0.241203
17 0.232508 1.580990 -1.763869
1 0.159916 -1.634030 1.482239
78 1.130936 0.030281 -0.291183
17 2.649430 -1.466315 0.670794
1 1.136442 0.350182 2.261892

PtCl₂: ts3-Hc-1c

E(Gas Phase) = -1429.011582

G(Solv.=Toluene) = -1429.031651

1 Imaginary Frequency = -678.7 cm⁻¹

6 0.649562 1.871097 -0.368623
6 0.461170 0.522813 -0.002600
6 1.843246 2.631010 -0.832803
6 2.967389 -0.049325 0.445504
6 1.557469 -0.527147 -0.003289
6 1.269628 -1.742189 0.918362
1 0.624936 -2.462627 0.410656
1 0.730256 -1.412235 1.812771
1 1.475521 3.037652 -1.795308
6 3.704664 -1.386721 0.658872
6 2.659687 -2.325401 1.300289
1 2.781958 -3.354893 0.950602
1 2.776780 -2.346532 2.388982
1 4.018988 -1.773530 -0.319554
1 4.609781 -1.267664 1.264511
1 1.626927 -0.879083 -1.040732

6 3.679391 0.886238 -0.495573
6 3.194280 2.003943 -1.040660
1 2.860698 0.441166 1.427799
1 1.925344 3.539217 -0.210828
1 3.841472 2.585912 -1.694318
1 4.702889 0.614635 -0.751980
17 -1.971559 1.296731 1.758828
1 -0.241966 2.488908 -0.266938
78 -1.411220 -0.100027 -0.057101
17 -1.204929 -1.523607 -1.890057
1 0.422952 1.142171 1.032201

PtCl₂: 4-Hc-1c

E(Gas Phase) = -1429.072423

G(Solv.=Toluene) = -1429.078887

6 -0.024539 1.421840 -0.034629
6 -0.536911 0.283176 -0.754016
6 -0.678179 1.897649 1.247831
6 -2.992403 0.499509 -0.536137
6 -1.765978 -0.418113 -0.263799
6 -2.140860 -1.746778 -0.944268
1 -1.636126 -2.591655 -0.467020
1 -1.821687 -1.733749 -1.993910
1 -0.693445 1.103997 2.000368
6 -4.164109 -0.473005 -0.262176
6 -3.694793 -1.830451 -0.846658
1 -4.018214 -2.664125 -0.216248
1 -4.130571 -1.997685 -1.837239
1 -4.314544 -0.549521 0.821665
1 -5.105460 -0.121563 -0.698112
1 -1.704711 -0.571789 0.816958
6 -3.044676 1.798758 0.227267
6 -2.092834 2.393604 0.962123
1 -3.009736 0.737948 -1.614123
1 -0.084068 2.712670 1.670847
1 -2.342522 3.346349 1.425705
1 -3.998855 2.321695 0.147136
17 2.442720 0.623450 -1.824586
1 0.469589 2.190925 -0.626342
78 1.353389 -0.183905 0.075001
17 0.734820 -1.274537 2.046972
1 -0.380467 0.272438 -1.833544

Ring contraction pathway:

PtCl₂: ts3"-1c

E(Gas Phase) = -1428.999701

G(Solv.=Toluene) = -1429.016761

1 Imaginary Frequency = -346.4 cm⁻¹

6 -0.138626 0.677547 2.204676
6 0.318294 0.193727 0.958242
6 0.739823 -1.206432 1.923376
6 2.516979 -0.229437 -0.295805
6 1.590578 0.800917 0.376189

6	1.455358	1.905400	-0.689160
1	1.139329	2.861709	-0.262326
1	0.694051	1.613760	-1.419093
1	0.538954	-1.136587	3.005328
6	3.609504	0.662462	-0.918610
6	2.864194	1.960194	-1.351478
1	3.419107	2.848750	-1.033138
1	2.771339	2.021375	-2.440101
1	4.373444	0.893118	-0.164929
1	4.119196	0.169356	-1.752430
78	-1.179220	-0.151581	-0.292031
1	2.159072	1.212804	1.227817
17	-2.055710	1.863111	0.601859
17	-0.506478	-2.157195	-1.259184
6	2.952471	-1.255583	0.703186
6	2.168367	-1.617774	1.724984
1	1.954621	-0.726955	-1.099823
1	0.013535	-1.917953	1.527536
1	2.529165	-2.321592	2.473611
1	3.946437	-1.691393	0.617934
1	-1.093661	0.372482	2.612873
1	0.510106	1.277780	2.846058

PtCl₂: [4+2]-product-1c

E(Gas Phase) = -1429.067136
G(Solv.=Toluene) = -1429.068367

6	0.485520	0.182263	1.768500
6	-0.457662	0.854480	0.915199
6	-0.297338	2.320650	0.534373
6	-2.375493	0.575600	-0.706267
6	-1.891409	0.433408	0.753268
6	-2.494355	-0.886712	1.264076
1	-2.728909	-0.824679	2.332220
1	-1.812898	-1.727084	1.122164
1	-0.619709	2.900601	1.418999
6	-3.845539	0.138825	-0.575273
6	-3.776694	-1.076647	0.388489
1	-4.682009	-1.161048	0.997397
1	-3.691182	-2.003499	-0.187426
1	-4.436180	0.953906	-0.136066
1	-4.300718	-0.114687	-1.538256
78	1.118870	-0.399270	-0.110220
1	-2.415792	1.246619	1.290475
17	-0.041137	-2.346795	-0.638859
17	2.845310	1.177716	-0.054566
6	-2.059527	1.946266	-1.236431
6	-1.133560	2.725035	-0.663811
1	-1.854626	-0.181995	-1.311201
1	0.751421	2.576707	0.376381
1	-0.924323	3.713948	-1.066282
1	-2.588086	2.294262	-2.122476
1	1.282271	0.759544	2.234983
1	0.154267	-0.694234	2.321783

Direct Diels Alder mechanism:

PtCl₂: DA-1-1c

E(Gas Phase) = -1429.006600
G(Solv.=Toluene) = -1429.038549

6	1.046992	0.998204	1.463300
6	0.238435	1.144123	0.310709
6	-3.553449	-2.793203	-0.622398
6	-3.576150	0.206867	0.164972
6	-0.705249	1.696558	-0.417667
6	-1.536586	2.869045	0.062130
1	-1.208012	3.753546	-0.502712
1	-1.314154	3.071329	1.116968
1	-3.576837	-3.774526	-1.087632
6	-3.742372	1.603510	0.702492
6	-3.057377	2.712357	-0.132964
1	-3.278494	2.552188	-1.196269
1	-3.508954	3.676341	0.135695
1	-4.813585	1.834122	0.759335
1	-3.360711	1.658008	1.734335
78	1.566675	-0.372438	-0.008502
1	-0.893164	1.323122	-1.422000
17	0.209277	-2.063919	0.843802
17	3.160254	0.984466	-1.021847
6	-4.586672	-0.519930	-0.341063
6	-4.505422	-1.884629	-0.878835
1	-2.573397	-0.217392	0.184255
1	-2.725265	-2.596388	0.053546
1	-5.324877	-2.168843	-1.539720
1	-5.577029	-0.061896	-0.378776
1	1.876865	1.683436	1.633430
1	0.662073	0.470451	2.335375

PtCl₂: DA-ts1-1c

E(Gas Phase) = -1428.965661
G(Solv.=Toluene) = -1428.979919
1 Imaginary Frequency = -406.9 cm⁻¹

6	-0.291121	-0.145389	1.654091
6	0.613261	0.062054	0.569643
6	0.909261	2.377961	0.253284
6	3.414141	0.987020	0.049204
6	1.697995	-0.582359	0.049601
6	2.657666	-1.483679	0.800531
1	2.263460	-2.509724	0.770997
1	2.716603	-1.193369	1.856910
1	-0.091817	2.790619	0.240186
6	4.564841	0.022260	0.001854
6	4.038539	-1.443153	0.128710
1	3.938703	-1.869592	-0.877211
1	4.755712	-2.071915	0.667493
1	5.137076	0.135245	-0.925788
1	5.249846	0.237279	0.831945
78	-1.400465	-0.209504	-0.093088
1	1.720388	-0.696277	-1.031173
17	-2.494219	1.825996	0.247853
17	-0.921806	-2.425267	-0.666376
6	2.941386	1.775102	-0.980053

6	1.701037	2.444116	-0.877204
1	3.064451	1.213954	1.051705
1	1.349204	2.266112	1.238854
1	1.268716	2.853171	-1.788051
1	3.422554	1.716508	-1.955748
1	-0.326068	-1.120626	2.144530
1	-0.642131	0.693942	2.253142

PtCl₂: DA-2-1c

E(Gas Phase) = -1429.063627
G(Solv.=Toluene) = -1429.070018

6	-0.266477	-0.015480	1.645995
6	0.614934	0.592103	0.679688
6	0.655559	2.114055	0.558956
6	3.034458	0.890361	-0.064068
6	1.851953	-0.099675	0.132943
6	2.498458	-1.260620	0.911820
1	1.939340	-2.192975	0.813485
1	2.548962	-1.009951	1.979364
1	-0.342419	2.543593	0.621173
6	4.155307	-0.052688	-0.521704
6	3.933280	-1.354440	0.307920
1	4.033883	-2.240290	-0.326373
1	4.679535	-1.450129	1.102977
1	4.045918	-0.258103	-1.593925
1	5.151254	0.377183	-0.374226
78	-1.295704	-0.294232	-0.114219
1	1.603452	-0.459613	-0.872930
17	-2.659537	1.595058	0.065866
17	-0.490014	-2.436364	-0.577045
6	2.604224	2.038881	-0.933710
6	1.431510	2.611335	-0.639930
1	3.306300	1.282565	0.932333
1	1.186841	2.428459	1.479275
1	1.021881	3.437936	-1.213432
1	3.216424	2.363676	-1.772064
1	-0.007602	-0.986195	2.062892
1	-0.855704	0.633126	2.293126

Stepwise mechansim:

PtCl₂: 5

E(Gas Phase) = -1429.006081
G(Solv.=Toluene) = -1429.026744

6	-2.347423	2.937237	-0.510235
6	-2.838233	1.816024	-0.969922
6	1.230326	-1.646331	0.947082
6	-1.888452	-1.360688	0.983715
6	-3.335002	0.689316	-1.417986
6	-4.538645	-0.016064	-0.830549
1	-5.278914	-0.176282	-1.627349
1	-5.012605	0.636988	-0.088021
1	2.167248	-2.189310	0.839480
6	-3.382630	-1.320817	1.097253

6	-4.242358	-1.385164	-0.178883
1	-3.793695	-2.066623	-0.913143
1	-5.206166	-1.835157	0.089697
1	-3.659320	-2.152800	1.765923
1	-3.642009	-0.418014	1.672046
78	1.441426	0.194002	0.060145
1	-2.861950	0.215244	-2.280676
17	0.369388	1.316834	1.815414
17	2.789168	-0.492967	-1.716938
6	-1.148420	-1.593699	-0.119970
6	0.300126	-1.693697	-0.155621
1	-1.368524	-1.184356	1.924355
1	0.871401	-1.537709	1.967517
1	0.701783	-2.101560	-1.080402
1	-1.636626	-1.726927	-1.080200
1	-2.688159	3.902766	-0.880815
1	-1.574875	2.939181	0.256925

PtCl₂: ts5

E(Gas Phase) = -1429.01905
G(Solv.=Toluene) = -1429.008478
1 Imaginary Frequency = -28.1 cm⁻¹

6	0.184657	1.983756	1.710300
6	-0.796281	1.708963	0.855465
6	1.221655	-1.854931	-0.892224
6	-2.070626	-1.367149	-0.260965
6	-1.780842	1.537327	0.005337
6	-3.264844	1.466503	0.306383
1	-3.745128	2.414698	0.025046
1	-3.428437	1.335595	1.381813
1	2.168178	-1.851357	-1.428774
6	-3.558468	-1.131926	-0.196710
6	-3.956940	0.342821	-0.504983
1	-3.770334	0.531562	-1.570801
1	-5.041017	0.432875	-0.361690
1	-4.086676	-1.766614	-0.920464
1	-3.926536	-1.406106	0.798793
78	0.983513	-0.012086	0.095629
1	-1.497076	1.322836	-1.021955
17	0.556466	-1.281822	2.062521
17	1.745687	1.382776	-1.636403
6	-1.353964	-1.427840	-1.399723
6	0.100339	-1.249005	-1.541640
1	-1.536363	-1.334278	0.683518
1	1.075009	-2.661309	-0.179985
1	0.355602	-0.724779	-2.462127
1	-1.883703	-1.376932	-2.353396
1	0.576259	2.998293	1.779919
1	0.541523	1.260845	2.439639

PtCl₂: 6

E(Gas Phase) = -1429.001983
G(Solv.=Toluene) = -1429.010140

6	0.293990	1.613873	1.912028
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6	-0.725550	1.500315	1.052946
6	1.210536	-1.695724	-1.185635
6	-2.084019	-1.297030	-0.448213
6	-1.742780	1.509042	0.223129
6	-3.222393	1.453600	0.544551
1	-3.679317	2.442276	0.395811
1	-3.377212	1.185688	1.595436
1	2.152597	-1.588775	-1.719139
6	-3.567414	-1.048371	-0.329058
6	-3.948549	0.462885	-0.403421
1	-3.781162	0.803583	-1.434044
1	-5.027881	0.544015	-0.223830
1	-4.116575	-1.555581	-1.133354
1	-3.928327	-1.466454	0.617927
78	0.970324	-0.019372	0.100286
1	-1.499573	1.409747	-0.830948
17	0.546403	-1.616885	1.823790
17	1.734010	1.618986	-1.407330
6	-1.375236	-1.209476	-1.589910
6	0.080883	-1.011129	-1.717835
1	-1.541742	-1.401962	0.485886
1	1.084383	-2.602028	-0.601989
1	0.322853	-0.338389	-2.540429
1	-1.909985	-1.023065	-2.523960
1	0.749886	2.589854	2.076103
1	0.582938	0.808447	2.582875

PtCl₂: ts6

E(Gas Phase) = -1428.996991
G(Solv.=Toluene) = -1429.006528
1 Imaginary Frequency = -143.4 cm⁻¹

6	0.240505	-1.871840	1.704874
6	-0.500993	-0.844236	1.210939
6	0.752393	1.113691	-1.772925
6	-2.163095	0.219113	-1.296048
6	-1.622582	-0.095693	1.309943
6	-3.016764	-0.629384	1.494611
1	-3.375116	-0.391013	2.508095
1	-3.027005	-1.720333	1.394951
1	1.691400	1.656986	-1.888795
6	-3.576728	-0.198795	-0.996690
6	-3.983101	0.027322	0.485976
1	-4.014367	1.107236	0.682009
1	-5.001845	-0.349457	0.638188
1	-4.276177	0.369256	-1.625479
1	-3.700783	-1.257758	-1.247611
78	1.038704	-0.066584	0.048112
1	-1.521658	0.981918	1.244221
17	1.033763	-1.964759	-1.392835
17	1.342239	1.817223	1.433596
6	-1.730051	1.524474	-1.354898
6	-0.367858	1.908260	-1.420187
1	-1.444711	-0.571024	-1.495799
1	0.605571	0.315757	-2.496588
1	-0.152834	2.920151	-1.080728
1	-2.445557	2.317401	-1.138309
1	0.265789	-2.031285	2.783113

1	0.795971	-2.563650	1.083476
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PtCl₂: 7

E(Gas Phase) = -1429.044798
G(Solv.=Toluene) = -1429.049610

6	0.284938	-2.138045	-1.298037
6	0.532186	-0.961438	-0.722765
6	-0.582509	1.083172	1.618308
6	2.202262	0.187567	0.912643
6	1.842614	-0.251393	-0.579988
6	3.070157	-1.077296	-1.033277
1	3.144593	-1.133127	-2.124222
1	2.997750	-2.100542	-0.644138
1	-1.533512	1.568584	1.860102
6	3.733016	-0.063591	1.051599
6	4.246848	-0.351113	-0.370758
1	4.452978	0.587082	-0.902501
1	5.169934	-0.940247	-0.379355
1	4.245457	0.781161	1.524800
1	3.903041	-0.936492	1.691817
78	-1.119827	0.009592	-0.112969
1	1.796606	0.658657	-1.190336
17	-1.848856	-1.753116	1.259254
17	-0.926128	1.783010	-1.642209
6	1.787639	1.610880	1.124417
6	0.523383	2.009705	1.370157
1	1.652733	-0.466381	1.597733
1	-0.373674	0.272681	2.315756
1	0.281948	3.068789	1.320444
1	2.542621	2.372687	0.929658
1	1.090242	-2.674148	-1.797507
1	-0.692671	-2.605778	-1.314179

PtCl₂: ts7

E(Gas Phase) = -1429.025797
G(Solv.=Toluene) = -1429.030966
1 Imaginary Frequency = -93.4 cm⁻¹

6	-0.256291	-2.022847	-1.426700
6	-0.536978	-1.027514	-0.592205
6	0.485081	1.753625	-1.133803
6	-2.312207	0.823646	-0.315866
6	-1.877403	-0.652868	-0.020635
6	-3.080414	-1.455578	-0.560954
1	-3.093105	-2.482837	-0.185160
1	-3.025629	-1.499952	-1.655261
1	1.395853	2.271814	-1.427912
6	-3.813457	0.833223	0.059742
6	-4.311805	-0.631732	-0.117874
1	-4.706377	-1.014093	0.829086
1	-5.121486	-0.705634	-0.850353
1	-3.935270	1.153434	1.101377
1	-4.371090	1.545566	-0.556236
78	0.941644	0.136383	0.149837
1	-1.827215	-0.776185	1.069180

17	2.699478	-0.395879	-1.293559
17	0.835202	-0.921040	2.311781
6	-1.474634	1.833888	0.403002
6	-0.262888	2.314029	-0.020533
1	-2.208833	0.967825	-1.399443
1	-0.063451	1.352057	-1.985119
1	0.241073	3.046457	0.607391
1	-1.858936	2.203942	1.352616
1	-1.061456	-2.668166	-1.773843
1	0.744136	-2.251691	-1.768423

PtCl₂: 8

E(Gas Phase) = -1429.034420

G(Solv.=Toluene) = -1429.042248

6	-0.229725	-1.906716	-1.670852
6	-0.558974	-1.045062	-0.721187
6	0.423078	1.730054	-1.479652
6	-2.184036	0.730687	-0.129690
6	-1.863714	-0.778846	-0.044150
6	-3.153313	-1.426645	-0.581216
1	-3.254700	-2.471589	-0.274877
1	-3.157399	-1.398598	-1.677222
1	1.303360	2.202426	-1.904757
6	-3.591289	0.797825	0.488060
6	-4.281134	-0.513097	-0.005303
1	-4.804525	-1.005321	0.819881
1	-5.031571	-0.300679	-0.773112
1	-3.512132	0.801636	1.582030
1	-4.138464	1.700034	0.197451
78	0.821876	0.255728	0.084213
1	-1.746914	-1.033364	1.017961
17	2.812727	-0.721339	-0.761787
17	0.904387	-0.983008	2.138318
6	-1.078097	1.540738	0.495875
6	-0.076799	2.223722	-0.233496
1	-2.254076	0.987780	-1.195879
1	-0.232515	1.244149	-2.196600
1	0.521858	2.961107	0.301953
1	-1.189763	1.810158	1.543894
1	-1.001050	-2.586098	-2.035136
1	0.764614	-2.000533	-2.085586

PtCl₂: ts8

E(Gas Phase) = -1429.029929

G(Solv.=Toluene) = -1429.034183

1 Imaginary Frequency = -41.7 cm⁻¹

6	-0.579313	2.619375	0.097132
6	-0.700628	1.313146	-0.101376
6	0.230596	-0.004230	2.179882
6	-2.239562	-0.566626	0.466273
6	-1.893301	0.536459	-0.570607
6	-3.250478	1.239813	-0.762960
1	-3.295849	1.808298	-1.696124
1	-3.421186	1.941435	0.061975

1	1.096917	0.085400	2.830087
6	-3.539175	-1.158886	-0.105747
6	-4.282847	0.072092	-0.712905
1	-4.660781	-0.163719	-1.712274
1	-5.149872	0.351001	-0.106037
1	-3.297388	-1.887188	-0.889462
1	-4.132388	-1.681031	0.651297
78	0.796866	-0.091024	0.124372
1	-1.632334	0.024684	-1.508926
17	2.466256	1.483654	-0.353810
17	1.737125	-1.673592	-1.440787
6	-1.074541	-1.492035	0.684407
6	-0.095877	-1.325771	1.675140
1	-2.467901	-0.054954	1.411187
1	-0.550767	0.726059	2.363650
1	0.582267	-2.152849	1.874645
1	-1.056725	-2.428401	0.130679
1	-1.407003	3.279949	-0.160849
1	0.330720	3.080123	0.461878

PtCl₂: 9

E(Gas Phase) = -1429.033745

G(Solv.=Toluene) = -1429.041836

6	-0.949401	2.276955	1.126451
6	-0.907401	1.187775	0.359599
6	0.333315	-0.989180	1.872008
6	-2.204318	-0.905478	0.117009
6	-2.077617	0.571079	-0.355281
6	-3.516243	1.085635	-0.180182
1	-3.713227	1.985265	-0.770296
1	-3.691542	1.336927	0.872798
1	1.243456	-1.124464	2.449195
6	-3.478275	-1.381889	-0.605305
6	-4.403597	-0.122681	-0.607264
1	-4.832084	0.031772	-1.602306
1	-5.245441	-0.249709	0.080386
1	-3.232037	-1.680930	-1.631652
1	-3.939618	-2.246301	-0.117825
78	0.767068	0.027313	0.029783
1	-1.851128	0.541471	-1.432510
17	2.757855	-1.308711	-0.588882
17	1.862379	1.949082	-0.613497
6	-0.932158	-1.648332	-0.137978
6	0.082156	-1.908505	0.806020
1	-2.393917	-0.877232	1.197965
1	-0.462753	-0.434407	2.357197
1	0.845741	-2.639265	0.562313
1	-0.837947	-2.168083	-1.091204
1	-1.876386	2.834717	1.260323
1	-0.067193	2.681277	1.612553

PtCl₂: ts9

E(Gas Phase) = -1429.003668

G(Solv.=Toluene) = -1429.011064

1 Imaginary Frequency = -392.5 cm⁻¹

6	-0.736410	2.636057	0.477834
6	-0.862783	1.313010	0.328526
6	-0.343892	0.313883	2.089571
6	-2.174843	-0.848656	0.282694
6	-1.950105	0.539157	-0.370897
6	-3.391144	1.042511	-0.554159
1	-3.468393	1.838470	-1.300511
1	-3.782569	1.437387	0.391796
1	0.407850	0.812288	2.696289
6	-3.211387	-1.464521	-0.663446
6	-4.154608	-0.256126	-0.981998
1	-4.405835	-0.232817	-2.046429
1	-5.099641	-0.342994	-0.436943
1	-2.721300	-1.827660	-1.574645
1	-3.748255	-2.308345	-0.219158
78	0.799016	-0.047160	0.088163
1	-1.558597	0.327055	-1.377078
17	2.209691	-1.737566	-0.744052
17	2.153115	1.614191	-0.871650
6	-0.868360	-1.542629	0.609514
6	-0.096445	-1.074680	1.694021
1	-2.689149	-0.671285	1.241160
1	-1.355480	0.598301	2.358839
1	0.668754	-1.679248	2.172369
1	-0.647043	-2.522149	0.195348
1	-1.477428	3.315695	0.058745
1	0.126000	3.083142	0.960455

PtCl₂: 10

E(Gas Phase) = -1429.073318
G(Solv.=Toluene) = -1429.071687

6	0.156338	-2.112372	0.570795
6	1.122953	-1.176627	0.865407
6	1.052199	-0.386702	2.175990
6	2.171982	0.895576	0.037254
6	2.079089	-0.629075	-0.172182
6	3.562770	-0.998329	-0.346510
1	3.705034	-1.977024	-0.813268
1	4.087608	-1.009064	0.616109
1	0.459305	-0.912571	2.928247
6	2.983716	1.316795	-1.189343
6	4.068196	0.181636	-1.253895
1	4.213738	-0.156175	-2.284060
1	5.037241	0.547145	-0.900781
1	2.359235	1.319750	-2.089728
1	3.430212	2.310884	-1.091016
78	-0.812789	-0.028638	0.073549
1	1.609023	-0.796857	-1.149399
17	-2.196950	1.810029	-0.319974
17	-2.294452	-1.400014	-1.158175
6	0.833767	1.439890	0.495639
6	0.332922	0.868257	1.685018
1	2.841569	1.055367	0.901141
1	2.045636	-0.179683	2.597088
1	-0.357854	1.402435	2.331034
1	0.477645	2.412634	0.171604

1	0.159946	-2.643088	-0.375610
1	-0.500540	-2.504552	1.341354

Substrate 1d:

PtCl₂: 1-1d

E(Gas Phase) = -1660.065816
G(Solv.=Toluene) = -1660.070374

6	0.779111	1.024523	-0.059515
6	-0.098887	0.204529	0.707543
6	-3.764551	2.912870	-1.427054
6	-3.843176	0.533749	0.545264
6	-0.889824	0.102172	1.759154
6	-1.637706	-1.117002	2.231327
1	-1.130058	-1.477496	3.138074
1	-1.546178	-1.917367	1.488889
1	-3.665727	3.859489	-1.951015
6	-4.084851	-0.687725	1.390069
6	-3.118216	-0.867399	2.584102
1	-3.193043	0.009305	3.242291
1	-3.466215	-1.726556	3.172072
1	-5.107417	-0.658002	1.788262
1	-4.021645	-1.585709	0.757188
78	0.473221	-1.046955	-0.744766
1	-1.000454	1.011203	2.356345
17	1.814270	-2.383323	0.619251
17	-0.908297	-0.216140	-2.438916
6	-4.629249	1.623273	0.546920
6	-4.439163	2.828954	-0.270923
1	-2.966928	0.515889	-0.099660
1	-3.300207	2.046902	-1.892558
1	-4.918765	3.730480	0.112531
1	-5.487544	1.642063	1.221517
6	2.125909	1.438889	0.322381
6	2.780190	2.396309	-0.478741
6	2.762829	0.960730	1.485149
6	4.037575	2.872770	-0.121659
1	2.291206	2.761717	-1.378078
6	4.016944	1.441993	1.838616
1	2.273755	0.200571	2.084611
6	4.656608	2.396353	1.037520
1	4.534866	3.611639	-0.742960
1	4.505066	1.069370	2.734233
1	5.640103	2.764642	1.316098
1	0.325110	1.605262	-0.862708

PtCl₂: ts1-1d

E(Gas Phase) = -1660.58154
G(Solv.=Toluene) = -1660.063844
1 Imaginary Frequency = -36.4 cm⁻¹

6	1.216085	0.347096	-0.579094
6	0.139876	0.114568	0.314279
6	-0.763857	3.417451	-2.112684
6	-2.368197	2.511461	0.365556
6	-0.172287	0.792656	1.445193

6	-1.252239	0.477112	2.431915
1	-0.751578	0.166420	3.363341
1	-1.836371	-0.381877	2.089907
1	-0.173091	3.842589	-2.919446
6	-3.100463	2.126425	1.625123
6	-2.165401	1.673256	2.772224
1	-1.542505	2.524971	3.078690
1	-2.778177	1.403323	3.641599
1	-3.688727	2.977424	1.993573
1	-3.811042	1.319897	1.405551
78	-0.651306	-1.514650	-0.414036
1	0.415330	1.691223	1.644919
17	0.093342	-2.861333	1.349580
17	-1.591583	-0.501587	-2.311867
6	-1.828194	3.727698	0.150233
6	-1.049718	4.145815	-1.019102
1	-2.267722	1.740035	-0.394883
1	-1.120148	2.400323	-2.255337
1	-0.667445	5.165738	-0.972581
1	-1.958182	4.490894	0.919769
6	2.585610	0.526901	-0.204113
6	3.502681	1.011440	-1.171203
6	3.047508	0.252434	1.107971
6	4.820604	1.265384	-0.822433
1	3.152722	1.202267	-2.181979
6	4.370510	0.503769	1.445861
1	2.367957	-0.200922	1.821276
6	5.253853	1.014442	0.486800
1	5.516371	1.650218	-1.561719
1	4.725705	0.282445	2.447675
1	6.290626	1.199185	0.754280
1	0.979984	0.390718	-1.640153

PtCl₂: 2-1d

E(Gas Phase) = -1660.059665
G(Solv.=Toluene) = -1660.064928

6	1.195791	-0.584065	-0.619943
6	0.133584	-0.198041	0.222881
6	1.598707	2.447781	-2.144252
6	-0.187264	3.109935	0.273204
6	0.360330	0.566181	1.355490
6	-0.630681	1.003774	2.378643
1	-0.389914	0.444714	3.299110
1	-1.639815	0.706176	2.085915
1	2.322963	2.270039	-2.934818
6	-0.972297	3.409959	1.523482
6	-0.556002	2.508252	2.710122
1	0.469135	2.763179	3.011587
1	-1.200791	2.715036	3.572671
1	-0.828365	4.456210	1.824786
1	-2.041930	3.276456	1.327225
78	-1.624008	-0.786749	-0.365453
1	1.389304	0.879457	1.530959
17	-1.965750	-2.207213	1.465505
17	-1.646909	0.502849	-2.330604
6	1.094456	3.501871	0.080266
6	1.940552	3.177050	-1.062941
1	-0.696831	2.543395	-0.503339

1	0.602270	2.043078	-2.297622
1	2.957707	3.564506	-1.007455
1	1.570757	4.100096	0.859139
6	2.535685	-0.925345	-0.219333
6	3.563646	-0.918766	-1.195110
6	2.860003	-1.311799	1.104452
6	4.871412	-1.220034	-0.846100
1	3.317359	-0.643591	-2.216747
6	4.172853	-1.619258	1.445279
1	2.064386	-1.428747	1.832034
6	5.179903	-1.565752	0.476964
1	5.654153	-1.195368	-1.598384
1	4.409163	-1.928289	2.459128
1	6.202154	-1.817753	0.744904
1	0.962046	-0.698443	-1.675746

Allene s-a:

PtCl₂: 1_s-a

E(Gas Phase) = -1274.232639
G(Solv.=Toluene) = -1274.266994

6	-0.022959	1.255062	-1.181591
6	0.122239	1.415435	0.229132
6	0.263321	2.224359	1.261297
6	0.367904	1.838512	2.708640
1	1.346885	2.125851	3.112038
1	0.239992	0.761924	2.844028
6	-1.348325	1.548548	-1.850543
1	-1.540035	0.850804	-2.671649
1	-1.272333	2.555949	-2.286890
1	-2.184750	1.518651	-1.154334
6	1.179738	1.341132	-2.096825
1	1.184739	2.351315	-2.532990
1	1.095006	0.629564	-2.924231
1	2.118406	1.168519	-1.573315
78	-0.035744	-0.572808	0.033405
1	0.315651	3.289608	1.022807
17	2.253281	-1.024591	0.018256
17	-2.341045	-0.779552	0.325167
1	-0.395023	2.358960	3.300113

PtCl₂: ts1_s-a

E(Gas Phase) = -1274.218899
G(Solv.=Toluene) = -1274.262301
1 Imaginary Frequency = -84.6 cm⁻¹

6	-1.747873	-1.007509	-0.569271
6	-0.949383	-0.647338	0.547795
6	-1.284984	-0.830607	1.849785
6	-0.469427	-0.425532	3.029519
1	-1.117744	-0.078428	3.843082
1	0.248383	0.354567	2.762092
6	-1.228768	-1.751654	-1.751850
1	-1.299787	-1.133053	-2.657311
1	-1.894375	-2.611884	-1.922554
1	-0.195610	-2.077078	-1.623704

6	-3.178423	-0.594023	-0.583701
1	-3.616207	-0.639817	0.420834
1	-3.779632	-1.152739	-1.305754
1	-3.195688	0.471699	-0.862145
78	0.583192	0.334445	-0.155521
1	-2.194797	-1.399198	2.055018
17	-0.623053	2.347238	-0.260556
17	2.070758	-1.464665	-0.158705
1	0.098657	-1.284553	3.414878

PtCl₂: 2_s-a

E(Gas Phase) = -1274.223158
G(Solv.=Toluene) = -1274.264520

6	2.179840	0.256539	-0.507463
6	1.032096	0.622921	0.231213
6	1.103733	1.675181	1.129433
6	-0.021970	2.185896	1.939658
1	0.306302	2.888015	2.709858
1	-0.591392	1.355854	2.375838
6	2.076200	-0.752100	-1.594166
1	1.890365	-1.731887	-1.122606
1	2.982018	-0.807201	-2.203995
1	1.191447	-0.565575	-2.213787
6	3.566730	0.761296	-0.253354
1	3.674789	1.458456	0.575929
1	3.956774	1.222876	-1.170583
1	4.212621	-0.106008	-0.056095
78	-0.659196	-0.305289	-0.051840
1	2.045568	2.213199	1.222178
17	0.089716	-2.289059	0.947735
17	-1.686032	1.506534	-1.124694
1	-0.733605	2.689379	1.263185

Allene s-b:

PtCl₂: 1_s-b

E(Gas Phase) = -1234.917013
G(Solv.=Toluene) = -1234.979341

6	0.155697	0.249488	1.744601
6	0.789657	1.046635	0.755284
6	1.615291	2.003063	0.385836
6	1.974823	2.403358	-1.015824
1	1.650037	3.431837	-1.216222
1	1.512422	1.740036	-1.750363
6	0.869329	-0.789635	2.568625
1	0.196766	-1.613013	2.827416
1	1.178627	-0.310265	3.509921
1	1.748237	-1.186037	2.059447
78	-0.347888	-0.294563	-0.243304
1	2.075213	2.565061	1.202478
17	-2.377862	0.835481	-0.064500
17	1.439470	-1.667653	-0.836096
1	3.062246	2.370627	-1.152604
1	-0.764409	0.647140	2.176681

PtCl₂: ts1_s-b

E(Gas Phase) = -1234.896150
G(Solv.=Toluene) = -1234.958512
1 Imaginary Frequency = -92.5 cm⁻¹

6	2.058058	0.444834	1.179672
6	1.071059	0.734842	0.280929
6	1.097394	1.755175	-0.679919
6	2.286672	2.130292	-1.479772
1	2.204142	1.645272	-2.466087
1	3.220198	1.779140	-1.029360
6	2.069598	-0.680870	2.148908
1	1.715894	-0.333943	3.131957
1	3.091768	-1.049739	2.294045
1	1.415997	-1.492967	1.819906
78	-0.557053	-0.266781	-0.087543
1	0.164435	2.275018	-0.887859
17	-1.997057	1.448374	0.599973
17	0.523408	-2.194873	-0.853710
1	2.312982	3.209863	-1.667286
1	2.880057	1.161104	1.247656

PtCl₂: 2_s-b

E(Gas Phase) = -1234.904067
G(Solv.=Toluene) = -1234.965586

6	-0.871684	2.135634	-0.787700
6	0.000804	1.385101	0.000206
6	0.874437	2.134427	0.788012
6	1.898752	1.585282	1.692731
1	2.407938	2.355587	2.274801
1	2.626663	1.024493	1.079935
6	-1.897705	1.587958	-1.691390
1	-1.456151	0.829897	-2.352371
1	-2.408553	2.359252	-2.270643
1	-2.623762	1.024679	-1.078790
78	-0.000272	-0.550943	-0.000053
1	0.803000	3.221200	0.706147
17	2.112314	-0.731707	-0.994132
17	-2.113182	-0.730598	0.993555
1	1.456701	0.824955	2.350634
1	-0.797517	3.222284	-0.706898

Allene s-c:

PtCl₂: 1_s-c

E(Gas Phase) = -1195.596857
G(Solv.=Toluene) = -1195.670961

6	-0.033244	0.317297	1.837885
6	-0.167990	1.335858	0.865583
6	-0.330212	2.571828	0.452058
6	-0.400662	3.053757	-0.968206
1	-1.355840	3.560436	-1.150629

1	-0.303719	2.226841	-1.675640
78	0.058662	-0.456538	-0.086725
1	-0.423291	3.318773	1.244082
17	-2.218791	-0.910639	-0.241137
17	2.377311	-0.327347	-0.246864
1	0.398957	3.777990	-1.164566
1	-0.916987	-0.068292	2.345396
1	0.923088	0.167545	2.338015

PtCl₂: ts1_s-c

E(Gas Phase) = -1195.565919

G(Solv.=Toluene) = -1195.641982

1 Imaginary Frequency = -318.7 cm⁻¹

6	0.145083	1.550667	1.746304
6	-0.502216	1.303720	0.541044
6	-1.573643	1.974955	0.015034
6	-2.329198	1.616548	-1.208916
1	-3.388690	1.872548	-1.091754
1	-2.215556	0.556180	-1.449995
78	0.277717	-0.384802	-0.036965
1	-1.843922	2.910108	0.510727
17	-1.647619	-1.676877	0.253230
17	2.382502	0.531056	-0.492372
1	-1.956616	2.203274	-2.063434
1	-0.403563	1.883059	2.630323
1	1.213225	1.393010	1.852023

PtCl₂: 2_s-c

E(Gas Phase) = -1195.573819

G(Solv.=Toluene) = -1195.651600

6	0.687587	2.059273	1.353126
6	-0.120609	1.396284	0.445053
6	-1.138752	2.173581	-0.127741
6	-2.111724	1.726696	-1.129002
1	-2.812327	2.508603	-1.424866
1	-2.642738	0.845543	-0.716425
78	0.184425	-0.453498	-0.019195
1	-1.216945	3.202824	0.230878
17	-1.947628	-1.329298	0.397096
17	2.415962	0.076028	-0.472797
1	-1.591880	1.317115	-2.006531
1	0.486425	3.095813	1.623890
1	1.531654	1.573555	1.828564

Metal free [4+2] cycloaddition:

Reactant

E(Gas Phase) = -389.390098
G(Solv.=Toluene) = -389.324969

6	2.620252	2.467727	-0.457510
6	2.281608	1.359677	0.149307
6	-3.085223	1.793067	0.031805
6	-1.064038	-0.525573	-0.334240
6	1.949496	0.245933	0.752720
6	2.166967	-1.145182	0.192429
1	2.953385	-1.631637	0.789083
1	2.555948	-1.069494	-0.830276
1	-3.766868	2.556553	0.395405
6	-0.215632	-1.693177	-0.757314
6	0.929737	-2.064447	0.215573
1	0.530722	-2.121964	1.237403
1	1.271517	-3.076651	-0.038775
1	-0.860949	-2.572046	-0.883984
1	0.225524	-1.488962	-1.745773
1	1.500984	0.304190	1.747045
6	-2.370459	-0.610416	-0.035290
6	-3.239175	0.504197	0.364716
1	-0.563472	0.437506	-0.252448
1	-2.280867	2.127213	-0.618878
1	-4.097669	0.229578	0.979172
1	-2.846947	-1.592189	-0.067798
1	3.609969	2.905595	-0.337121
1	1.927519	3.001476	-1.106226

Transition state

E(Gas Phase) = -389.347659
G(Solv.=Toluene) = -389.276712
1 Imaginary Frequency = -506.7 cm⁻¹

6	-1.529170	2.121103	-0.428396
6	-1.206803	0.922307	0.063115
6	-2.245795	-0.155512	0.341678
6	0.537564	-0.795448	-0.450583
6	0.191243	0.463810	0.377717
6	1.413408	1.360612	0.149086
1	1.526664	2.132627	0.917387
1	1.323538	1.875344	-0.815489
1	-2.573203	-0.083027	1.393243
6	1.994428	-1.063986	-0.033752
6	2.612427	0.360959	0.119293
1	3.209136	0.429272	1.034902
1	3.288574	0.591100	-0.710793
1	2.011381	-1.596293	0.925868
1	2.536978	-1.683408	-0.756285
1	0.199229	0.135990	1.431952
6	-0.496862	-1.870550	-0.261973
6	-1.749880	-1.566708	0.096009
1	0.546469	-0.497029	-1.513115

1	-3.150176	0.031496	-0.253827
1	-2.485251	-2.360030	0.225774
1	-0.215273	-2.907641	-0.441893
1	-0.784284	2.893592	-0.596830
1	-2.557144	2.378484	-0.674059

Product

E(Gas Phase) = -389.456601
G(Solv.=Toluene) = -389.375828

6	-1.529170	2.121103	-0.428396
6	-1.206803	0.922307	0.063115
6	-2.245795	-0.155512	0.341678
6	0.537564	-0.795448	-0.450583
6	0.191243	0.463810	0.377717
6	1.413408	1.360612	0.149086
1	1.526664	2.132627	0.917387
1	1.323538	1.875344	-0.815489
1	-2.573203	-0.083027	1.393243
6	1.994428	-1.063986	-0.033752
6	2.612427	0.360959	0.119293
1	3.209136	0.429272	1.034902
1	3.288574	0.591100	-0.710793
1	2.011381	-1.596293	0.925868
1	2.536978	-1.683408	-0.756285
1	0.199229	0.135990	1.431952
6	-0.496862	-1.870550	-0.261973
6	-1.749880	-1.566708	0.096009
1	0.546469	-0.497029	-1.513115
1	-3.150176	0.031496	-0.253827
1	-2.485251	-2.360030	0.225774
1	-0.215273	-2.907641	-0.441893
1	-0.784284	2.893592	-0.596830
1	-2.557144	2.378484	-0.674059

AuCl

Substrate 1a:

AuCl: 1

E(Gas Phase) = -1063.741313
G(Solv.=Dichlorometane) = -1063.690966

6	-3.101622	0.417409	0.619490
6	-1.825025	0.711660	0.438645
6	3.440470	-0.970906	1.846989
6	2.597238	0.969805	-0.411995
6	-0.708287	1.505788	0.374391
6	-0.451390	2.500699	-0.748921
1	-1.056963	3.387519	-0.501631
1	-0.858597	2.105591	-1.686217
1	3.953480	-1.549553	2.610208
6	-3.707019	-0.945898	0.397651
1	-4.511854	-0.886425	-0.346769
1	-4.158601	-1.316517	1.327206
1	-2.971084	-1.677020	0.055330
6	-4.049762	1.500804	1.096005
1	-3.545637	2.460178	1.237830
1	-4.512138	1.208354	2.047775
1	-4.863490	1.639015	0.372081
6	1.987842	1.890459	-1.448118
6	1.001970	2.966078	-0.952883
1	1.372005	3.432205	-0.031160
1	0.969691	3.771890	-1.696790
1	2.810805	2.392955	-1.980468
1	1.490766	1.278147	-2.213261
1	-0.128393	1.649615	1.288194
6	2.863137	1.268602	0.872500
6	3.487022	0.369353	1.853540
1	2.902601	-0.006618	-0.785516
1	2.885690	-1.531641	1.098705
1	4.018356	0.867333	2.665745
1	2.629333	2.266640	1.246315
79	-0.242748	-0.613424	-0.177097
17	0.796688	-2.596134	-0.843571

AuCl: ts1

E(Gas Phase) = -1063.719444
G(Solv.=Dichlorometane) = -1063.676181
Imaginary Frequency = -91.5 cm⁻¹

6	-0.782335	2.608198	0.066387
6	-0.223400	1.478542	-0.456116
6	2.804070	0.387307	2.884696
6	2.529252	-1.126117	0.211200
6	0.927279	1.263627	-1.173358
6	1.127622	0.365526	-2.352194
1	1.289539	1.055087	-3.200718
1	0.216374	-0.201670	-2.564336
1	3.055640	0.750782	3.876783
6	-1.708177	2.613298	1.249162
1	-2.747019	2.777418	0.929939

1	-1.450570	3.444420	1.918307
1	-1.675750	1.671911	1.802929
6	-0.593893	3.930633	-0.632245
1	0.295699	3.926028	-1.271072
1	-0.522147	4.747396	0.095929
1	-1.455745	4.157355	-1.275537
6	2.306536	-1.640122	-1.194594
6	2.357292	-0.571265	-2.302454
1	3.267427	0.033672	-2.201091
1	2.425580	-1.067885	-3.277946
1	3.064871	-2.403089	-1.425317
1	1.341072	-2.158437	-1.236370
1	1.826045	1.804284	-0.859121
6	3.536554	-0.321279	0.595732
6	3.750293	0.193049	1.954271
1	1.825748	-1.474144	0.965741
1	1.753140	0.189476	2.688220
1	4.780572	0.452329	2.200537
1	4.287118	-0.024935	-0.139655
79	-1.046085	-0.398041	-0.000833
17	-2.066082	-2.430774	0.584452

AuCl: 2

E(Gas Phase) = -1063.721150
G(Solv.=Dichlorometane) = -1063.683685

6	0.768276	2.058252	-0.784671
6	0.457910	0.684953	-0.804630
6	2.125381	1.480231	2.170010
6	2.268320	-1.360369	1.028959
6	1.415911	-0.187851	-1.317713
6	1.217628	-1.616554	-1.693769
1	1.226432	-1.637354	-2.798552
1	0.233456	-1.970360	-1.372470
1	2.185601	2.485936	2.575873
6	-0.152992	3.031249	-0.113611
1	-0.947926	3.302095	-0.825828
1	0.359727	3.956609	0.169816
1	-0.656178	2.585332	0.748130
6	1.884073	2.718148	-1.548040
1	2.576054	2.033134	-2.037961
1	2.445700	3.387128	-0.885657
1	1.446326	3.357468	-2.328924
6	2.366604	-2.693974	0.338765
6	2.347979	-2.544288	-1.203105
1	3.312850	-2.136612	-1.534150
1	2.241921	-3.529864	-1.671029
1	3.290620	-3.212742	0.624871
1	1.528876	-3.328097	0.649398
1	2.418714	0.180900	-1.539221
6	3.311336	-0.521225	1.231041
6	3.240429	0.820969	1.797405
1	1.277710	-1.068644	1.369349
1	1.136695	1.033184	2.128221
1	4.196188	1.334473	1.896861
1	4.304269	-0.850441	0.920718
79	-1.311069	-0.026556	-0.058127
17	-3.323981	-0.884792	0.817572

AuCl: ts2

E(Gas Phase) = -1063.717993
G(Solv.=Dichlorometane) = -1063.674053
l Imaginary Frequency = -215.9 cm⁻¹

6	1.030402	1.874017	-0.634265
6	0.577837	0.518464	-0.689480
6	1.738942	1.707187	1.603412
6	2.159984	-1.197764	1.046361
6	1.488343	-0.459385	-1.112423
6	1.180873	-1.889730	-1.448905
1	1.152507	-1.986134	-2.545643
1	0.190805	-2.168933	-1.074177
1	1.693843	2.774994	1.794423
6	0.016590	2.969901	-0.394362
1	-0.520276	3.148935	-1.337710
1	0.490234	3.913134	-0.102647
1	-0.735651	2.683566	0.343787
6	2.286461	2.377840	-1.322649
1	3.121607	1.676354	-1.305385
1	2.623056	3.318727	-0.877248
1	2.049472	2.588111	-2.375628
6	2.368811	-2.636777	0.651051
6	2.278481	-2.808919	-0.888670
1	3.243342	-2.533369	-1.335111
1	2.092085	-3.856012	-1.151120
1	3.342259	-2.997452	1.005296
1	1.595627	-3.248705	1.128323
1	2.478778	-0.154642	-1.451342
6	3.177052	-0.287760	1.265411
6	2.970742	1.087047	1.534501
1	1.154337	-0.936716	1.361312
1	0.828517	1.157388	1.811172
1	3.858937	1.716470	1.554154
1	4.204732	-0.617209	1.112404
79	-1.291756	-0.011636	-0.070131
17	-3.438977	-0.652001	0.666211

AuCl: 3

E(Gas Phase) = -1063.758139
G(Solv.=Dichlorometane) = -1063.699166

6	-1.047886	1.848943	0.446746
6	-0.577168	0.420715	0.462165
6	-1.609650	2.041886	-1.039152
6	-2.191184	-1.003415	-0.765435
6	-1.579929	-0.641083	0.676579
6	-1.114985	-2.017685	1.183421
1	-0.886244	-2.004833	2.254308
1	-0.203161	-2.319068	0.655477
1	-1.741569	3.124427	-1.145153
6	0.115730	2.848301	0.624450
1	0.607343	2.703775	1.592227
1	-0.265834	3.875310	0.586299
1	0.873455	2.733296	-0.156104

6	-2.152785	2.188732	1.474477
1	-3.083783	1.648255	1.292176
1	-2.376883	3.259727	1.423408
1	-1.815481	1.970970	2.494359
6	-2.798543	-2.424077	-0.548862
6	-2.288078	-2.942508	0.818222
1	-3.079545	-2.858114	1.572678
1	-1.988626	-3.994513	0.786146
1	-3.892845	-2.378661	-0.571672
1	-2.488811	-3.080319	-1.368448
1	-2.423093	-0.301519	1.287125
6	-3.150529	0.033238	-1.277923
6	-2.900466	1.346191	-1.381448
1	-1.334995	-1.086552	-1.446526
1	-0.811557	1.757603	-1.736405
1	-3.705691	1.987089	-1.736098
1	-4.141971	-0.323650	-1.553937
79	1.281284	-0.054467	0.005939
17	3.488867	-0.623868	-0.514026

AuCl: ts3

E(Gas Phase) = -1063.734925
G(Solv.=Dichlorometane) = -1063.686844
l Imaginary Frequency = -676.4 cm⁻¹

6	1.013521	1.813226	0.170193
6	0.600475	0.320588	0.098206
6	2.536863	2.119113	0.329524
6	3.039629	-0.713979	0.407927
6	1.509480	-0.753213	0.227396
6	1.087083	-2.211773	0.190011
1	0.180627	-2.373929	-0.399417
1	0.835787	-2.484656	1.226110
1	2.650276	3.207858	0.295707
6	0.304099	2.400986	1.414562
1	-0.783860	2.340638	1.321733
1	0.583771	3.455047	1.528770
1	0.594406	1.871046	2.329354
6	0.494145	2.529173	-1.097194
1	0.989128	2.152508	-2.000608
1	0.694265	3.604932	-1.026341
1	-0.583364	2.386606	-1.219852
6	3.486420	-2.200391	0.395687
6	2.337181	-2.967788	-0.282026
1	2.420533	-2.903771	-1.374761
1	2.316260	-4.028353	-0.016476
1	4.449105	-2.330291	-0.108750
1	3.611564	-2.555414	1.424973
1	1.044322	-0.220544	-0.956742
6	3.687566	0.159684	-0.649544
6	3.442832	1.472046	-0.686546
1	3.237829	-0.267131	1.392981
1	2.851250	1.816165	1.338951
1	3.903160	2.090820	-1.453701
1	4.343167	-0.323008	-1.371572
79	-1.412121	-0.097525	-0.028717
17	-3.706849	-0.561180	-0.104171

AuCl: 4

E(Gas Phase) = -1063.799915
G(Solv.=Dichlorometane) = -1063.735854

6	1.402571	-1.865235	0.269024
6	0.827564	-0.577708	0.871535
6	1.939943	-1.677035	-1.175783
6	1.587743	1.253095	-0.871255
6	0.945934	0.747819	0.446296
6	0.878143	1.929046	1.431749
1	1.115889	1.615390	2.453329
1	-0.124981	2.369702	1.452058
1	2.243943	-2.661087	-1.550524
6	0.336792	-2.981368	0.270599
1	-0.125345	-3.086775	1.259213
1	0.796090	-3.942240	0.009300
1	-0.461981	-2.777440	-0.450495
6	2.556846	-2.294943	1.210272
1	3.328881	-1.522561	1.281817
1	3.024849	-3.212375	0.833943
1	2.182584	-2.502692	2.219356
6	1.673936	2.783726	-0.670126
6	1.866084	2.954590	0.844234
1	2.894751	2.696683	1.127729
1	1.669497	3.972489	1.194257
1	2.474999	3.231611	-1.267160
1	0.731507	3.252252	-0.978506
1	0.599291	-0.694086	1.933871
6	2.942008	0.610044	-1.113891
6	3.091458	-0.706804	-1.280636
1	0.939757	1.016186	-1.724021
1	1.106789	-1.347320	-1.814290
1	4.083133	-1.110427	-1.476384
1	3.803448	1.273632	-1.178447
79	-1.173347	0.024825	0.066042
17	-3.404871	0.024503	-0.584379

AuCl: ts3"

E(Gas Phase) = -1063.729953
G(Solv.=Dichlorometane) = -1063.681170
1 Imaginary Frequency = -244.3 cm⁻¹

6	0.862461	2.066754	-0.603962
6	0.688163	0.717649	-0.223575
6	1.082594	1.665876	1.349590
6	1.997358	-1.234288	0.728527
6	1.819057	-0.266620	-0.452780
6	1.668156	-1.219639	-1.658453
1	1.923567	-0.735507	-2.607295
1	0.628643	-1.556042	-1.735422
1	1.527781	2.669634	1.312900
6	-0.297870	3.026287	-0.626538
1	-0.613543	3.123991	-1.674572
1	-0.009362	4.024710	-0.277885
1	-1.158281	2.653533	-0.066903

6	2.124664	2.617213	-1.233796
1	3.038121	2.185197	-0.822174
1	2.173591	3.706198	-1.144718
1	2.100854	2.372179	-2.303970
6	3.016645	-2.248745	0.175599
6	2.612333	-2.415595	-1.318563
1	3.496506	-2.424980	-1.964143
1	2.093180	-3.365103	-1.481568
1	4.031939	-1.839363	0.257250
1	3.004665	-3.195878	0.724606
1	2.782911	0.250127	-0.559771
6	2.355651	-0.477027	1.968685
6	1.987725	0.791976	2.176782
1	1.041799	-1.755873	0.890911
1	0.082880	1.763440	1.768448
1	2.323168	1.301287	3.081003
1	2.964715	-0.969614	2.725073
79	-1.195056	-0.102444	-0.008899
17	-3.325020	-1.073996	0.170126

Substrate 1b:

AuCl: 1-1b

E(Gas Phase) = -1024.424400
G(Solv.=Dichlorometane) = -1024.395085

6	0.571778	1.794840	0.975414
6	-0.093761	0.637202	1.272248
6	-3.932549	2.173882	-1.771199
6	-3.246911	-0.537238	-0.443603
6	-0.964795	-0.179017	1.829249
6	-1.068908	-1.675938	1.677645
1	-0.740262	-2.120910	2.628603
1	-0.367322	-2.026937	0.911863
1	-4.192065	3.203643	-1.999474
6	1.602583	2.440008	1.879646
1	1.117288	3.251454	2.439207
1	2.421760	2.878353	1.301814
1	2.015021	1.723446	2.593527
6	-3.013606	-1.972581	-0.057805
6	-2.491018	-2.195056	1.381064
1	-3.198710	-1.751582	2.094891
1	-2.492103	-3.275366	1.573990
1	-3.951811	-2.531855	-0.164871
1	-2.297682	-2.427221	-0.758758
1	-1.690291	0.290033	2.499145
6	-4.458359	0.020512	-0.602222
6	-4.718360	1.410891	-0.998338
1	-2.362945	0.081411	-0.587787
1	-3.017368	1.790388	-2.215949
1	-5.655214	1.835184	-0.634748
1	-5.341521	-0.590906	-0.407246
79	1.440286	0.081608	-0.169919
17	2.746640	-1.218198	-1.581712
1	0.161194	2.428136	0.185909

AuCl: ts1-1b

E(Gas Phase) = -1024.400314
G(Solv.=Dichlorometane) = -1024.376216
1 Imaginary Frequency = -88.1 cm⁻¹

6	-0.607111	1.836320	0.816340
6	-0.324156	0.498033	0.843281
6	-4.088044	2.218554	-1.293153
6	-3.356380	-0.723352	-0.676635
6	-1.071375	-0.569756	1.256804
6	-0.977309	-1.987994	0.793395
1	-0.392753	-2.545520	1.541915
1	-0.403793	-2.047534	-0.140333
1	-4.283397	3.286976	-1.291943
6	0.359264	2.965442	0.933491
1	-0.059462	3.731768	1.600244
1	0.508797	3.453273	-0.040001
1	1.335708	2.637316	1.299986
6	-3.182019	-2.214431	-0.566467
6	-2.357390	-2.665878	0.663104
1	-2.940259	-2.475504	1.574650
1	-2.209307	-3.750744	0.607119
1	-4.162405	-2.704510	-0.518035
1	-2.686792	-2.585611	-1.473953
1	-1.744658	-0.413978	2.105014
6	-4.443499	-0.043610	-0.269325
6	-4.641103	1.407927	-0.377576
1	-2.525503	-0.169098	-1.111463
1	-3.448213	1.840755	-2.086894
1	-5.326522	1.842591	0.350763
1	-5.258549	-0.599009	0.198069
79	1.543409	0.035728	0.003975
17	3.614283	-0.516344	-0.957154
1	-1.640310	2.126667	0.602902

AuCl: 2-1b

E(Gas Phase) = -1024.407233
G(Solv.=Dichlorometane) = -1024.383282

6	-0.776866	1.923077	1.156659
6	-0.478685	0.578675	0.920465
6	-1.923147	2.258234	-1.396826
6	-2.520214	-0.707765	-1.041773
6	-1.514477	-0.286827	1.305620
6	-1.458385	-1.775652	1.376960
1	-1.397016	-2.044276	2.445095
1	-0.545226	-2.144062	0.898487
1	-1.811179	3.335025	-1.481918
6	0.184574	3.054560	1.040547
1	0.657187	3.202714	2.025584
1	-0.315558	3.995155	0.787007
1	0.985470	2.838303	0.328993
6	-2.831261	-2.147954	-0.737748
6	-2.718282	-2.433581	0.782381
1	-3.607061	-2.033995	1.288876
1	-2.703785	-3.513740	0.965908
1	-3.843164	-2.406002	-1.074322
1	-2.130710	-2.792268	-1.279834
1	-2.417074	0.151046	1.743524

6	-3.427545	0.306590	-0.977828
6	-3.139531	1.712063	-1.149065
1	-1.507692	-0.494033	-1.374671
1	-1.043547	1.664645	-1.622560
1	-3.982096	2.386659	-1.003370
1	-4.456827	0.057602	-0.716829
79	1.248168	-0.065628	0.064799
17	3.228128	-0.828244	-0.960620
1	-1.742263	2.173448	1.605126

AuCl: ts2-1b

E(Gas Phase) = -1024.406888
G(Solv.=Dichlorometane) = -1024.379723
1 Imaginary Frequency = -128.8 cm⁻¹

6	-0.848473	1.926856	1.030092
6	-0.527186	0.565177	0.866126
6	-1.767694	2.248528	-1.222710
6	-2.472832	-0.671871	-1.024485
6	-1.558235	-0.309804	1.236674
6	-1.480580	-1.800176	1.346466
1	-1.434363	-2.059664	2.416252
1	-0.557635	-2.165483	0.884216
1	-1.615467	3.322743	-1.256339
6	0.151625	3.039922	0.981751
1	0.663863	3.076271	1.955809
1	-0.319033	4.015612	0.825661
1	0.922856	2.864272	0.226955
6	-2.822677	-2.115716	-0.781741
6	-2.723521	-2.463381	0.727268
1	-3.622716	-2.094333	1.238476
1	-2.697279	-3.549425	0.869262
1	-3.837522	-2.332211	-1.137657
1	-2.131868	-2.751525	-1.345786
1	-2.467475	0.121274	1.666959
6	-3.376219	0.362504	-0.997631
6	-3.036420	1.744693	-1.091275
1	-1.457136	-0.475650	-1.355383
1	-0.928473	1.641283	-1.542493
1	-3.849826	2.451266	-0.932928
1	-4.420101	0.127737	-0.788770
79	1.229667	-0.069983	0.069500
17	3.246093	-0.823684	-0.890475
1	-1.801853	2.178750	1.500165

AuCl: 3-1b

E(Gas Phase) = -1024.450228
G(Solv.=Dichlorometane) = -1024.408086

6	-0.887729	1.933434	0.824896
6	-0.582521	0.488928	0.622712
6	-1.345468	2.482271	-0.584994
6	-2.420672	-0.539201	-0.668911
6	-1.730167	-0.425157	0.764779
6	-1.471716	-1.903184	1.110053
1	-1.280152	-2.040670	2.179144

1	-0.579994	-2.247525	0.575181
1	-1.414131	3.569220	-0.463282
6	0.288168	2.771176	1.352114
1	0.662609	2.369602	2.298956
1	-0.040535	3.802672	1.523948
1	1.120223	2.783727	0.640888
6	-3.376621	-1.741822	-0.461294
6	-2.731793	-2.654814	0.613763
1	-3.433274	-2.829033	1.436445
1	-2.464966	-3.637784	0.214339
1	-4.350171	-1.370971	-0.119629
1	-3.546225	-2.258816	-1.411930
1	-2.492928	-0.005200	1.435232
6	-3.102786	0.704257	-1.167217
6	-2.654454	1.966855	-1.126776
1	-1.624865	-0.834513	-1.366188
1	-0.529394	2.301519	-1.296838
1	-3.307807	2.732795	-1.542033
1	-4.084328	0.540449	-1.611259
79	1.182577	-0.116482	0.007943
17	3.281504	-0.836392	-0.723091
1	-1.748640	2.048814	1.497366

AuCl: ts3*-1b

E(Gas Phase) = -1024.441714
G(Solv.=Dichlorometane) = -1024.399723
1 Imaginary Frequency = -101.3 cm⁻¹

6	0.935707	1.942105	-0.845557
6	0.587915	0.515951	-0.567189
6	2.143363	2.489592	0.021546
6	2.229672	-0.746200	0.742063
6	1.719461	-0.423008	-0.704894
6	1.459552	-1.828978	-1.291921
1	1.483448	-1.811091	-2.386066
1	0.461909	-2.169725	-0.996749
1	2.950187	2.796597	-0.658278
6	-0.241099	2.925657	-0.807755
1	-1.049933	2.601986	-1.469635
1	0.086913	3.920802	-1.130487
1	-0.647528	3.009347	0.205968
6	3.210641	-1.913519	0.467231
6	2.561023	-2.738092	-0.671663
1	3.307218	-3.030427	-1.416913
1	2.116516	-3.662577	-0.290282
1	4.176050	-1.501682	0.149678
1	3.389287	-2.500876	1.374265
1	2.561955	0.047114	-1.233875
6	2.820347	0.417474	1.475638
6	2.771050	1.718955	1.164983
1	1.375657	-1.142469	1.310853
1	1.776123	3.425950	0.457470
1	3.306676	2.387315	1.839759
1	3.364553	0.149001	2.381244
79	-1.197969	-0.070319	-0.016290
17	-3.324272	-0.765898	0.655369
1	1.307340	1.896596	-1.886164

AuCl: 3*-1b

E(Gas Phase) = -1024.446477
G(Solv.=Dichlorometane) = -1024.406740

6	1.020485	1.841576	-0.678067
6	0.566268	0.425936	-0.470000
6	2.550878	2.076526	-0.784698
6	2.364536	-0.693305	0.768290
6	1.587354	-0.629330	-0.610415
6	1.158454	-2.088421	-0.819395
1	0.826841	-2.280379	-1.844891
1	0.316398	-2.319907	-0.157337
1	2.945102	1.601444	-1.693593
6	0.370510	2.843515	0.304350
1	-0.719058	2.760333	0.299171
1	0.643925	3.866020	0.023892
1	0.723489	2.660683	1.323984
6	3.136914	-2.047452	0.655768
6	2.407120	-2.901244	-0.416818
1	3.059131	-3.052627	-1.284225
1	2.137619	-3.894945	-0.046838
1	4.173069	-1.851103	0.360254
1	3.167742	-2.540312	1.632812
1	2.336342	-0.352890	-1.365549
6	3.252301	0.478500	1.084596
6	3.349743	1.640826	0.427886
1	1.609563	-0.799192	1.561363
1	2.702523	3.150258	-0.938427
1	4.075797	2.362777	0.797696
1	3.892055	0.329917	1.955046
79	-1.302987	0.011090	-0.038349
17	-3.536624	-0.485412	0.430119
1	0.580699	2.053073	-1.674760

AuCl: ts3-Hb-1b

E(Gas Phase) = -1024.424827
G(Solv.=Dichlorometane) = -1024.395103
1 Imaginary Frequency = -790.4 cm⁻¹

6	1.075041	1.842783	-0.447386
6	0.608865	0.507188	-0.468767
6	2.562196	2.171528	-0.540397
6	2.418804	-0.742516	0.746495
6	1.682242	-0.561764	-0.604435
6	1.235363	-1.991771	-0.944887
1	0.957165	-2.107480	-1.997580
1	0.350601	-2.245065	-0.349881
1	2.976423	1.773119	-1.476515
6	0.158988	3.008876	-0.187761
1	-0.894225	2.735112	-0.281241
1	0.395045	3.859985	-0.835909
1	0.329588	3.327204	0.849645
6	3.226269	-2.055309	0.535586
6	2.439603	-2.873018	-0.531557
1	3.081065	-3.084393	-1.393971
1	2.106447	-3.840269	-0.143683

1	4.231321	-1.812754	0.171415
1	3.350512	-2.598877	1.477589
1	2.434763	-0.257971	-1.347800
6	3.257993	0.420848	1.200338
6	3.336221	1.643855	0.660482
1	1.652729	-0.936146	1.514943
1	2.681506	3.256972	-0.599540
1	4.009254	2.365660	1.118318
1	3.873673	0.226372	2.079094
79	-1.321391	0.002069	-0.035987
17	-3.509717	-0.602291	0.534531
1	0.509704	1.189813	-1.535165

AuCl: 4-Hb-1b

E(Gas Phase) = -1024.487831
G(Solv.=Dichlorometane) = -1024.442487

6	0.002320	1.758157	-0.537920
6	0.681537	0.703402	-1.149257
6	0.460933	2.470461	0.724327
6	2.159530	-0.354749	0.734634
6	2.017364	0.142686	-0.717325
6	2.494450	-1.071568	-1.540813
1	2.818924	-0.788274	-2.548107
1	1.661016	-1.775979	-1.657123
1	0.983933	3.379507	0.373169
6	-0.990190	2.577395	-1.348166
1	-1.323576	2.047118	-2.244090
1	-0.508823	3.514525	-1.663113
1	-1.871927	2.846344	-0.757844
6	3.540907	-1.047817	0.707940
6	3.632466	-1.708663	-0.695187
1	4.613994	-1.532450	-1.146846
1	3.505861	-2.794045	-0.633379
1	4.328427	-0.293153	0.830993
1	3.654957	-1.766790	1.525810
1	2.748734	0.958565	-0.848840
6	2.000583	0.674936	1.816492
6	1.309066	1.819296	1.792422
1	1.400093	-1.138911	0.888732
1	-0.438601	2.861402	1.219581
1	1.335297	2.421769	2.700502
1	2.510358	0.436136	2.750377
79	-1.071765	-0.198943	-0.094271
17	-2.648625	-1.703146	0.713375
1	0.423561	0.512967	-2.192627

Substrate 1c:

AuCl: 1-1c

E(Gas Phase) = -985.103153
G(Solv.=Dichlorometane) = -985.086630

6	-3.010935	1.266480	1.352371
6	-1.758728	1.253657	0.948450
6	2.923291	-1.911687	1.336377

6	2.351239	0.383981	-0.655845
6	-0.489438	1.708746	0.712047
6	-0.149139	2.707375	-0.384933
1	-0.430843	3.693344	0.017525
1	-0.797362	2.535138	-1.251073
1	3.355037	-2.678863	1.973070
6	1.880298	1.527365	-1.529482
6	1.324631	2.779328	-0.823551
1	1.950325	3.044277	0.037839
1	1.401696	3.627792	-1.514649
1	2.723131	1.836231	-2.167605
1	1.123767	1.146972	-2.229832
1	0.248638	1.581773	1.505191
6	2.877938	0.479382	0.578367
6	3.355748	-0.643718	1.397265
1	2.307071	-0.600237	-1.120048
1	2.125391	-2.224151	0.667027
1	4.123319	-0.390150	2.129581
1	2.996499	1.464717	1.031806
79	-0.781792	-0.388178	-0.034037
17	-0.476911	-2.485151	-1.002725
1	-3.684218	0.429383	1.201685
1	-3.402825	2.141923	1.868371

AuCl: ts1'-1c

E(Gas Phase) = -985.073471
G(Solv.=Dichlorometane) = -985.066462
1 Imaginary Frequency = -129.4 cm⁻¹

6	-0.156461	1.306494	2.499736
6	-0.308313	0.334534	1.556428
6	-2.209155	2.786361	-0.802143
6	-2.214139	-0.250647	-1.275736
6	-1.414658	-0.512985	1.484914
6	-1.411701	-1.959630	1.148699
1	-1.678303	-2.471095	2.091978
1	-0.409180	-2.288133	0.859934
1	-2.325582	3.864451	-0.743988
6	-2.207845	-1.760097	-1.289131
6	-2.465168	-2.382903	0.097299
1	-3.462288	-2.095057	0.455021
1	-2.460827	-3.476470	0.021012
1	-2.975030	-2.138132	-1.979670
1	-1.244119	-2.112953	-1.671994
1	-2.392398	-0.098373	1.741594
6	-3.262929	0.514707	-0.899427
6	-3.281786	1.976614	-0.821716
1	-1.302502	0.240191	-1.608016
1	-1.190558	2.410141	-0.847475
1	-4.271214	2.426718	-0.746614
1	-4.195980	0.019953	-0.622883
79	1.176057	0.065421	0.151175
17	2.864885	-0.184123	-1.466829
1	0.625244	2.056196	2.425975
1	-0.735873	1.309672	3.424838

AuCl: 3-1c

E(Gas Phase) = -985.136759
G(Solv.=Dichlorometane) = -985.111247

6	1.028770	-1.913965	1.007312
6	0.623326	-0.502466	0.752207
6	1.689192	-2.517221	-0.297321
6	2.403855	0.455984	-0.597440
6	1.694412	0.498020	0.865394
6	1.332339	1.991720	1.091718
1	1.819857	2.327869	2.013361
1	0.255721	2.129391	1.226248
1	1.748719	-3.597480	-0.136052
6	2.979297	1.879675	-0.699238
6	1.868801	2.770623	-0.131743
1	2.217853	3.774223	0.130758
1	1.074399	2.887232	-0.878510
1	3.890461	1.952972	-0.089766
1	3.248078	2.125075	-1.733055
1	2.465206	0.172158	1.573164
6	3.373380	-0.678119	-0.745290
6	3.058906	-1.974906	-0.616282
1	1.600778	0.365549	-1.339814
1	0.992794	-2.362294	-1.130905
1	3.855240	-2.710012	-0.717128
1	4.410900	-0.408007	-0.938487
79	-1.179190	-0.101888	0.089145
17	-3.332662	0.344537	-0.697825
1	1.760321	-1.991195	1.821309
1	0.157235	-2.529497	1.243515

AuCl: ts3*-1c

E(Gas Phase) = -985.128661
G(Solv.=Dichlorometane) = -985.105890
1 Imaginary Frequency = -28.1 cm⁻¹

6	-0.940297	-1.969605	-0.162426
6	-0.547612	-0.520843	-0.160265
6	-2.239468	-2.438704	0.547424
6	-2.985254	0.432706	0.289393
6	-1.568174	0.538871	-0.390168
6	-1.115731	2.011560	-0.156200
1	-0.669559	2.420254	-1.067741
1	-0.340712	2.053074	0.613878
1	-2.202242	-3.532499	0.570960
6	-3.560151	1.837189	0.045497
6	-2.380853	2.793813	0.285539
1	-2.497869	3.739354	-0.252331
1	-2.313753	3.040618	1.351334
1	-3.903458	1.903743	-0.996572
1	-4.423938	2.047025	0.685970
1	-1.755578	0.400242	-1.474992
6	-3.854642	-0.690868	-0.209038
6	-3.524822	-1.979335	-0.092525
1	-2.815164	0.311024	1.370730
1	-2.196969	-2.113799	1.596680
1	-4.195736	-2.744219	-0.478718
1	-4.792380	-0.415180	-0.689797
79	1.361982	-0.106285	-0.032814

17	3.642836	0.351609	0.141904
1	-1.015419	-2.214634	-1.238513
1	-0.099988	-2.564543	0.205621

AuCl: 3*-1c

E(Gas Phase) = -985.128712
G(Solv.=Dichlorometane) = -985.108021

6	-0.939611	-1.968167	0.010788
6	-0.547971	-0.522635	-0.067116
6	-2.304796	-2.417365	0.587725
6	-3.020980	0.427698	0.227191
6	-1.554998	0.543277	-0.315507
6	-1.115107	2.005828	0.004342
1	-0.566135	2.433343	-0.839459
1	-0.430929	2.015965	0.857250
1	-2.273068	-3.509882	0.653202
6	-3.571744	1.836391	-0.046341
6	-2.418574	2.786343	0.322644
1	-2.476957	3.736842	-0.216076
1	-2.460077	3.023916	1.391719
1	-3.813073	1.922555	-1.115325
1	-4.492689	2.039472	0.511008
1	-1.638128	0.449525	-1.420021
6	-3.830726	-0.693962	-0.368518
6	-3.510160	-1.979905	-0.207079
1	-2.953781	0.289746	1.318081
1	-2.380559	-2.056523	1.623407
1	-4.124220	-2.753636	-0.663600
1	-4.705211	-0.421112	-0.957760
79	1.368514	-0.108775	-0.028574
17	3.652583	0.360447	0.044734
1	-0.868438	-2.292255	-1.045668
1	-0.135285	-2.517389	0.511317

AuCl: ts3-1c

E(Gas Phase) = -985.111001
G(Solv.=Dichlorometane) = -985.099286
1 Imaginary Frequency = -716.3 cm⁻¹

6	-0.966329	-1.996539	0.205738
6	-0.623203	-0.512289	0.039792
6	-2.394856	-2.413407	0.610470
6	-3.108766	0.423363	0.203654
6	-1.581147	0.520306	0.109355
6	-1.192604	1.996180	0.084499
1	-0.761659	2.246808	-0.893659
1	-0.405044	2.190635	0.817208
1	-2.406186	-3.500928	0.738640
6	-3.594139	1.835840	-0.189631
6	-2.501419	2.771175	0.342287
1	-2.504556	3.753187	-0.138339
1	-2.634341	2.933391	1.418791
1	-3.654056	1.904103	-1.284401
1	-4.590424	2.052772	0.207497
1	-0.976414	-0.076930	-1.055677

6	-3.750686	-0.703205	-0.576653
6	-3.439793	-1.987295	-0.387818
1	-3.308590	0.281987	1.282257
1	-2.625473	-1.987189	1.597990
1	-3.934307	-2.752390	-0.983040
1	-4.500734	-0.414201	-1.310429
79	1.386044	-0.091472	-0.034643
17	3.685835	0.345036	-0.033209
1	-0.667009	-2.512240	-0.714900
1	-0.270273	-2.363077	0.969242

AuCl: 4-1c

E(Gas Phase) = -985.176304

G(Solv.=Dichlorometane) = -985.146114

6	1.186167	-2.127170	0.960491
6	0.797646	-0.690627	1.263059
6	1.737291	-2.408396	-0.448945
6	1.990548	0.572794	-0.727439
6	1.176146	0.467086	0.586929
6	1.157365	1.849119	1.236365
1	2.025308	1.906157	1.912368
1	0.263229	2.040346	1.835612
1	1.858322	-3.490677	-0.562914
6	2.386236	2.072429	-0.810298
6	1.360533	2.815010	0.061000
1	1.705688	3.804171	0.376923
1	0.415546	2.946334	-0.480779
1	3.391239	2.208495	-0.388884
1	2.416714	2.429335	-1.844190
1	0.455466	-0.542415	2.289764
6	3.167692	-0.381072	-0.799870
6	3.051451	-1.708206	-0.701832
1	1.317536	0.348536	-1.566143
1	0.987093	-2.100917	-1.192768
1	3.946211	-2.324011	-0.775959
1	4.147423	0.066441	-0.961522
79	-1.010506	-0.068486	0.107386
17	-3.143078	0.031431	-0.806048
1	1.946034	-2.410395	1.705496
1	0.320086	-2.771120	1.155574

[AuPH₃]⁺

Substrate 1a:

[AuPH₃]⁺: 1

E(Gas Phase) = -946.4494081
G(Solv.=Dichlorometane) = -946.371929

6	0.498521	1.799276	1.203877
6	-0.132200	0.613298	1.470981
6	-2.776216	1.769979	-2.502902
6	-2.935296	-0.629267	-0.549943
6	-1.015221	-0.164395	2.069814
6	-1.256153	-1.643852	1.914948
1	-0.971792	-2.109688	2.868872
1	-0.588340	-2.068052	1.153006
1	-2.692731	2.747293	-2.969207
6	-0.080859	2.802012	0.230939
1	0.688690	3.218287	-0.427940
1	-0.473086	3.638943	0.827263
1	-0.899493	2.391764	-0.363629
6	1.694588	2.248934	2.015283
1	2.095594	1.451381	2.643272
1	1.357513	3.067249	2.667694
1	2.488571	2.656658	1.380871
6	-3.145570	-1.955400	0.127802
6	-2.727704	-2.015416	1.615508
1	-3.388419	-1.366940	2.205142
1	-2.899256	-3.037507	1.972285
1	-4.202939	-2.238141	0.063214
1	-2.585879	-2.730830	-0.417073
1	-1.643847	0.336733	2.811007
6	-3.908567	0.233068	-0.883661
6	-3.710685	1.514415	-1.574230
1	-1.904371	-0.355665	-0.779148
1	-2.100177	0.996899	-2.861496
1	-4.418280	2.303667	-1.319074
1	-4.937141	-0.009162	-0.612084
79	1.242690	-0.138270	-0.101111
15	2.493410	-1.356850	-1.691134
1	2.530301	-2.749532	-1.502567
1	2.082647	-1.259192	-3.032114
1	3.860958	-1.043995	-1.783967

[AuPH₃]⁺: ts1

E(Gas Phase) = -946.4443428
G(Solv.=Dichlorometane) = -946.364342
1 Imaginary Frequency = -84.0 cm⁻¹

6	-0.327339	2.430611	-0.006804
6	0.131692	1.301657	-0.673969
6	2.560381	-0.186905	3.117659
6	2.812713	-0.986297	0.148298
6	1.075074	1.062872	-1.603436
6	1.281621	-0.154442	-2.454767
1	1.094114	0.170825	-3.490512
1	0.535670	-0.926595	-2.227696

1	2.455724	0.320797	4.072020
6	-0.286440	2.558750	1.485335
1	-1.275801	2.785859	1.902933
1	0.343839	3.431020	1.715423
1	0.140387	1.681525	1.974629
6	-0.916003	3.574737	-0.775799
1	-0.542733	3.598757	-1.803358
1	-0.724648	4.526621	-0.268566
1	-2.008518	3.463009	-0.826120
6	3.040139	-1.633558	-1.190491
6	2.713276	-0.740979	-2.410652
1	3.434171	0.085753	-2.458011
1	2.864287	-1.335305	-3.319186
1	4.085974	-1.951068	-1.279391
1	2.432683	-2.548046	-1.256938
1	1.833101	1.839622	-1.736494
6	3.768404	-0.476513	0.942715
6	3.536821	0.138375	2.255925
1	1.779127	-0.920245	0.485914
1	1.870511	-1.004277	2.919954
1	4.252372	0.906410	2.550291
1	4.802479	-0.489593	0.595152
79	-1.204399	-0.221663	-0.018564
15	-2.634609	-2.000799	0.579623
1	-3.749309	-2.225464	-0.248436
1	-2.058150	-3.283064	0.619248
1	-3.240668	-1.933045	1.847256

[AuPH₃]⁺: 2

E(Gas Phase) = -946.4551805
G(Solv.=Dichlorometane) = -946.369234

6	0.902862	1.945749	-0.790531
6	0.538580	0.586515	-0.745600
6	2.154093	1.607701	2.017133
6	2.428925	-1.281781	1.057611
6	1.450170	-0.365046	-1.210245
6	1.205512	-1.812832	-1.469155
1	1.089692	-1.912089	-2.562567
1	0.263699	-2.144591	-1.018324
1	2.160352	2.644942	2.338173
6	-0.052802	3.009069	-0.331202
1	-0.649933	3.335084	-1.197681
1	0.469992	3.896101	0.039165
1	-0.750980	2.647097	0.427027
6	2.125535	2.506336	-1.466768
1	2.905733	1.783096	-1.700590
1	2.561191	3.307402	-0.862825
1	1.809357	2.971014	-2.413077
6	2.581775	-2.672734	0.505651
6	2.388663	-2.698230	-1.033117
1	3.302788	-2.333005	-1.518332
1	2.235892	-3.725718	-1.379080
1	3.572941	-3.077006	0.742627
1	1.843926	-3.332427	0.975394
1	2.422679	-0.030051	-1.566299
6	3.422376	-0.354553	1.116812
6	3.287593	1.014166	1.581083

1	1.455839	-1.030925	1.473635
1	1.219263	1.070505	2.140849
1	4.194660	1.614353	1.537574
1	4.412310	-0.641203	0.761432
79	-1.324747	-0.010125	-0.059171
15	-3.482337	-0.699333	0.692206
1	-4.355183	-1.253375	-0.264295
1	-3.552682	-1.687429	1.693500
1	-4.321152	0.281939	1.255115

[AuPH₃]⁺: ts2

E(Gas Phase) = -946.451821
G(Solv.=Dichlorometane) = -946.360439
1 Imaginary Frequency = -239.1 cm⁻¹

6	-1.089202	1.849044	0.576915
6	-0.621842	0.490765	0.657126
6	-1.904080	1.733458	-1.509037
6	-2.342459	-1.195180	-1.089398
6	-1.475317	-0.493914	1.133196
6	-1.178442	-1.943703	1.372306
1	-1.086420	-2.103815	2.457591
1	-0.220914	-2.229486	0.921472
1	-1.874499	2.801469	-1.700431
6	-0.081131	2.946369	0.298932
1	0.488140	3.126512	1.222313
1	-0.563952	3.889513	0.027761
1	0.636145	2.672285	-0.479112
6	-2.280574	2.349474	1.376363
1	-3.115327	1.649936	1.428478
1	-2.652709	3.294891	0.972399
1	-1.946435	2.546952	2.404583
6	-2.512889	-2.632222	-0.689245
6	-2.329846	-2.819487	0.843977
1	-3.259071	-2.529940	1.350281
1	-2.156713	-3.875124	1.076281
1	-3.506844	-2.994893	-0.976401
1	-1.772693	-3.241345	-1.219150
1	-2.447608	-0.195874	1.523686
6	-3.355595	-0.261543	-1.156149
6	-3.141177	1.120319	-1.375242
1	-1.365370	-0.918457	-1.472228
1	-1.037761	1.180611	-1.852477
1	-4.014900	1.763876	-1.292396
1	-4.371067	-0.579598	-0.924471
79	1.299083	-0.004294	0.057611
15	3.537209	-0.573077	-0.564481
1	4.387024	-1.056462	0.449523
1	3.723610	-1.572710	-1.539336
1	4.347036	0.446765	-1.100905

[AuPH₃]⁺: 3

E(Gas Phase) = -946.473026
G(Solv.=Dichlorometane) = -946.300035

6	-1.166964	1.831956	0.437392
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6	-0.690447	0.428487	0.487594
6	-1.708575	1.946220	-1.096805
6	-2.178277	-1.051360	-0.791504
6	-1.624242	-0.659529	0.717455
6	-1.125184	-2.020596	1.231422
1	-0.947681	-2.003669	2.311719
1	-0.178886	-2.283553	0.740903
1	-1.821263	3.025161	-1.241894
6	-0.025761	2.861474	0.583777
1	0.457895	2.769085	1.562102
1	-0.427134	3.876976	0.503957
1	0.738247	2.740560	-0.192000
6	-2.306924	2.192477	1.417236
1	-3.208514	1.598686	1.258605
1	-2.576332	3.245272	1.286815
1	-1.978415	2.061785	2.454098
6	-2.655840	-2.525148	-0.603954
6	-2.240575	-2.988867	0.809410
1	-3.086023	-2.902561	1.501371
1	-1.913323	-4.032089	0.832905
1	-3.739085	-2.591481	-0.744702
1	-2.192526	-3.145961	-1.376985
1	-2.510325	-0.354635	1.280246
6	-3.207048	-0.075197	-1.261850
6	-2.999821	1.245891	-1.387163
1	-1.303978	-1.036197	-1.451045
1	-0.903034	1.619620	-1.764037
1	-3.840727	1.874792	-1.669654
1	-4.205427	-0.468042	-1.444530
79	1.258565	-0.014521	0.022164
15	3.552777	-0.530015	-0.469846
1	4.164580	-1.533370	0.304475
1	3.840139	-0.988772	-1.769003
1	4.491514	0.510900	-0.344638

[AuPH₃]⁺: ts3*

E(Gas Phase) = -946.463187
G(Solv.=Dichlorometane) = -946.372147
1 Imaginary Frequency = --39.5 cm⁻¹

6	1.102917	-1.764935	-0.015894
6	0.635511	-0.346584	0.083390
6	2.468419	-2.008408	-0.757923
6	2.931933	0.889909	-0.384054
6	1.537592	0.781484	0.388357
6	0.943637	2.224862	0.375275
1	0.666663	2.520037	1.392593
1	0.032029	2.275164	-0.228891
1	2.561426	-3.094462	-0.850565
6	0.048356	-2.674620	-0.692460
1	-0.900794	-2.671677	-0.146169
1	0.410138	-3.707411	-0.716166
1	-0.144046	-2.362691	-1.724657
6	1.231652	-2.206905	1.490867
1	2.076820	-1.715065	1.976604
1	1.399067	-3.289522	1.490381
1	0.318885	-2.009492	2.062481
6	3.342041	2.341767	-0.094817

6	2.041902	3.147040	-0.208967
1	2.094809	4.109231	0.307274
1	1.829386	3.358334	-1.263321
1	3.749377	2.405830	0.923324
1	4.121874	2.684816	-0.782336
1	1.833756	0.537843	1.428048
6	3.938077	-0.146844	0.019276
6	3.721588	-1.455481	-0.134212
1	2.706130	0.794946	-1.456244
1	2.358150	-1.629609	-1.783569
1	4.475037	-2.168242	0.192263
1	4.861990	0.204768	0.474857
79	-1.378086	0.028221	-0.000822
15	-3.741900	0.472456	-0.086884
1	-4.389937	0.201086	-1.306229
1	-4.558107	-0.239761	0.811373
1	-4.167063	1.791853	0.154119

[AuPH₃]⁺: 3*

E(Gas Phase) = -946.463773
G(Solv.=Dichlorometane) = -946.373974

6	1.099314	-1.764395	-0.184608
6	0.638573	-0.348995	-0.053206
6	2.575750	-2.002815	-0.637214
6	3.029444	0.854067	-0.198418
6	1.514770	0.807358	0.192529
6	0.946467	2.220689	-0.174248
1	0.287728	2.587350	0.619250
1	0.349166	2.163582	-1.089595
1	2.684924	-3.083866	-0.768250
6	0.172015	-2.547912	-1.153715
1	-0.872156	-2.531875	-0.825540
1	0.495458	-3.592990	-1.191456
1	0.222405	-2.141629	-2.169240
6	0.894146	-2.350262	1.262705
1	1.562860	-1.878039	1.985838
1	1.137317	-3.417191	1.204783
1	-0.139688	-2.253165	1.606520
6	3.391342	2.311375	0.127253
6	2.189063	3.130309	-0.375026
1	2.088090	4.084392	0.149062
1	2.311799	3.359381	-1.438794
1	3.507861	2.421647	1.214161
1	4.336192	2.614996	-0.333427
1	1.495739	0.735948	1.309322
6	3.875762	-0.192609	0.472469
6	3.658849	-1.495846	0.282297
1	3.082308	0.723639	-1.290890
1	2.698566	-1.567967	-1.639164
1	4.282112	-2.231111	0.785546
1	4.675134	0.144618	1.129506
79	-1.380778	0.031620	0.015176
15	-3.731213	0.513846	0.115613
1	-4.598981	-0.344900	-0.583830
1	-4.320860	0.507276	1.393302
1	-4.149274	1.768469	-0.365100

[AuPH₃]⁺: ts3

E(Gas Phase) = -946.460595
G(Solv.=Dichlorometane) = -946.372225
1 Imaginary Frequency = -309.3 cm⁻¹

6	-1.078021	-1.793071	0.228729
6	-0.662065	-0.321458	0.118853
6	-2.590786	-2.055994	0.490394
6	-3.095506	0.794973	0.156399
6	-1.549440	0.782488	0.069782
6	-1.057084	2.242205	0.152112
1	-0.621513	2.544786	-0.807623
1	-0.273825	2.343065	0.908742
1	-2.710178	-3.138132	0.603643
6	-0.301817	-2.342293	1.458534
1	0.781471	-2.327135	1.299871
1	-0.600858	-3.382273	1.627144
1	-0.525068	-1.775924	2.369522
6	-0.623285	-2.552335	-1.039462
1	-1.163145	-2.207366	-1.927891
1	-0.824244	-3.621926	-0.915307
1	0.450128	-2.431179	-1.221756
6	-3.460423	2.259871	-0.157882
6	-2.319569	3.073010	0.464834
1	-2.250851	4.090192	0.071095
1	-2.458234	3.149038	1.549666
1	-3.485917	2.407201	-1.245970
1	-4.446912	2.525728	0.232085
1	-1.217752	0.291296	-1.024027
6	-3.778061	-0.238000	-0.708460
6	-3.534908	-1.542688	-0.567010
1	-3.330574	0.603886	1.217137
1	-2.855522	-1.619504	1.463877
1	-4.036350	-2.261829	-1.210130
1	-4.480712	0.126112	-1.454840
79	1.385612	0.070030	-0.028199
15	3.722309	0.498503	-0.176728
1	4.565302	-0.241962	0.672693
1	4.333209	0.267147	-1.423219
1	4.159331	1.808616	0.092967

[AuPH₃]⁺: 4

E(Gas Phase) = -946.512289
G(Solv.=Dichlorometane) = -946.421629

6	1.606163	-1.758367	0.296847
6	0.975548	-0.512604	0.925251
6	2.013686	-1.548966	-1.186780
6	1.663734	1.411411	-0.751225
6	1.085500	0.822229	0.550336
6	0.823750	1.973173	1.513841
1	1.727950	2.062901	2.136690
1	-0.014490	1.803919	2.196236
1	2.322102	-2.520336	-1.587281
6	0.620611	-2.943345	0.388452

1	0.238053	-3.068565	1.408355
1	1.120124	-3.875433	0.103816
1	-0.236427	-2.810454	-0.284870
6	2.849180	-2.092348	1.161965
1	3.575327	-1.274772	1.160790
1	3.341696	-2.987949	0.766864
1	2.564456	-2.300718	2.199314
6	1.758857	2.935141	-0.469736
6	0.703602	3.210469	0.612094
1	0.875871	4.145164	1.151865
1	-0.301120	3.262645	0.170847
1	2.756495	3.170498	-0.078231
1	1.618438	3.526611	-1.378471
1	0.687545	-0.666436	1.970500
6	2.963826	0.773902	-1.201536
6	3.111978	-0.536800	-1.407698
1	0.916928	1.259913	-1.547632
1	1.114951	-1.257666	-1.755929
1	4.077064	-0.908282	-1.744689
1	3.795257	1.452865	-1.379220
79	-1.124670	-0.084921	0.072831
15	-3.366641	-0.146902	-0.628136
1	-3.600257	-0.055691	-2.011599
1	-4.081196	-1.310443	-0.292979
1	-4.208815	0.861179	-0.126877

[AuPH₃]⁺: ts3[”]

E(Gas Phase) = -946.459459
G(Solv.=Dichlorometane) = -946.367904
1 Imaginary Frequency = -166.4cm⁻¹

6	0.977011	1.983458	-0.695245
6	0.740619	0.657662	-0.264172
6	1.266834	1.595699	1.306370
6	2.192024	-1.191808	0.758013
6	1.770337	-0.427706	-0.524312
6	1.342774	-1.568790	-1.470399
1	1.304332	-1.259319	-2.519928
1	0.338470	-1.920860	-1.200033
1	1.327096	2.687269	1.276166
6	-0.133901	2.995674	-0.774127
1	-0.470899	3.022868	-1.820467
1	0.208636	4.004142	-0.520903
1	-0.995991	2.726687	-0.158683
6	2.289111	2.438131	-1.290287
1	3.154937	2.021599	-0.770361
1	2.367646	3.527869	-1.300249
1	2.335061	2.090212	-2.331122
6	2.987740	-2.397013	0.208288
6	2.392931	-2.681749	-1.203772
1	3.180755	-2.654740	-1.962623
1	1.933978	-3.672587	-1.264242
1	4.049930	-2.137859	0.130784
1	2.919626	-3.261493	0.874968
1	2.690134	0.003071	-0.936398
6	2.915894	-0.259346	1.681593
6	2.526739	1.014194	1.844594
1	1.275966	-1.559716	1.247161

1	0.361542	1.348036	1.857310
1	3.131682	1.697058	2.437714
1	3.826363	-0.601955	2.169135
79	-1.226042	-0.035503	0.020841
15	-3.437829	-0.862660	0.303342
1	-3.856845	-1.169809	1.611933
1	-4.497496	-0.036371	-0.116728
1	-3.768810	-2.059927	-0.359273

Substrate 1b:

[AuPH₃]⁺: 1-1b

E(Gas Phase) = -907.128505
G(Solv.=Dichlorometane) = -907.072878

6	0.457082	-0.789905	1.999908
6	-0.335637	-1.403652	1.086682
6	-2.012112	2.848560	1.459956
6	-2.720183	0.613331	-0.550243
6	-1.250462	-2.075402	0.434054
6	-1.495772	-2.201560	-1.050422
1	-1.354240	-3.260253	-1.305295
1	-0.740869	-1.638930	-1.614681
1	-1.753767	3.440318	2.333078
6	1.623679	-1.451519	2.708734
1	1.273727	-1.784797	3.694590
1	2.445205	-0.749278	2.877994
1	1.993839	-2.321605	2.162084
6	-3.140215	-0.264489	-1.696462
6	-2.924841	-1.780907	-1.471192
1	-3.637836	-2.140851	-0.718789
1	-3.169790	-2.302134	-2.403763
1	-4.200985	-0.103931	-1.921811
1	-2.584671	0.031267	-2.599020
1	-1.938044	-2.632870	1.076822
6	-3.538979	1.218274	0.324377
6	-3.101641	2.065633	1.442461
1	-1.645710	0.747429	-0.413784
1	-1.374414	2.963045	0.585723
1	-3.750624	2.061784	2.318289
1	-4.614239	1.057804	0.235112
79	1.174767	0.041387	-0.031777
1	0.075278	0.138081	2.436925
15	2.327657	1.201195	-1.724173
1	3.464169	0.568567	-2.256672
1	1.591119	1.508331	-2.881495
1	2.834927	2.460336	-1.359447

[AuPH₃]⁺: ts1-1b

E(Gas Phase) = -907.120680
G(Solv.=Dichlorometane) = -907.061974
1 Imaginary Frequency = -183.1cm⁻¹

6	-0.400125	1.822185	0.946901
6	-0.393123	0.461792	1.106094
6	-3.585748	2.275974	-1.659028

6	-3.172046	-0.659523	-0.774224
6	-1.214300	-0.543341	1.462002
6	-1.145775	-1.993991	1.092068
1	-0.720555	-2.538847	1.948285
1	-0.456482	-2.149570	0.250142
1	-3.665727	3.354989	-1.752953
6	0.604840	2.804979	1.451263
1	0.068379	3.501650	2.113724
1	1.016373	3.421901	0.643081
1	1.416415	2.336385	2.012831
6	-3.156405	-2.150771	-0.558714
6	-2.537487	-2.590728	0.790057
1	-3.220646	-2.317264	1.604794
1	-2.457012	-3.683500	0.805542
1	-4.176552	-2.549545	-0.605053
1	-2.597677	-2.626733	-1.375635
1	-1.973316	-0.295017	2.207409
6	-4.194849	0.158422	-0.465461
6	-4.224420	1.611455	-0.682816
1	-2.273855	-0.221170	-1.209747
1	-3.008517	1.760814	-2.423123
1	-4.858748	2.176514	0.000373
1	-5.085087	-0.270444	-0.002798
79	1.416476	0.030903	0.011992
1	-1.234988	2.246820	0.379258
15	3.349561	-0.624200	-1.158969
1	4.386283	0.322093	-1.244283
1	4.032400	-1.745166	-0.654845
1	3.180888	-0.981001	-2.508706

[AuPH₃]⁺: 2-1b

E(Gas Phase) = -907.140347
G(Solv.=Dichlorometane) = -907.075165

6	-0.863259	1.888499	1.094493
6	-0.546476	0.553227	0.853277
6	-2.188419	2.258175	-1.347152
6	-2.683783	-0.729090	-1.030826
6	-1.544863	-0.363818	1.219924
6	-1.446654	-1.851009	1.263595
1	-1.321675	-2.131341	2.322901
1	-0.554218	-2.199496	0.731533
1	-2.105202	3.338269	-1.417467
6	0.060257	3.051391	0.974708
1	0.496463	3.244648	1.968259
1	-0.468533	3.965826	0.688861
1	0.884510	2.864530	0.281238
6	-2.939231	-2.188330	-0.767103
6	-2.722957	-2.529148	0.729792
1	-3.584662	-2.175731	1.309741
1	-2.665980	-3.613120	0.871709
1	-3.964003	-2.457963	-1.049036
1	-2.264196	-2.793340	-1.381626
1	-2.438076	0.037849	1.703781
6	-3.597505	0.265060	-0.823276
6	-3.360201	1.679386	-0.979433
1	-1.729579	-0.475093	-1.485476
1	-1.335893	1.686423	-1.697458

1	-4.192536	2.330924	-0.720353
1	-4.584209	-0.017240	-0.456104
79	1.265545	-0.034338	0.062604
15	3.384709	-0.703459	-0.811414
1	4.257157	-1.382029	0.061194
1	3.401962	-1.580518	-1.913184
1	4.241958	0.307909	-1.285878
1	-1.823447	2.108047	1.564884

[AuPH₃]⁺: ts2-1b

E(Gas Phase) = -907.139773
G(Solv.=Dichlorometane) = -907.070648
1 Imaginary Frequency = -154.6cm⁻¹

6	-0.940697	1.897569	0.964640
6	-0.594522	0.537775	0.810751
6	-1.956868	2.239609	-1.150790
6	-2.637440	-0.687694	-1.036163
6	-1.571349	-0.381403	1.194791
6	-1.470117	-1.872566	1.250158
1	-1.367419	-2.166886	2.306433
1	-0.571691	-2.222295	0.728457
1	-1.821079	3.315845	-1.177357
6	0.034779	3.034907	0.905595
1	0.559992	3.078635	1.871924
1	-0.460492	3.999719	0.767688
1	0.792582	2.896638	0.128848
6	-2.939742	-2.142766	-0.810335
6	-2.741346	-2.530375	0.680558
1	-3.609465	-2.189121	1.258113
1	-2.695630	-3.618892	0.786977
1	-3.971350	-2.369919	-1.104315
1	-2.278405	-2.750847	-1.436526
1	-2.470749	0.015965	1.671276
6	-3.540880	0.336440	-0.874393
6	-3.214038	1.720509	-0.938847
1	-1.665314	-0.456937	-1.461434
1	-1.158897	1.653545	-1.591556
1	-4.010986	2.416519	-0.683600
1	-4.559124	0.084667	-0.580599
79	1.238697	-0.043244	0.064999
15	3.386859	-0.708791	-0.746438
1	4.258977	-1.329538	0.168694
1	3.438037	-1.635105	-1.806106
1	4.232441	0.295884	-1.255063
1	-1.868035	2.118219	1.494003

[AuPH₃]⁺: 3-1b

E(Gas Phase) = -907.163451
G(Solv.=Dichlorometane) = -907.091469

6	-1.038321	1.936130	0.756253
6	-0.697723	0.506705	0.633663
6	-1.614874	2.346752	-0.696912
6	-2.416620	-0.595457	-0.712150
6	-1.751299	-0.471147	0.810983

6	-1.432619	-1.936540	1.140623
1	-1.227113	-2.073022	2.207404
1	-0.544392	-2.262428	0.583670
1	-1.609579	3.440484	-0.691045
6	0.126169	2.867063	1.126589
1	0.586020	2.565788	2.073086
1	-0.242839	3.891191	1.242663
1	0.900427	2.869737	0.351164
6	-3.042822	-2.025557	-0.688153
6	-2.680434	-2.688829	0.657059
1	-3.494773	-2.555522	1.378489
1	-2.507438	-3.764636	0.563885
1	-4.126343	-1.964862	-0.829120
1	-2.639880	-2.598084	-1.529252
1	-2.563199	-0.102338	1.447150
6	-3.349366	0.539061	-0.982024
6	-2.994144	1.834297	-0.976300
1	-1.578059	-0.579784	-1.415720
1	-0.886960	2.028504	-1.452153
1	-3.769992	2.583088	-1.117828
1	-4.398131	0.285315	-1.122957
79	1.171269	-0.056530	0.028797
15	3.389988	-0.707398	-0.628183
1	4.438280	0.174867	-0.307849
1	3.887869	-1.914798	-0.104191
1	3.617856	-0.901403	-2.003302
1	-1.869517	2.079872	1.455918

[AuPH₃]⁺: ts3*-1b

E(Gas Phase) = -907.153956
G(Solv.=Dichlorometane) = -907.083157
1 Imaginary Frequency = -98.0cm⁻¹

6	1.047277	1.941291	-0.842291
6	0.704001	0.521162	-0.593376
6	2.242743	2.465383	0.066064
6	2.219442	-0.778013	0.763174
6	1.780659	-0.445025	-0.730109
6	1.491583	-1.850431	-1.304748
1	1.526180	-1.839963	-2.398150
1	0.482327	-2.167466	-1.016279
1	3.067010	2.773579	-0.589760
6	-0.128936	2.925706	-0.816009
1	-0.924922	2.615689	-1.501402
1	0.205098	3.921574	-1.125305
1	-0.548921	3.009118	0.192996
6	3.174439	-1.977738	0.514088
6	2.565480	-2.775270	-0.662943
1	3.336519	-3.046407	-1.389134
1	2.107241	-3.709106	-0.324913
1	4.167014	-1.592159	0.257647
1	3.279723	-2.570937	1.428320
1	2.661951	-0.006628	-1.217179
6	2.826599	0.364703	1.513965
6	2.826771	1.668940	1.210531
1	1.330607	-1.150886	1.292429
1	1.863877	3.396786	0.501872
1	3.382883	2.314107	1.889863

1	3.357913	0.068822	2.417750
79	-1.168945	-0.045214	-0.036641
15	-3.396035	-0.678727	0.616991
1	-3.587463	-1.016123	1.969578
1	-4.413062	0.275865	0.432917
1	-3.959963	-1.799135	-0.020466
1	1.452855	1.911791	-1.871090

[AuPH₃]⁺: 3*-1b

E(Gas Phase) = -907.160111
G(Solv.=Dichlorometane) = -907.089527

6	1.340601	-1.783178	0.501799
6	0.759244	-0.407057	0.517338
6	2.868401	-1.899708	0.740867
6	2.263529	0.836952	-0.687876
6	1.620995	0.710528	0.817879
6	1.050682	2.103469	1.168810
1	1.617456	2.503889	2.015549
1	0.003251	2.051648	1.484212
1	3.117948	-1.564794	1.757794
6	0.892406	-2.625409	-0.718587
1	-0.194634	-2.615147	-0.844258
1	1.209261	-3.662896	-0.581325
1	1.353403	-2.246890	-1.635656
6	2.483476	2.368713	-0.765276
6	1.255701	2.979563	-0.083985
1	1.387054	4.037549	0.159229
1	0.386736	2.904823	-0.750704
1	3.399129	2.622898	-0.217661
1	2.609800	2.684520	-1.806208
1	2.470499	0.439883	1.450225
6	3.476025	-0.029667	-0.885817
6	3.738408	-1.190742	-0.274855
1	1.502067	0.592486	-1.447280
1	3.115162	-2.966729	0.729505
1	4.672031	-1.690803	-0.522651
1	4.186633	0.349219	-1.619338
79	-1.218816	-0.136303	0.072335
15	-3.555604	0.163823	-0.383129
1	-4.025930	-0.273604	-1.635098
1	-4.451645	-0.489756	0.482684
1	-4.060581	1.476637	-0.350724
1	0.826059	-2.223104	1.382377

[AuPH₃]⁺: ts3-Hb-1b

E(Gas Phase) = -907.148110
G(Solv.=Dichlorometane) = -907.082756
1 Imaginary Frequency = -579.1cm⁻¹

6	1.169017	1.830925	-0.462661
6	0.683094	0.501789	-0.439280
6	2.669890	2.112499	-0.578787
6	2.453596	-0.782111	0.750959
6	1.701570	-0.599296	-0.599700
6	1.210805	-2.018552	-0.926789

1	0.945291	-2.139165	-1.981966
1	0.309817	-2.238585	-0.338673
1	3.069605	1.695053	-1.512006
6	0.309210	3.022915	-0.110973
1	-0.758246	2.789716	-0.115649
1	0.504904	3.865222	-0.781643
1	0.587823	3.337939	0.902517
6	3.234776	-2.105464	0.512734
6	2.376753	-2.939929	-0.481382
1	2.979451	-3.248498	-1.340640
1	1.995354	-3.855944	-0.021774
1	4.211635	-1.871310	0.075942
1	3.420820	-2.627818	1.455620
1	2.454631	-0.312754	-1.345899
6	3.318349	0.369577	1.188027
6	3.429598	1.581632	0.629137
1	1.701343	-0.972991	1.534633
1	2.813573	3.193325	-0.653315
1	4.127090	2.288213	1.072169
1	3.929010	0.168634	2.067732
79	-1.298064	0.038439	-0.037184
15	-3.551939	-0.544063	0.454332
1	-4.167547	0.115603	1.533907
1	-4.498758	-0.330323	-0.564406
1	-3.809819	-1.888249	0.780329
1	0.670200	1.312296	-1.532052

[AuPH₃]⁺: 4-Hb-1b

E(Gas Phase) = -907.198441
G(Solv.=Dichlorometane) = -907.128059

6	0.234575	1.900358	-0.355376
6	0.835768	0.859058	-1.051202
6	0.725151	2.344639	1.010743
6	2.061308	-0.633898	0.700558
6	2.117190	0.194816	-0.597417
6	2.760378	-0.784206	-1.596749
1	3.200454	-0.272812	-2.458449
1	1.993023	-1.467361	-1.984807
1	1.587126	3.008096	0.812156
6	-0.714837	2.855275	-1.043603
1	-1.025759	2.498657	-2.029422
1	-0.196681	3.815359	-1.178431
1	-1.602914	3.061419	-0.437396
6	3.472988	-1.267013	0.738100
6	3.811062	-1.561308	-0.752191
1	4.827707	-1.235965	-0.989623
1	3.765943	-2.632437	-0.968922
1	4.181774	-0.546840	1.163559
1	3.506049	-2.161369	1.367422
1	2.831873	1.014886	-0.414939
6	1.648751	0.100138	1.945285
6	1.106343	1.320947	2.064896
1	1.349458	-1.463012	0.533595
1	-0.033887	3.005303	1.443182
1	0.917972	1.676321	3.076359
1	1.824817	-0.445205	2.872694
79	-1.057750	-0.142782	-0.163242

15	-2.837930	-1.564994	0.409666
1	-4.133806	-1.082337	0.156729
1	-2.865607	-2.810942	-0.241210
1	-2.929862	-1.945256	1.760067
1	0.581428	0.765376	-2.109717

Substrate 1c:

[AuPH₃]⁺: 1-1c

E(Gas Phase) = -867.810058
G(Solv.=Dichlorometane) = -867.777704

6	-0.225340	-0.450434	-2.212199
6	0.713235	-1.178113	-1.563380
6	0.899010	3.205361	-0.411449
6	2.400009	0.781996	0.778559
6	1.695962	-1.849681	-1.039198
6	1.965221	-2.234282	0.399913
1	2.036782	-3.328530	0.422237
1	1.113693	-1.959603	1.033680
1	0.384319	3.917698	-1.049431
6	3.161478	-0.227826	1.590126
6	3.286001	-1.628420	0.939918
1	4.018914	-1.586917	0.124990
1	3.695798	-2.315770	1.688347
1	4.171972	0.140980	1.800218
1	2.665570	-0.345354	2.564825
1	2.441140	-2.180425	-1.769425
6	2.918910	1.807208	0.085436
6	2.136037	2.770437	-0.701130
1	1.316468	0.646497	0.745821
1	0.390863	2.912389	0.505096
1	2.634860	3.177747	-1.580753
1	4.001693	1.936166	0.065659
1	0.003031	0.580395	-2.491351
1	-1.011578	-0.956749	-2.776086
79	-1.197581	-0.162849	-0.219626
15	-2.548418	0.324642	1.634207
1	-3.460950	1.377678	1.450574
1	-3.381745	-0.711102	2.090210
1	-1.888824	0.712876	2.813155

[AuPH₃]⁺: ts1'-1c

E(Gas Phase) = -867.797007
G(Solv.=Dichlorometane) = -867.763043
1 Imaginary Frequency = -203.6cm⁻¹

6	-0.477327	-1.738611	-1.033685
6	-0.439047	-0.386509	-1.077506
6	-4.014215	-2.558313	0.924871
6	-3.299092	0.447428	0.790945
6	-1.188633	0.722826	-1.236846
6	-1.072923	2.044919	-0.542219
1	-0.555707	2.734584	-1.225918
1	-0.443831	1.960486	0.354865
1	-4.158001	-3.622564	0.763447

6	-3.197461	1.943574	0.950213
6	-2.451115	2.652296	-0.204316
1	-3.076186	2.629766	-1.106391
1	-2.310307	3.708464	0.051084
1	-4.198130	2.385577	1.022367
1	-2.687540	2.170961	1.895115
1	-1.887351	0.696435	-2.076480
6	-4.292777	-0.196520	0.148540
6	-4.427748	-1.654141	0.023044
1	-2.506274	-0.148012	1.244404
1	-3.565284	-2.263936	1.870487
1	-4.949704	-2.006231	-0.866702
1	-5.075899	0.395853	-0.327812
1	-1.328682	0.253464	-0.584780
1	0.340152	-2.363730	-1.386874
79	1.507022	-0.189880	-0.110677
15	3.602322	0.167658	0.881444
1	4.170886	-0.921895	1.564569
1	4.645094	0.542333	0.016395
1	3.659187	1.179299	1.855826

[AuPH₃]⁺: 3-1c

E(Gas Phase) = -867.849732
G(Solv.=Dichlorometane) = -867.799199

6	1.168059	-1.905343	0.971743
6	0.748189	-0.501492	0.767566
6	1.839726	-2.461515	-0.371501
6	2.429104	0.483214	-0.627082
6	1.734390	0.535701	0.923886
6	1.325155	2.017573	1.110648
1	1.864420	2.407786	1.979641
1	0.256822	2.116781	1.329468
1	1.894925	-3.545425	-0.246560
6	2.881804	1.946724	-0.755644
6	1.733311	2.772748	-0.173961
1	2.013506	3.810949	0.024672
1	0.897314	2.793287	-0.884493
1	3.803461	2.096724	-0.179710
1	3.097711	2.182621	-1.803797
1	2.552904	0.244570	1.587665
6	3.467694	-0.577591	-0.718508
6	3.203734	-1.891024	-0.618568
1	1.614367	0.306101	-1.336671
1	1.151096	-2.267655	-1.201787
1	4.033499	-2.593567	-0.638582
1	4.500905	-0.245838	-0.803339
79	-1.139949	-0.129711	0.099555
15	-3.400885	0.260355	-0.618713
1	-4.419775	-0.209416	0.230542
1	-3.802747	1.595763	-0.805695
1	-3.791689	-0.309738	-1.844418
1	1.906164	-2.007462	1.774293
1	0.309357	-2.547624	1.183140

[AuPH₃]⁺: ts3*-1c

E(Gas Phase) = -867.838709
G(Solv.=Dichlorometane) = -867.792997
1 Imaginary Frequency = -50.3cm⁻¹

6	-1.031493	-1.961480	-0.121090
6	-0.648358	-0.524669	-0.165139
6	-2.368850	-2.432814	0.524686
6	-3.044078	0.455144	0.304029
6	-1.625785	0.537964	-0.426761
6	-1.167568	2.022759	-0.308114
1	-0.939694	2.420283	-1.302284
1	-0.253690	2.113001	0.288255
1	-2.339663	-3.525962	0.501791
6	-3.570544	1.886765	0.124100
6	-2.345406	2.782972	0.348968
1	-2.474324	3.786716	-0.064356
1	-2.163554	2.896942	1.424012
1	-3.954742	2.006058	-0.898027
1	-4.393506	2.103530	0.812602
1	-1.863879	0.322208	-1.489627
6	-3.939329	-0.634758	-0.211915
6	-3.634433	-1.932384	-0.121000
1	-2.836605	0.291836	1.371426
1	-2.344594	-2.152468	1.586562
1	-4.317812	-2.676059	-0.523691
1	-4.865118	-0.328161	-0.695374
79	1.337842	-0.119694	-0.028228
15	3.704865	0.303680	0.127685
1	4.533943	-0.407027	-0.759353
1	4.143493	1.622993	-0.086869
1	4.314755	0.011434	1.361387
1	-1.045099	-2.234565	-1.196365
1	-0.207385	-2.547149	0.298033

[AuPH₃]⁺: 3*-1c

E(Gas Phase) = -867.839191
G(Solv.=Dichlorometane) = -867.795683

6	-1.026114	-1.955768	0.180203
6	-0.646146	-0.528959	0.023728
6	-2.445365	-2.399367	0.601674
6	-3.114756	0.437750	0.170352
6	-1.604940	0.546190	-0.229323
6	-1.168414	2.011954	0.101396
1	-0.608008	2.442513	-0.734145
1	-0.509657	2.028897	0.975074
1	-2.419114	-3.490687	0.677152
6	-3.617122	1.859810	-0.126417
6	-2.489899	2.778958	0.375886
1	-2.503199	3.758961	-0.108295
1	-2.601634	2.949601	1.452036
1	-3.757668	1.976797	-1.209833
1	-4.579706	2.066308	0.350910
1	-1.582714	0.444152	-1.345379
6	-3.859044	-0.677498	-0.516465
6	-3.553182	-1.963735	-0.327409
1	-3.146873	0.283691	1.260161
1	-2.635235	-2.032120	1.619715

1	-4.115058	-2.738516	-0.843306
1	-4.668792	-0.401249	-1.189235
79	1.349989	-0.120291	-0.019416
15	3.712000	0.333036	-0.048673
1	4.574612	-0.764552	-0.221254
1	4.181715	1.209841	-1.043554
1	4.250035	0.923299	1.109631
1	-0.787515	-2.367184	-0.823734
1	-0.270395	-2.438289	0.816287

[AuPH₃]⁺: ts3-1c

E(Gas Phase) = -867.835302
G(Solv.=Dichlorometane) = -867.791149
1 Imaginary Frequency = -321.5cm⁻¹

6	-1.010629	-1.982673	0.256875
6	-0.667730	-0.511299	0.116701
6	-2.451790	-2.414569	0.591157
6	-3.161340	0.414048	0.168878
6	-1.623642	0.527140	0.054877
6	-1.242959	2.018207	0.081663
1	-0.836667	2.318558	-0.891525
1	-0.464264	2.204269	0.827034
1	-2.448191	-3.503318	0.701576
6	-3.646657	1.832132	-0.195906
6	-2.565804	2.758602	0.375943
1	-2.582639	3.759866	-0.061530
1	-2.698443	2.870607	1.458304
1	-3.698489	1.932325	-1.288391
1	-4.645660	2.034844	0.199838
1	-1.254789	0.022714	-1.030553
6	-3.784244	-0.707107	-0.632454
6	-3.464877	-1.990071	-0.443739
1	-3.356592	0.252226	1.242750
1	-2.726410	-2.009635	1.575286
1	-3.943921	-2.759927	-1.043971
1	-4.527336	-0.423387	-1.374622
79	1.358443	-0.094282	-0.011701
15	3.704876	0.310522	-0.108869
1	4.539819	-0.808365	-0.282613
1	4.166735	1.152944	-1.136834
1	4.294495	0.913946	1.017229
1	-0.652828	-2.493911	-0.647945
1	-0.336915	-2.339779	1.049457

[AuPH₃]⁺: 4-1c

E(Gas Phase) = -867.885777
G(Solv.=Dichlorometane) = -867.837449

6	1.204280	-2.117254	0.948578
6	0.872331	-0.664927	1.253050
6	1.739595	-2.422183	-0.462033
6	2.112597	0.547492	-0.727673
6	1.333534	0.471900	0.598787
6	1.305996	1.861269	1.214852
1	2.172171	1.913578	1.893906

1	0.417769	2.066086	1.819735
1	1.818282	-3.507948	-0.570720
6	2.547099	2.034418	-0.828500
6	1.532224	2.809103	0.026987
1	1.893542	3.793601	0.334725
1	0.592703	2.957324	-0.522469
1	3.551252	2.149961	-0.401859
1	2.593930	2.375992	-1.865945
1	0.513128	-0.498624	2.273076
6	3.250473	-0.453488	-0.818171
6	3.078748	-1.774529	-0.723780
1	1.405087	0.340539	-1.545752
1	1.000398	-2.092242	-1.210533
1	3.944188	-2.427112	-0.815240
1	4.242862	-0.040929	-0.987490
79	-1.025773	-0.070972	0.128173
15	-3.195514	0.103211	-0.754580
1	-4.025178	-1.013981	-0.555479
1	-3.991671	1.148347	-0.254544
1	-3.299550	0.296623	-2.143177
1	1.956425	-2.418913	1.693056
1	0.322194	-2.734520	1.159169

[AuNHC]⁺

Substrate 1a:

[AuNHC]⁺: 1

E(Gas Phase) = -908.169245
G(Solv.=Dichlorometane) = -908.076063

6	0.867666	-2.087992	-1.168485
6	1.237214	-1.707412	0.084769
6	3.318730	2.150591	-2.233238
6	3.108777	1.405730	0.768468
6	1.975553	-1.638962	1.175208
6	1.732606	-0.881928	2.456589
1	1.540898	-1.633290	3.235859
1	0.821853	-0.274627	2.379535
1	3.446843	2.147037	-3.311667
6	1.433921	-1.411345	-2.403141
1	0.653528	-1.208135	-3.144702
1	2.143901	-2.109398	-2.868581
1	1.967941	-0.488194	-2.168141
6	0.091476	-3.371306	-1.403586
1	-0.324496	-3.777572	-0.479442
1	0.785607	-4.111653	-1.824785
1	-0.711901	-3.230597	-2.134538
6	3.027516	1.388515	2.270252
6	2.927932	-0.014359	2.913570
1	3.861017	-0.563399	2.732000
1	2.855269	0.120149	3.999317
1	3.905481	1.892123	2.692354
1	2.151951	1.974341	2.589379
1	2.884823	-2.246447	1.157121
6	4.212806	1.683923	0.057111
6	4.288890	1.727011	-1.409088
1	2.194940	1.157281	0.228540
1	2.385061	2.558036	-1.851195
1	5.237720	1.411793	-1.844271
1	5.145466	1.874360	0.590482
79	-0.665295	-0.543199	-0.185284
6	-2.276034	0.690985	0.048304
7	-3.420765	0.429944	0.729800
6	-3.657778	2.463646	-0.080428
6	-4.281663	1.510142	0.660278
1	-3.977200	3.451850	-0.373918
1	-5.248725	1.507970	1.139383
7	-2.428418	1.946298	-0.446075
6	-3.734638	-0.807029	1.447999
1	-2.887510	-1.487632	1.366194
1	-3.920273	-0.584783	2.501837
1	-4.619904	-1.274724	1.009576
6	-1.461963	2.670826	-1.273907
1	-0.533253	2.102161	-1.314381
1	-1.856794	2.795169	-2.285767
1	-1.265760	3.651042	-0.832889

[AuNHC]⁺: ts1

E(Gas Phase) = -908.169245

G(Solv.=Dichlorometane) = -908,067807
1 Imaginary Frequency = -72.5cm⁻¹

6	-1.163080	2.372404	-1.084988
6	-1.156210	1.516973	0.005128
6	-3.720196	-2.100852	-2.338233
6	-3.157187	-1.575585	0.659025
6	-2.006698	1.385098	1.049088
6	-1.767006	0.726001	2.372892
1	-1.731001	1.548157	3.107703
1	-0.784480	0.240488	2.396266
1	-3.994991	-2.044130	-3.387279
6	-0.991042	1.907598	-2.498511
1	-0.129129	2.389799	-2.978477
1	-1.875208	2.233712	-3.065634
1	-0.894064	0.823833	-2.578458
6	-1.298852	3.851572	-0.872390
1	-1.954911	4.057730	-0.018885
1	-1.660819	4.360334	-1.771010
1	-0.319403	4.284707	-0.627145
6	-2.900601	-1.624689	2.141428
6	-2.872360	-0.246934	2.841542
1	-3.849814	0.238702	2.720959
1	-2.737720	-0.411187	3.917340
1	-3.674983	-2.229711	2.628586
1	-1.943760	-2.132928	2.332715
1	-3.023737	1.764541	0.911352
6	-4.335057	-1.855349	0.076200
6	-4.602596	-1.824112	-1.367305
1	-2.324566	-1.271044	0.026844
1	-2.707184	-2.428004	-2.114664
1	-5.625846	-1.577849	-1.651759
1	-5.184335	-2.109853	0.712586
79	0.693817	0.449922	-0.080149
6	2.441646	-0.619984	-0.031745
7	3.617988	-0.253060	0.539394
6	3.971801	-2.252881	-0.310893
6	4.569608	-1.245439	0.375776
1	4.354108	-3.205223	-0.644794
1	5.574206	-1.149152	0.758036
7	2.667623	-1.854516	-0.550896
6	3.877453	1.005335	1.239122
1	2.967873	1.605619	1.231476
1	4.168182	0.801588	2.273029
1	4.678133	1.552378	0.734415
6	1.695699	-2.671586	-1.277794
1	0.732570	-2.161827	-1.270153
1	2.024858	-2.812615	-2.310844
1	1.593296	-3.644293	-0.789991

[AuNHC]⁺: 2

E(Gas Phase) = -908.169245
G(Solv.=Dichlorometane) = -908,068223

6	-1.908228	-1.822422	-0.922550
6	-1.336332	-0.536476	-0.830379
6	-2.970756	-1.436839	2.112531
6	-2.898167	1.488476	1.215810

6	-2.155817	0.537364	-1.194143
6	-1.749040	1.957621	-1.387337
1	-1.675058	2.106544	-2.479208
1	-0.751927	2.143158	-0.973424
1	-3.103615	-2.464512	2.437081
6	-1.094930	-3.051569	-0.651623
1	-1.029306	-3.652123	-1.571879
1	-1.600155	-3.691018	0.083464
1	-0.085009	-2.825849	-0.306311
6	-3.292909	-2.138411	-1.433852
1	-4.039082	-1.370739	-1.228077
1	-3.650431	-3.083224	-1.015372
1	-3.244244	-2.275988	-2.524394
6	-2.891488	2.902259	0.701479
6	-2.791115	2.955089	-0.844618
1	-3.771086	2.715731	-1.277017
1	-2.540749	3.970265	-1.170607
1	-3.801215	3.430424	1.011048
1	-2.042346	3.441434	1.136695
1	-3.181970	0.346527	-1.507350
6	-4.005157	0.715387	1.351309
6	-4.035622	-0.669401	1.801231
1	-1.937712	1.084090	1.527870
1	-1.953518	-1.057912	2.107908
1	-5.025610	-1.118125	1.863348
1	-4.970639	1.152289	1.094740
79	0.642569	-0.219713	-0.270345
6	2.621409	0.104088	0.243361
7	3.646192	0.420325	-0.593100
6	4.546441	0.316581	1.412204
6	4.833779	0.554804	0.107247
1	5.178376	0.316140	2.286972
1	5.765109	0.803750	-0.377763
7	3.189872	0.042891	1.477177
6	3.537644	0.605938	-2.039131
1	2.514622	0.385901	-2.343912
1	3.782080	1.638452	-2.304166
1	4.222348	-0.074140	-2.552886
6	2.489491	-0.273652	2.719887
1	1.435886	-0.435713	2.493248
1	2.908586	-1.180231	3.165248
1	2.586012	0.556648	3.424871

[AuNHC]⁺: ts2

E(Gas Phase) = -908.158423
G(Solv.=Dichlorometane) = -908,056840
1 Imaginary Frequency = -224.9cm⁻¹

6	-2.105228	-1.801661	-0.050706
6	-1.455297	-0.613431	-0.533645
6	-2.857650	-0.927903	1.929925
6	-2.878354	1.709762	0.578704
6	-2.202788	0.285386	-1.293690
6	-1.671896	1.471941	-2.063525
1	-2.340659	1.656567	-2.911839
1	-0.680777	1.236089	-2.469468
1	-2.959298	-1.878799	2.442843
6	-1.255511	-2.887364	0.577886

1	-0.758416	-3.442633	-0.230930
1	-1.857121	-3.608792	1.138838
1	-0.469882	-2.485642	1.222759
6	-3.382777	-2.352942	-0.659674
1	-4.115042	-1.594168	-0.937630
1	-3.865623	-3.061412	0.019063
1	-3.120124	-2.908517	-1.571064
6	-2.782364	2.922153	-0.290028
6	-1.562943	2.767337	-1.216337
1	-1.452259	3.638784	-1.870096
1	-0.657462	2.710288	-0.599077
1	-3.706581	3.074306	-0.860037
1	-2.638854	3.812358	0.340769
1	-3.234296	0.038406	-1.533348
6	-4.021051	1.012440	0.904657
6	-4.001418	-0.231745	1.580605
1	-1.958662	1.454972	1.098484
1	-1.906220	-0.428012	2.065616
1	-4.956680	-0.740911	1.692197
1	-4.975942	1.360809	0.514167
79	0.552642	-0.241828	-0.141079
6	4.549494	0.751504	1.069538
6	4.824005	0.073239	-0.073492
1	5.203483	1.224693	1.785775
1	5.764212	-0.158582	-0.549821
6	2.476310	1.378414	2.332136
1	2.739588	2.438104	2.390524
1	1.402460	1.280161	2.174413
1	2.752319	0.882927	3.267277
6	3.478461	-1.081967	-1.846627
1	4.031913	-2.021555	-1.767028
1	2.423781	-1.297590	-2.017168
1	3.869922	-0.498038	-2.684293
6	2.576125	0.092200	0.180396
7	3.606969	-0.323018	-0.603555
7	3.170864	0.753939	1.208919

[AuNHC]⁺: 3

E(Gas Phase) = -908.186708
G(Solv.=Dichlorometane) = -908,081001

6	-2.066733	-1.634195	-0.739900
6	-1.439596	-0.296598	-0.539445
6	-2.485505	-2.041397	0.768055
6	-2.729727	1.018211	1.100744
6	-2.299459	0.883503	-0.467271
6	-1.707883	2.276594	-0.744291
1	-1.571807	2.457796	-1.815818
1	-0.727180	2.364131	-0.259990
1	-2.710167	-3.110750	0.695501
6	-1.056193	-2.695997	-1.225262
1	-0.651049	-2.429049	-2.207062
1	-1.551880	-3.668094	-1.319148
1	-0.217749	-2.809110	-0.530438
6	-3.312338	-1.674835	-1.654546
1	-4.140224	-1.073422	-1.275639
1	-3.666484	-2.707363	-1.737714
1	-3.062489	-1.330728	-2.664435

6	-3.164063	2.513161	1.208601
6	-2.719026	3.230415	-0.087564
1	-3.576963	3.376167	-0.753373
1	-2.290769	4.219095	0.101195
1	-4.247697	2.582357	1.346102
1	-2.699864	2.956714	2.094981
1	-3.235384	0.768331	-1.021624
6	-3.765709	0.014661	1.507419
6	-3.660795	-1.313939	1.354206
1	-1.810228	0.871305	1.679580
1	-1.596268	-1.950957	1.403281
1	-4.510036	-1.929227	1.642861
1	-4.692253	0.415741	1.914103
79	0.563970	-0.117146	-0.181982
6	4.740161	-0.335258	0.744457
6	4.712713	0.887596	0.153321
1	5.557073	-0.894726	1.173791
1	5.502187	1.598140	-0.037843
6	3.057098	-2.111562	1.283488
1	3.198424	-2.106832	2.367767
1	2.006933	-2.292774	1.056744
1	3.664978	-2.903435	0.838513
6	2.962426	2.336702	-0.903188
1	3.429180	2.393937	-1.890303
1	1.879437	2.304523	-1.018348
1	3.239388	3.216049	-0.315934
6	2.605209	0.075788	0.132851
7	3.399560	1.123638	-0.212704
7	3.443843	-0.817973	0.721247

[AuNHC]⁺: ts3*

E(Gas Phase) = -908.178477
G(Solv.=Dichlorometane) = -908,075904
1 Imaginary Frequency = -36.2 cm⁻¹

6	1.948173	-1.716005	0.264805
6	1.360679	-0.335394	0.141255
6	3.288389	-1.981304	-0.513145
6	3.564999	0.962256	-0.588833
6	2.208374	0.880292	0.240533
6	1.515476	2.262480	0.020368
1	1.216598	2.684823	0.985935
1	0.605399	2.154420	-0.577241
1	3.454555	-3.061358	-0.457688
6	0.945475	-2.805956	-0.185030
1	0.022428	-2.768568	0.402264
1	1.386234	-3.798576	-0.045735
1	0.690116	-2.697848	-1.245088
6	2.184077	-1.890673	1.807496
1	2.998627	-1.255762	2.162071
1	2.453349	-2.938725	1.979589
1	1.280342	-1.677148	2.387798
6	3.893000	2.461305	-0.521367
6	2.543682	3.166234	-0.704828
1	2.547150	4.189333	-0.318672
1	2.299976	3.226521	-1.771899
1	4.318309	2.692435	0.464821
1	4.634957	2.748686	-1.273540

1	2.543585	0.827072	1.294304
6	4.656738	0.060869	-0.090031
6	4.527219	-1.266621	-0.043746
1	3.317760	0.704760	-1.629649
1	3.106436	-1.762471	-1.575015
1	5.342103	-1.875174	0.341346
1	5.573312	0.533106	0.259202
79	-0.662935	-0.112643	0.046034
6	-4.918750	-0.250285	-0.394019
6	-4.797251	0.991587	0.144788
1	-5.791389	-0.801062	-0.710069
1	-5.544084	1.729424	0.394871
6	-3.348294	-2.087747	-1.053192
1	-3.605729	-2.111155	-2.115625
1	-2.284909	-2.291832	-0.934494
1	-3.924997	-2.847728	-0.519960
6	-2.908199	2.430339	0.943395
1	-3.253413	2.532434	1.975819
1	-1.820060	2.378414	0.929614
1	-3.237327	3.294307	0.360381
6	-2.720919	0.123565	-0.036966
7	-3.447383	1.204267	0.354705
7	-3.640431	-0.767010	-0.495979

[AuNHC]⁺: 3*

E(Gas Phase) = -908.178685
G(Solv.=Dichlorometane) = -908,077254

6	1.965040	-1.721545	-0.113601
6	1.374284	-0.342903	-0.053108
6	3.466508	-1.860216	-0.518276
6	3.680989	1.032330	-0.217155
6	2.166626	0.888846	0.143043
6	1.504657	2.229957	-0.325840
1	0.787631	2.587449	0.419325
1	0.946471	2.072326	-1.253544
1	3.666685	-2.933293	-0.600838
6	1.135127	-2.614175	-1.076355
1	0.081931	-2.659884	-0.784393
1	1.537342	-3.632452	-1.057695
1	1.193318	-2.247915	-2.107030
6	1.766028	-2.272123	1.344535
1	2.352673	-1.707288	2.073180
1	2.118902	-3.309736	1.344657
1	0.714122	-2.267107	1.643681
6	3.925131	2.528496	0.031752
6	2.677703	3.224167	-0.541284
1	2.488324	4.192307	-0.069409
1	2.814056	3.411341	-1.611851
1	4.004032	2.706454	1.113267
1	4.856748	2.878656	-0.423329
1	2.124249	0.887683	1.259685
6	4.587120	0.094755	0.533187
6	4.479353	-1.229329	0.405214
1	3.776456	0.845716	-1.298797
1	3.584893	-1.457414	-1.534334
1	5.140943	-1.888258	0.962671
1	5.335448	0.528913	1.193722

79	-0.665527	-0.124349	-0.009960
6	-4.835554	0.441120	0.780714
6	-4.888041	0.305673	-0.569138
1	-5.617139	0.608523	1.505780
1	-5.724327	0.331725	-1.250730
6	-3.031515	0.418354	2.523015
1	-3.498480	-0.362408	3.129184
1	-1.949816	0.284967	2.535094
1	-3.279908	1.399790	2.935648
6	-3.224680	-0.088411	-2.404599
1	-3.557553	0.767531	-2.997417
1	-2.141038	-0.178319	-2.479818
1	-3.691001	-1.000997	-2.785537
6	-2.724693	0.119500	0.048170
7	-3.586928	0.109141	-1.001072
7	-3.503473	0.324903	1.141641

[AuNHC]⁺: ts3

E(Gas Phase) = -908.173682
G(Solv.=Dichlorometane) = -908,072981
1 Imaginary Frequency = -349.5cm⁻¹

6	-1.948400	-1.705039	0.463344
6	-1.414622	-0.289115	0.136095
6	-3.479898	-1.821685	0.717269
6	-3.759020	0.990413	-0.002892
6	-2.224998	0.860511	-0.009681
6	-1.632728	2.266581	-0.173224
1	-1.196604	2.366443	-1.175412
1	-0.821507	2.430074	0.540712
1	-3.686816	-2.866052	0.972712
6	-1.243950	-2.127880	1.778226
1	-0.158248	-2.193549	1.655380
1	-1.609118	-3.115067	2.082531
1	-1.454033	-1.425793	2.593413
6	-1.535799	-2.674471	-0.666040
1	-2.039280	-2.429895	-1.608358
1	-1.808675	-3.700469	-0.395353
1	-0.454580	-2.648065	-0.838996
6	-4.018376	2.421220	-0.520422
6	-2.824490	3.229687	-0.001331
1	-2.674828	4.171196	-0.535881
1	-2.961703	3.471882	1.059304
1	-4.027103	2.416902	-1.618556
1	-4.985856	2.806367	-0.186554
1	-1.800029	0.088856	-1.028172
6	-4.491843	-0.100395	-0.750007
6	-4.357733	-1.388004	-0.427474
1	-4.039788	0.956815	1.065009
1	-3.731152	-1.237415	1.614416
1	-4.896613	-2.146468	-0.990420
1	-5.141558	0.214097	-1.563837
79	0.676642	-0.070033	0.015274
6	4.863238	0.079164	-0.808767
6	4.878897	0.527751	0.472342
1	5.666357	-0.084387	-1.510790
1	5.698341	0.831333	1.105525
6	3.104145	-0.669275	-2.431904

1	3.541317	-1.654398	-2.615980
1	2.017404	-0.750483	-2.431171
1	3.415536	0.021570	-3.219956
6	3.161447	0.968667	2.245579
1	3.491635	1.995111	2.426275
1	2.075023	0.920022	2.317702
1	3.603852	0.305872	2.994231
6	2.726380	0.119007	-0.077553
7	3.563104	0.546663	0.904284
7	3.538299	-0.165913	-1.129391

[AuNHC]⁺: 4

E(Gas Phase) = -908.230504
G(Solv.=Dichlorometane) = -908,125008

6	-2.247374	-1.753447	-0.492636
6	-1.704105	-0.413706	-0.994323
6	-2.509755	-1.766685	1.037379
6	-2.292367	1.249974	0.970858
6	-1.797394	0.849195	-0.436746
6	-1.656741	2.126167	-1.265543
1	-2.598225	2.246915	-1.823225
1	-0.851529	2.089572	-2.005493
1	-2.756588	-2.794610	1.324241
6	-1.257073	-2.884802	-0.842069
1	-0.983885	-2.862401	-1.903719
1	-1.710016	-3.860671	-0.635807
1	-0.334231	-2.813115	-0.253815
6	-3.564585	-2.004151	-1.270874
1	-4.301653	-1.218809	-1.081672
1	-3.998940	-2.962662	-0.964379
1	-3.381284	-2.053038	-2.350122
6	-2.494417	2.785718	0.877265
6	-1.533854	3.250133	-0.226538
1	-1.790885	4.232122	-0.632819
1	-0.504986	3.305501	0.153294
1	-3.528654	2.997000	0.576833
1	-2.328121	3.278822	1.839305
1	-1.493441	-0.423608	-2.068258
6	-3.510908	0.496718	1.464239
6	-3.601110	-0.834562	1.506432
1	-1.467148	1.064671	1.677620
1	-1.563938	-1.526234	1.550095
1	-4.514390	-1.284930	1.889146
1	-4.338012	1.107066	1.822210
79	0.452773	0.019985	-0.242074
6	4.684686	-0.043574	-0.014499
6	4.393688	-0.341395	1.278659
1	5.632665	0.067357	-0.518218
1	5.038842	-0.539915	2.120723
6	3.370252	0.443961	-2.093448
1	3.833959	-0.345074	-2.691004
1	2.316373	0.525497	-2.358114
1	3.868822	1.396257	-2.291363
6	2.306546	-0.644151	2.634337
1	2.594705	0.083721	3.397066
1	1.233909	-0.574516	2.455632
1	2.552462	-1.652445	2.977294

6	2.442093	-0.076599	0.186687
7	3.014312	-0.358015	1.385419
7	3.477057	0.116009	-0.670654

[AuNHC]⁺: ts3''

E(Gas Phase) = -908.169931

G(Solv.=Dichlorometane) = -908.065417

1 Imaginary Frequency = -202.7cm⁻¹

6	2.072548	1.971888	-0.047922
6	1.558711	0.655887	-0.081250
6	2.152162	1.006838	1.689947
6	2.447813	-1.705541	0.262907
6	2.412789	-0.461046	-0.646809
6	1.963065	-1.043911	-2.005453
1	2.236257	-0.399527	-2.847466
1	0.871872	-1.153134	-2.022740
1	2.678428	1.933649	1.947014
6	1.175649	3.153250	0.223377
1	0.952448	3.619518	-0.746239
1	1.672191	3.912616	0.837055
1	0.225249	2.864099	0.677805
6	3.462456	2.349516	-0.518016
1	4.226775	1.628997	-0.221371
1	3.749491	3.339579	-0.154235
1	3.456236	2.387293	-1.615158
6	3.154947	-2.749190	-0.624901
6	2.653285	-2.441212	-2.065424
1	3.485707	-2.440741	-2.775117
1	1.946357	-3.200766	-2.412515
1	4.241304	-2.613601	-0.558753
1	2.939522	-3.775280	-0.311598
1	3.457423	-0.146798	-0.759861
6	3.084770	-1.367017	1.575348
6	2.992880	-0.153917	2.135253
1	1.410889	-2.037506	0.432316
1	1.171628	1.062293	2.160032
1	3.543402	0.052217	3.052498
1	3.693894	-2.121259	2.070292
79	-0.509680	0.259670	0.009528
6	-4.556804	-0.945712	0.659039
6	-4.717517	-0.264774	-0.504169
1	-5.270587	-1.468539	1.276906
1	-5.598611	-0.078639	-1.098830
6	-2.634675	-1.486633	2.175950
1	-2.815314	-2.564871	2.164706
1	-1.560848	-1.300589	2.180839
1	-3.082876	-1.050860	3.073119
6	-3.220123	0.995587	-2.072386
1	-3.795358	1.924772	-2.035679
1	-2.156984	1.229414	-2.125708
1	-3.509562	0.421813	-2.956925
6	-2.528018	-0.161728	0.045561
7	-3.466752	0.208307	-0.865250
7	-3.211512	-0.872850	0.981048

[AuP(OMe)₃]⁺

Substrate 1a:

[AuP(OMe)₃]⁺: 1-PO

E(Gas Phase) = -1290.106440
G(Solv.=Dichlorometane) = -1290.011274

6	-1.126635	2.432287	-0.637096
6	-1.516385	1.705144	0.447560
6	-3.020632	-1.549442	-2.926147
6	-3.139058	-1.601143	0.169288
6	-2.300313	1.327021	1.438622
6	-2.080784	0.267795	2.488772
1	-1.991314	0.792785	3.450226
1	-1.123937	-0.245733	2.326674
1	-3.080864	-1.292975	-3.979668
6	-1.584219	2.079013	-2.037129
1	-0.755527	2.113347	-2.752784
1	-2.307332	2.845818	-2.349694
1	-2.073929	1.104348	-2.086489
6	-0.383457	3.742841	-0.475554
1	-0.034864	3.897934	0.547204
1	-1.080123	4.553341	-0.731798
1	0.462047	3.817865	-1.167711
6	-3.161006	-1.956396	1.630456
6	-3.232608	-0.757993	2.604855
1	-4.191792	-0.240402	2.475743
1	-3.231602	-1.156566	3.626079
1	-4.013790	-2.614377	1.835702
1	-2.258534	-2.538826	1.875113
1	-3.235917	1.885867	1.528517
6	-4.132260	-1.842029	-0.701449
6	-4.103789	-1.522219	-2.134939
1	-2.245190	-1.095793	-0.197950
1	-2.048765	-1.868710	-2.555855
1	-5.066157	-1.273006	-2.582358
1	-5.054644	-2.291479	-0.330620
79	0.450294	0.675983	0.016796
15	2.389965	-0.649429	-0.047744
8	2.175911	-2.206321	0.306905
8	3.050889	-0.509252	-1.488195
8	3.575984	-0.254559	0.948422
6	4.366779	-1.053892	-1.816330
1	5.135488	-0.468331	-1.310556
1	4.426095	-2.103895	-1.521907
1	4.457180	-0.956203	-2.897063
6	3.434641	-0.324150	2.388757
1	2.586354	0.285358	2.718147
1	3.306927	-1.362394	2.702071
1	4.359108	0.083356	2.796012
6	1.097047	-2.982340	-0.268407
1	0.136640	-2.478260	-0.117837
1	1.275278	-3.144982	-1.334364
1	1.100236	-3.935235	0.259852

[AuP(OMe)₃]⁺: ts1-PO

E(Gas Phase) = -1290.099698
G(Solv.=Dichlorometane) = -1290.005076
1 Imaginary Frequency = -69.0cm⁻¹

6	6	1.431234	2.572526	0.655609
6	1.456001	1.544712	-0.273219	
6	3.316026	-1.698467	2.920320	
6	3.115616	-1.747540	-0.163449	
6	2.326555	1.174920	-1.235430	
6	2.104230	0.268607	-2.408271	
1	2.176859	0.914451	-3.298780	
1	1.087119	-0.142402	-2.400882	
1	3.489346	-1.458437	3.965093	
6	1.239459	2.341374	2.123547	
1	0.370219	2.890415	2.508935	
1	2.115292	2.760584	2.640273	
1	1.150809	1.284046	2.378610	
6	1.548207	3.996807	0.201149	
1	2.128495	4.068597	-0.724081	
1	1.981622	4.629543	0.982547	
1	0.547929	4.399236	-0.013502	
6	2.999050	-2.068580	-1.629500	
6	3.149685	-0.857565	-2.578556	
1	4.154587	-0.431086	-2.462018	
1	3.084574	-1.220986	-3.610972	
1	3.761398	-2.806499	-1.907162	
1	2.025437	-2.543590	-1.826089	
1	3.352847	1.539868	-1.135673	
6	4.196421	-1.995888	0.594962	
6	4.317668	-1.700281	2.028368	
1	2.259648	-1.262311	0.302915	
1	2.300507	-1.973961	2.644432	
1	5.327516	-1.492789	2.382543	
1	5.076935	-2.433839	0.122005	
79	-0.438980	0.559484	-0.055375	
15	-2.514164	-0.530305	0.106620	
8	-2.573667	-2.029432	-0.490249	
8	-2.979781	-0.554002	1.631316	
8	-3.757887	0.149321	-0.641785	
6	-4.296141	-1.028546	2.045528	
1	-5.055817	-0.312843	1.728235	
1	-4.495081	-2.014122	1.618762	
1	-4.254075	-1.087441	3.132211	
6	-3.799312	0.284872	-2.081720	
1	-2.909303	0.812169	-2.442531	
1	-3.875270	-0.699538	-2.548621	
1	-4.688456	0.875745	-2.299194	
6	-1.513230	-2.983533	-0.254215	
1	-0.541640	-2.551316	-0.517271	
1	-1.512465	-3.301323	0.791770	
1	-1.725260	-3.834441	-0.901204	

[AuP(OMe)₃]⁺: 2-PO

E(Gas Phase) = -1290.106179
G(Solv.=Dichlorometane) = -1290.011232

6	-2.087943	-1.982920	-0.637145
6	-1.578508	-0.672717	-0.737044

6	-3.001439	-1.295178	2.264152
6	-3.049516	1.528808	1.094515
6	-2.430511	0.335339	-1.190484
6	-2.062389	1.724469	-1.589596
1	-2.064322	1.734713	-2.693613
1	-1.043475	1.971780	-1.272099
1	-3.090003	-2.298122	2.670716
6	-1.207860	-3.104585	-0.165154
1	-0.661959	-3.502727	-1.035248
1	-1.785972	-3.934310	0.252186
1	-0.458060	-2.773641	0.557478
6	-3.418019	-2.456447	-1.156990
1	-4.120442	-1.672049	-1.435380
1	-3.897680	-3.115012	-0.426563
1	-3.235943	-3.071844	-2.051131
6	-3.102309	2.883209	0.442722
6	-3.083409	2.772198	-1.104290
1	-4.081670	2.482337	-1.456264
1	-2.861306	3.746963	-1.551185
1	-4.006479	3.424785	0.745036
1	-2.244783	3.479817	0.774000
1	-3.469439	0.093993	-1.410497
6	-4.129284	0.741667	1.341397
6	-4.100779	-0.598529	1.901603
1	-2.068467	1.183955	1.413052
1	-2.002292	-0.872145	2.238294
1	-5.070407	-1.082023	2.006765
1	-5.114615	1.124637	1.074834
79	0.407818	-0.258710	-0.265669
15	2.705036	0.110208	0.206728
8	3.184005	1.636773	0.485202
8	3.169003	-0.789628	1.446380
8	3.756330	-0.313359	-0.936637
6	4.561643	-0.902124	1.853788
1	5.112451	-1.486311	1.114864
1	5.007764	0.089123	1.963907
1	4.546049	-1.417653	2.813473
6	3.750649	0.323346	-2.232282
1	2.756271	0.261252	-2.688701
1	4.061516	1.366894	-2.140823
1	4.466314	-0.228439	-2.841523
6	2.426001	2.504369	1.351441
1	1.369201	2.517584	1.060870
1	2.520882	2.184477	2.393211
1	2.851024	3.501231	1.231885

[AuP(OMe)₃]⁺: ts2-PO

E(Gas Phase) = -1290.102122
G(Solv.=Dichlorometane) = -1290.001134
1 Imaginary Frequency = -266.6cm⁻¹

6	-2.154377	-1.894220	-0.626088
6	-1.644237	-0.591995	-0.607455
6	-2.664280	-1.437313	2.016774
6	-2.955786	1.342824	0.940577
6	-2.517836	0.509982	-0.886549
6	-2.052514	1.836007	-1.452555
1	-2.022946	1.750081	-2.547890

1	-1.032223	2.057306	-1.117456
1	-2.631164	-2.484894	2.300688
6	-1.250628	-3.092272	-0.473803
1	-1.024515	-3.496710	-1.471861
1	-1.741315	-3.899929	0.080152
1	-0.301158	-2.849266	0.009183
6	-3.550741	-2.260424	-1.082801
1	-4.308301	-1.507657	-0.858027
1	-3.870168	-3.208014	-0.639532
1	-3.545141	-2.406702	-2.172605
6	-3.176218	2.793009	0.527894
6	-3.034401	2.923644	-1.006807
1	-4.007730	2.752734	-1.483166
1	-2.704790	3.923525	-1.304113
1	-4.156887	3.148007	0.862136
1	-2.424739	3.412938	1.029273
1	-3.523859	0.268801	-1.227905
6	-4.005223	0.526849	1.378926
6	-3.864859	-0.796269	1.863938
1	-1.967923	1.120809	1.335679
1	-1.716994	-0.913240	2.024100
1	-4.779506	-1.363635	2.019925
1	-5.021381	0.888793	1.222164
79	0.369538	-0.228874	-0.220377
15	2.694635	0.086475	0.171822
8	3.229532	1.607357	0.372858
8	3.164849	-0.775161	1.436881
8	3.703445	-0.417852	-0.977242
6	4.564181	-0.917935	1.809282
1	5.072093	-1.555791	1.084118
1	5.047547	0.060694	1.858351
1	4.560283	-1.386650	2.792839
6	3.698463	0.173800	-2.294240
1	2.694522	0.135797	-2.731808
1	4.051515	1.206700	-2.244598
1	4.380837	-0.426522	-2.895764
6	2.525175	2.534895	1.221110
1	1.455406	2.546408	0.982300
1	2.667813	2.274888	2.274141
1	2.954739	3.517235	1.022949

[AuP(OMe)₃]⁺: 3-PO

E(Gas Phase) = -1290.125666
G(Solv.=Dichlorometane) = -1290.019243

6	-2.257808	-1.823283	-0.205031
6	-1.682753	-0.472687	-0.421453
6	-2.668186	-1.753552	1.370591
6	-2.947949	1.232264	0.808300
6	-2.556088	0.659900	-0.686257
6	-2.001682	1.920002	-1.372482
1	-1.921596	1.787725	-2.456549
1	-0.997754	2.144727	-0.989993
1	-2.845416	-2.801967	1.630464
6	-1.210966	-2.950100	-0.342861
1	-0.805959	-2.981865	-1.359989
1	-1.677340	-3.919384	-0.137907
1	-0.377099	-2.823192	0.355665

6	-3.502642	-2.176444	-1.050381
1	-4.342942	-1.502852	-0.874425
1	-3.833301	-3.189876	-0.801968
1	-3.258809	-2.161490	-2.118420
6	-3.336806	2.715027	0.514975
6	-2.998907	3.014672	-0.962652
1	-3.901716	2.941793	-1.579564
1	-2.593414	4.020006	-1.108658
1	-4.399407	2.875078	0.722274
1	-2.776499	3.367696	1.191661
1	-3.505851	0.377688	-1.148729
6	-3.997122	0.388677	1.459605
6	-3.874796	-0.927183	1.696677
1	-2.023557	1.211890	1.396137
1	-1.785818	-1.432965	1.936184
1	-4.728202	-1.456814	2.113547
1	-4.942180	0.876424	1.690788
79	0.331270	-0.154271	-0.122354
15	2.691015	0.103911	0.178244
8	3.282559	1.610325	0.218222
8	3.134111	-0.658218	1.509636
8	3.634939	-0.556073	-0.940553
6	4.530003	-0.834116	1.890401
1	4.997128	-1.564885	1.228535
1	5.060466	0.119582	1.841600
1	4.508861	-1.203723	2.914788
6	3.665065	-0.066629	-2.300943
1	2.659798	-0.075929	-2.736488
1	4.081960	0.942591	-2.327532
1	4.307279	-0.754018	-2.850769
6	2.643347	2.651391	0.987493
1	1.564936	2.672054	0.793968
1	2.828499	2.502908	2.054939
1	3.092060	3.589419	0.660681

[AuP(OMe)₃]⁺: ts3*-PO

E(Gas Phase) = -1290.111998
G(Solv.=Dichlorometane) = -1290.007397
1 Imaginary Frequency = -39.0cm⁻¹

6	-2.098215	-1.753727	-0.005858
6	-1.536726	-0.368356	-0.116098
6	-3.450298	-1.908368	0.784258
6	-3.727505	1.015403	0.414213
6	-2.378610	0.807192	-0.421155
6	-1.696872	2.210761	-0.458182
1	-1.472219	2.483578	-1.494836
1	-0.745082	2.206487	0.082437
1	-3.612455	-2.986165	0.879494
6	-1.086555	-2.733064	0.637602
1	-0.154601	-2.788932	0.065592
1	-1.513334	-3.740676	0.671205
1	-0.842933	-2.436983	1.663735
6	-2.306501	-2.182752	-1.505355
1	-3.138037	-1.640686	-1.960378
1	-2.535427	-3.253992	-1.504459
1	-1.405030	-2.033315	-2.108927
6	-4.049817	2.491365	0.138923

6	-2.693287	3.204163	0.186950
1	-2.706130	4.172087	-0.321320
1	-2.411665	3.391524	1.229871
1	-4.499899	2.582849	-0.858960
1	-4.770386	2.887850	0.861677
1	-2.738026	0.567006	-1.439935
6	-4.818370	0.049489	0.058749
6	-4.686416	-1.270651	0.209403
1	-3.462168	0.905865	1.475897
1	-3.277800	-1.541868	1.805975
1	-5.499892	-1.930078	-0.083535
1	-5.733553	0.462579	-0.361678
79	0.511041	-0.120271	-0.040228
15	2.895164	0.173854	0.060802
8	3.533201	1.095553	-1.083788
8	3.764714	-1.168548	-0.038750
8	3.431991	0.848266	1.411450
6	3.125669	0.301709	2.715207
1	3.495438	1.028441	3.437817
1	2.044001	0.176393	2.838352
1	3.638177	-0.653808	2.847973
6	3.656703	-2.065404	-1.167595
1	4.207247	-2.963899	-0.890675
1	2.608677	-2.319982	-1.362958
1	4.106444	-1.605602	-2.050495
6	3.063396	2.438950	-1.339989
1	3.359072	3.098063	-0.520418
1	3.545677	2.753127	-2.265080
1	1.975354	2.451321	-1.468105

[AuP(OMe)₃]⁺: 3*-PO

E(Gas Phase) = -1290.112832
G(Solv.=Dichlorometane) = -1290.009185

6	-2.097341	-1.751097	0.189306
6	-1.538149	-0.369606	0.060307
6	-3.593252	-1.895663	0.614467
6	-3.853659	0.982818	0.173419
6	-2.339477	0.838965	-0.192809
6	-1.688185	2.212601	0.186971
1	-0.998086	2.540014	-0.596878
1	-1.104725	2.115492	1.107787
1	-3.774274	-2.967401	0.743703
6	-1.240916	-2.584108	1.182330
1	-0.189588	-2.628365	0.881353
1	-1.626029	-3.608377	1.215795
1	-1.292054	-2.170875	2.195171
6	-1.901352	-2.358862	-1.248591
1	-2.518317	-1.845625	-1.989825
1	-2.218626	-3.406362	-1.194458
1	-0.855854	-2.332867	-1.569081
6	-4.115858	2.461025	-0.152715
6	-2.872847	3.198349	0.375582
1	-2.702746	4.148540	-0.137897
1	-2.999074	3.426551	1.439290
1	-4.203272	2.581424	-1.241419
1	-5.047914	2.824466	0.290540
1	-2.306397	0.767310	-1.309311

6	-4.754332	-0.005783	-0.515211
6	-4.625627	-1.320488	-0.323703
1	-3.934047	0.853539	1.264502
1	-3.706763	-1.452837	1.614174
1	-5.286733	-2.013712	-0.838295
1	-5.519059	0.383497	-1.184649
79	0.517348	-0.123445	0.007493
15	2.895349	0.186588	-0.041818
8	3.464087	0.998159	-1.300792
8	3.765817	-1.158185	-0.063398
8	3.499083	0.984912	1.208973
6	3.235666	0.585470	2.573906
1	3.623896	1.387982	3.200246
1	2.158800	0.472824	2.743044
1	3.756659	-0.348864	2.795229
6	3.607019	-2.155860	-1.098007
1	4.186327	-3.019355	-0.772693
1	2.553590	-2.437974	-1.207551
1	3.998520	-1.774806	-2.043885
6	2.984926	2.318783	-1.642425
1	3.339023	3.043521	-0.905750
1	3.403866	2.545213	-2.622385
1	1.890533	2.332054	-1.696689

[AuP(OMe)₃]⁺: ts3-PO

E(Gas Phase) = -1290.109381
G(Solv.=Dichlorometane) = -1290.009233
1 Imaginary Frequency = -278.0cm⁻¹

6	2.102169	-1.783417	-0.227579
6	1.567647	-0.347120	-0.125674
6	3.633543	-1.931057	-0.467441
6	3.907728	0.955702	-0.137327
6	2.368575	0.819688	-0.086391
6	1.764104	2.235321	-0.169695
1	1.288712	2.495131	0.783735
1	0.985997	2.277390	-0.936880
1	3.839222	-3.001097	-0.573801
6	1.388694	-2.392069	-1.465901
1	0.303624	-2.443426	-1.328571
1	1.757725	-3.411355	-1.622360
1	1.591141	-1.816983	-2.376466
6	1.690624	-2.573847	1.035681
1	2.199061	-2.193827	1.928580
1	1.963772	-3.627797	0.914625
1	0.610337	-2.523021	1.210382
6	4.150844	2.444288	0.185099
6	2.960444	3.166801	-0.456126
1	2.803167	4.173519	-0.060751
1	3.112677	3.258680	-1.537978
1	4.145088	2.589425	1.273812
1	5.120216	2.788579	-0.186051
1	2.034554	0.284355	1.006062
6	4.654264	-0.020419	0.741175
6	4.518533	-1.340704	0.600526
1	4.179882	0.786148	-1.193275
1	3.879264	-1.479171	-1.439158
1	5.066263	-2.014980	1.254510

1	5.314425	0.400271	1.496583
79	-0.525095	-0.105881	-0.015177
15	-2.879796	0.199394	0.072678
8	-3.499975	0.411771	1.535127
8	-3.769947	-0.993520	-0.520586
8	-3.419733	1.474570	-0.735772
6	-3.170859	1.640303	-2.150156
1	-3.493863	2.651723	-2.394957
1	-2.103506	1.528673	-2.373209
1	-3.754471	0.911845	-2.717594
6	-3.695193	-2.340015	0.001085
1	-4.272363	-2.959233	-0.684900
1	-2.657273	-2.690223	0.029660
1	-4.135339	-2.375000	1.000212
6	-2.996160	1.412021	2.447999
1	-3.283004	2.408200	2.102827
1	-3.461674	1.201608	3.410473
1	-1.906673	1.338813	2.541481

[AuP(OMe)₃]⁺: 4-PO

E(Gas Phase) = -1290.165670
G(Solv.=Dichlorometane) = -1290.058673

6	-2.377771	-1.794633	-0.281579
6	-1.850751	-0.522474	-0.949690
6	-2.671910	-1.609337	1.231726
6	-2.464558	1.360852	0.790687
6	-1.970708	0.798979	-0.556902
6	-1.807890	1.966109	-1.524981
1	-2.747407	2.034412	-2.095128
1	-1.004419	1.829455	-2.255530
1	-2.910376	-2.593916	1.647996
6	-1.357933	-2.940506	-0.459073
1	-1.054436	-3.045473	-1.507702
1	-1.798915	-3.892401	-0.144293
1	-0.455107	-2.778844	0.144130
6	-3.672573	-2.176330	-1.044359
1	-4.427607	-1.388063	-0.977944
1	-4.096360	-3.093541	-0.619558
1	-3.465145	-2.366429	-2.103452
6	-2.639287	2.880133	0.527430
6	-1.671304	3.200536	-0.621200
1	-1.912109	4.133023	-1.138443
1	-0.642515	3.284961	-0.245091
1	-3.669827	3.076984	0.205777
1	-2.461052	3.473793	1.428296
1	-1.628966	-0.664725	-2.012552
6	-3.698964	0.676440	1.343618
6	-3.784857	-0.639752	1.549858
1	-1.647576	1.237403	1.521227
1	-1.741531	-1.286705	1.727870
1	-4.705621	-1.048082	1.960306
1	-4.536576	1.324364	1.594456
79	0.335516	-0.024015	-0.254446
15	2.621732	-0.049178	0.262204
8	3.527774	0.922417	-0.622062
8	3.317384	-1.474219	0.087335
8	2.975714	0.366016	1.761957

6	2.398581	-0.295754	2.914240
1	2.680825	0.308802	3.775290
1	1.306920	-0.334613	2.829367
1	2.812139	-1.302189	3.007030
6	3.297617	-2.200838	-1.167189
1	3.709147	-3.184541	-0.945199
1	2.271455	-2.301554	-1.536520
1	3.921585	-1.686013	-1.900665
6	3.286069	2.347586	-0.713105
1	3.526813	2.823955	0.239667
1	3.950812	2.711313	-1.495558
1	2.244584	2.543696	-0.990311

Ring contraction pathway:

[AuP(OMe)₃]⁺: ts3⁺-PO

E(Gas Phase) = -1290.111916
G(Solv.=Dichlorometane) = -1290.007811
1 Imaginary Frequency = -183.6cm⁻¹

6	-2.189961	-1.927892	-0.665778
6	-1.737838	-0.646581	-0.275383
6	-2.296910	-1.524527	1.323539
6	-2.821628	1.397061	0.816748
6	-2.623550	0.567816	-0.476351
6	-2.114727	1.625077	-1.479028
1	-2.223165	1.306432	-2.520991
1	-1.047222	1.815661	-1.308960
1	-2.572275	-2.583243	1.298841
6	-1.236490	-3.086838	-0.797967
1	-0.969511	-3.164837	-1.861501
1	-1.700084	-4.036411	-0.511513
1	-0.309228	-2.939221	-0.238575
6	-3.583145	-2.196587	-1.189430
1	-4.354459	-1.659155	-0.633385
1	-3.814436	-3.264540	-1.177147
1	-3.633227	-1.856246	-2.232279
6	-3.494696	2.688738	0.304333
6	-2.949954	2.892454	-1.141135
1	-3.776202	3.011277	-1.848451
1	-2.336119	3.794155	-1.222901
1	-4.583074	2.557960	0.287749
1	-3.287013	3.541707	0.957195
1	-3.627913	0.272757	-0.802054
6	-3.577668	0.587838	1.826382
6	-3.379092	-0.730072	1.973279
1	-1.824600	1.646181	1.214190
1	-1.321966	-1.468249	1.804690
1	-4.016226	-1.300909	2.646262
1	-4.363608	1.070008	2.404390
79	0.330761	-0.255638	-0.089813
15	2.660778	0.131685	0.052741
8	3.152459	1.424870	0.896387
8	3.379563	-1.165698	0.650918
8	3.455329	0.363459	-1.325649
6	4.828073	-1.301019	0.715505
1	5.225771	-1.445452	-0.290249
1	5.273020	-0.416796	1.177836

1	5.012741	-2.181589	1.329719
6	3.197283	1.513105	-2.161443
1	2.132544	1.575747	-2.412426
1	3.523052	2.425571	-1.656608
1	3.778073	1.359024	-3.070578
6	2.573411	1.748726	2.178328
1	1.479487	1.766206	2.117959
1	2.894455	1.027254	2.935040
1	2.941924	2.741965	2.434999

[AuP(OMe)₃]⁺: [4+2]-PO

E(Gas Phase) = -1290.166871
G(Solv.=Dichlorometane) = -1290.059721

6	1.547102	2.029947	-0.352721
6	2.046388	0.922259	0.342978
6	2.199922	0.989449	1.871463
6	2.434483	-1.601743	0.449952
6	2.829347	-0.259484	-0.217163
6	2.923922	-0.660849	-1.701258
1	3.502305	0.041259	-2.306826
1	1.919829	-0.731183	-2.139746
1	3.094843	1.602823	2.075141
6	1.153689	3.313993	0.365564
1	0.377733	3.846294	-0.191746
1	2.032795	3.973752	0.400759
1	0.805598	3.179152	1.389777
6	1.697670	2.255044	-1.847897
1	2.600481	2.858754	-2.018061
1	0.853317	2.836090	-2.231282
1	1.784524	1.347181	-2.436796
6	3.416483	-2.593354	-0.203609
6	3.580785	-2.073017	-1.661392
1	4.637908	-2.016881	-1.936542
1	3.104341	-2.739878	-2.385901
1	4.374076	-2.564905	0.329394
1	3.054259	-3.624841	-0.159705
1	3.858881	-0.054607	0.128031
6	2.427059	-1.517579	1.947210
6	2.338320	-0.340965	2.574104
1	1.419617	-1.863291	0.097636
1	1.375193	1.541922	2.331987
1	2.362051	-0.292169	3.660881
1	2.504625	-2.440089	2.519807
79	-0.283085	0.561935	-0.072474
15	-2.421712	-0.390227	-0.080344
8	-2.555213	-1.752312	0.770138
8	-3.468420	0.683477	0.451857
8	-3.029502	-0.834793	-1.492024
6	-4.912355	0.462607	0.439212
1	-5.270046	0.469710	-0.591179
1	-5.152994	-0.485705	0.924670
1	-5.335634	1.294873	0.999362
6	-2.441632	-1.895979	-2.282576
1	-1.384315	-1.685614	-2.476732
1	-2.553541	-2.851859	-1.766607
1	-2.992660	-1.905400	-3.222237
6	-1.968988	-1.896168	2.087639

1 -0.912979 -1.604908 2.076104
1 -2.520955 -1.293073 2.813186
1 -2.057914 -2.952834 2.338399

Diels Alder mechanism:

[AuP(OMe)₃]⁺: DA-1-PO

E(Gas Phase) = -1290.106970
G(Solv.=Dichlorometane) = -1290.012363

6 1.115439 -2.287066 0.784402
6 1.555612 -1.463825 -0.205594
6 1.849406 3.222820 1.771631
6 3.891471 1.439937 0.271870
6 2.358025 -0.906965 -1.093195
6 3.794516 -1.333880 -1.323925
1 3.803749 -1.953912 -2.232210
1 4.132298 -1.976662 -0.502318
1 1.010570 3.826030 2.107902
6 1.326843 -1.956603 2.249311
1 2.087981 -2.643108 2.644996
1 0.415324 -2.119639 2.834432
1 1.675093 -0.932383 2.396917
6 0.567571 -3.666506 0.475827
1 0.387380 -3.809380 -0.591322
1 -0.353947 -3.867956 1.032557
1 1.309407 -4.406864 0.805891
6 5.078998 0.712411 -0.301412
6 4.769206 -0.160392 -1.540745
1 4.382903 0.482300 -2.343057
1 5.713291 -0.580831 -1.908169
1 5.847645 1.438743 -0.591238
1 5.528754 0.076078 0.474265
1 1.991958 -0.100753 -1.726589
6 3.600150 2.731312 0.044273
6 2.451829 3.461910 0.596463
1 3.214630 0.858591 0.896490
1 2.209516 2.460785 2.458806
1 2.094565 4.297366 -0.006318
1 4.250957 3.304004 -0.618214
79 -0.531727 -0.646052 -0.032799
15 -2.525577 0.555861 -0.295092
8 -3.069988 1.295956 1.027561
8 -2.309055 1.619973 -1.456309
8 -3.819028 -0.256949 -0.767189
6 -3.388618 2.450344 -1.984967
1 -4.085177 1.824565 -2.544311
1 -3.900433 2.965801 -1.169461
1 -2.902721 3.168593 -2.643429
6 -4.416145 -1.291955 0.050988
1 -3.674254 -2.061462 0.290741
1 -4.826800 -0.856781 0.964476
1 -5.211760 -1.725046 -0.553906
6 -2.173967 1.951772 1.957915
1 -1.466123 1.227960 2.374285
1 -1.634104 2.764723 1.466093
1 -2.808087 2.347693 2.750613

[AuP(OMe)₃]⁺: DA-ts1-PO

E(Gas Phase) = -1290.101541
G(Solv.=Dichlorometane) = -1290.007582
1 Imaginary Frequency = -46.6cm⁻¹

6 1.380250 -2.223756 1.015068
6 1.342025 -1.307568 -0.006514
6 3.103335 3.225595 1.942714
6 4.371290 1.161944 0.012283
6 2.163330 -0.741483 -0.916946
6 3.364461 -1.427253 -1.514693
1 3.022130 -1.982746 -2.401172
1 3.741004 -2.185393 -0.813881
1 2.477106 3.942657 2.465009
6 2.378904 -2.088511 2.131639
1 2.834984 -3.064403 2.341944
1 1.871935 -1.782529 3.056821
1 3.155923 -1.355862 1.907473
6 0.406785 -3.364016 1.134424
1 -0.285907 -3.415146 0.291915
1 -0.165057 -3.310072 2.069396
1 0.980615 -4.299919 1.180122
6 5.237293 0.261790 -0.830313
6 4.483541 -0.468553 -1.965285
1 4.059870 0.277108 -2.650835
1 5.206160 -1.052108 -2.548283
1 6.040670 0.850329 -1.289038
1 5.727295 -0.486253 -0.190713
1 1.897849 0.218283 -1.356817
6 4.264151 2.491793 -0.151611
6 3.432924 3.395584 0.654042
1 3.781088 0.689972 0.798538
1 3.476886 2.387794 2.526658
1 3.089962 4.296294 0.144777
1 4.828192 2.960655 -0.959798
79 -0.647270 -0.466986 -0.035806
15 -2.724520 0.589750 -0.225917
8 -3.774321 0.317575 0.970187
8 -2.505726 2.159366 -0.384754
8 -3.609400 0.211521 -1.506233
6 -3.596427 3.080053 -0.687927
1 -3.926249 2.925109 -1.716125
1 -4.424434 2.928435 0.008141
1 -3.175738 4.077081 -0.565750
6 -4.071744 -1.139376 -1.738940
1 -3.224366 -1.833618 -1.756720
1 -4.788512 -1.429329 -0.967436
1 -4.553951 -1.124611 -2.715746
6 -3.371209 0.351779 2.357779
1 -2.500310 -0.292539 2.521359
1 -3.142252 1.376163 2.663040
1 -4.220656 -0.025576 2.926674

[AuP(OMe)₃]⁺: DA-2-PO

E(Gas Phase) = -1290.101820
G(Solv.=Dichlorometane) = -1290.009251

6	1.542195	-2.182957	1.017131
6	1.329397	-1.193273	0.090723
6	3.496171	3.030685	2.147544
6	4.469489	1.067418	-0.039119
6	2.113544	-0.580050	-0.851755
6	3.166295	-1.266846	-1.669491
1	2.661502	-1.691479	-2.552299
1	3.563367	-2.128743	-1.116394
1	2.956770	3.703739	2.806992
6	2.824417	-2.255160	1.799887
1	3.172194	-3.293780	1.862457
1	2.649386	-1.928154	2.834401
1	3.610063	-1.627116	1.377149
6	0.488047	-3.177618	1.411454
1	-0.383152	-3.149782	0.752369
1	0.151708	-3.003217	2.442592
1	0.919282	-4.186765	1.396724
6	5.200048	0.243475	-1.071329
6	4.285627	-0.336272	-2.174163
1	3.832709	0.491646	-2.734946
1	4.897376	-0.899241	-2.888881
1	5.963721	0.857329	-1.563673
1	5.735160	-0.579017	-0.578413
1	1.870858	0.436065	-1.158703
6	4.210824	2.383235	-0.162368
6	3.520497	3.226116	0.820694
1	4.135510	0.559033	0.865454
1	4.040626	2.217385	2.621126
1	3.017848	4.104119	0.415412
1	4.530323	2.888598	-1.075766
79	-0.652313	-0.398462	-0.034000
15	-2.794541	0.545033	-0.205510
8	-3.829794	0.167934	0.977564
8	-2.679362	2.132162	-0.306818
8	-3.660383	0.162148	-1.500193
6	-3.829997	2.989714	-0.565305
1	-4.163070	2.850654	-1.594835
1	-4.637956	2.760810	0.133310
1	-3.473746	4.007447	-0.411854
6	-4.036568	-1.206073	-1.777615
1	-3.148875	-1.848039	-1.804445
1	-4.742437	-1.562174	-1.023804
1	-4.508617	-1.192755	-2.759515
6	-3.420093	0.155426	2.362730
1	-2.517073	-0.451517	2.491255
1	-3.240157	1.173909	2.717287
1	-4.245525	-0.290845	2.917108

[AuP(OMe)₃]⁺: DA-ts2-PO

E(Gas Phase) = -1290.089089
G(Solv.=Dichlorometane) = -1289.989563
1 Imaginary Frequency = -219.5cm⁻¹

6	-2.061078	-1.909742	-0.591167
6	-1.583986	-0.784635	0.037322
6	-1.820105	1.549096	-2.675545
6	-3.684180	1.090739	-0.306607

6	-2.429679	0.151562	0.799413
6	-3.418471	-0.289744	1.885162
1	-2.843886	-0.479600	2.800536
1	-3.919921	-1.222808	1.617742
1	-1.079102	1.736091	-3.446448
6	-3.512335	-2.280339	-0.797487
1	-3.734865	-3.209710	-0.254508
1	-3.697570	-2.505007	-1.856694
1	-4.234170	-1.531310	-0.477509
6	-1.134865	-2.946397	-1.176081
1	-0.087139	-2.757947	-0.932705
1	-1.236455	-2.980249	-2.270440
1	-1.404827	-3.946916	-0.812923
6	-4.893100	1.191311	0.638269
6	-4.427508	0.845675	2.063259
1	-3.934890	1.712899	2.521829
1	-5.262021	0.569468	2.714664
1	-5.356667	2.181847	0.584816
1	-5.648806	0.471120	0.306035
1	-1.841631	0.978550	1.195462
6	-2.924145	2.239174	-0.580049
6	-2.005085	2.429796	-1.661374
1	-3.796182	0.400994	-1.136725
1	-2.399064	0.636596	-2.772032
1	-1.413510	3.341436	-1.642831
1	-2.977795	3.049512	0.148218
79	0.435286	-0.302953	0.063906
15	2.724963	0.299009	0.207015
8	3.781985	-0.633622	-0.601604
8	2.967365	1.818736	-0.246508
8	3.395033	0.277836	1.672299
6	4.258471	2.472179	-0.102761
1	4.445056	2.686618	0.950908
1	5.053861	1.841362	-0.506911
1	4.186494	3.398214	-0.672790
6	3.450125	-0.941680	2.442870
1	2.455657	-1.396014	2.518253
1	4.152925	-1.643555	1.987134
1	3.797736	-0.655734	3.435584
6	3.514849	-1.053975	-1.954151
1	2.498403	-1.452992	-2.046685
1	3.649977	-0.217840	-2.646705
1	4.237808	-1.838548	-2.179046

[AuP(OMe)₃]⁺: DA-3-PO

E(Gas Phase) = -1290.163438
G(Solv.=Dichlorometane) = -1290.056807

6	1.472043	-1.438365	-0.971804
6	1.902414	-0.674148	0.119397
6	2.102815	-1.284221	1.513511
6	4.103839	0.516553	0.245242
6	2.563816	0.697296	0.102730
6	2.475412	1.781829	-0.983402
1	1.475240	2.220381	-1.081738
1	2.770877	1.392917	-1.961076
1	1.465686	-0.758393	2.241686
6	1.569665	-0.979358	-2.419745

1	0.834630	-1.506168	-3.035130
1	2.562376	-1.239619	-2.812899
1	1.423474	0.089569	-2.558742
6	1.201900	-2.933251	-0.870362
1	0.898778	-3.275812	0.119154
1	2.117041	-3.475700	-1.147061
1	0.428142	-3.231413	-1.584066
6	4.600469	1.983505	0.292220
6	3.540152	2.805762	-0.506912
1	3.080041	3.560746	0.138713
1	3.980336	3.339476	-1.353644
1	4.652349	2.325789	1.331442
1	5.605824	2.077561	-0.128327
1	2.243016	1.179102	1.038979
6	4.454064	-0.372119	1.402991
6	3.549888	-1.173777	1.971618
1	4.477930	0.059296	-0.685516
1	1.796311	-2.331079	1.552688
1	3.819013	-1.800997	2.818619
1	5.478241	-0.358974	1.771061
79	-0.445102	-0.348592	-0.113467
15	-2.618777	0.446419	0.234405
8	-3.805593	-0.528696	-0.251987
8	-2.799930	0.784822	1.778538
8	-3.010661	1.813724	-0.496937
6	-3.981325	1.460388	2.310022
1	-3.964668	2.507646	2.005638
1	-4.889908	0.969979	1.953972
1	-3.900940	1.372663	3.392394
6	-3.109558	1.919210	-1.938257
1	-2.175876	1.594926	-2.410184
1	-3.948388	1.320684	-2.299277
1	-3.279319	2.974937	-2.146307
6	-3.801344	-1.947992	0.030588
1	-2.838440	-2.392237	-0.243767
1	-4.009753	-2.121866	1.089312
1	-4.593336	-2.377638	-0.582021

Stepwise mechanism

[AuP(OMe)₃]⁺: 5-PO

E(Gas Phase) = -1290.107751
G(Solv.=Dichlorometane) = -1290.013166

6	-1.179990	-2.189807	-0.904823
6	-1.599462	-1.372760	0.098988
6	-1.447043	2.685842	-1.527623
6	-4.023714	1.441779	-0.372229
6	-2.381592	-0.817294	1.005583
6	-3.812104	-1.239395	1.280901
1	-3.787783	-1.890589	2.166862
1	-4.193237	-1.851157	0.454643
1	-0.688256	3.243706	-2.068317
6	-1.397649	-1.841616	-2.364092
1	-2.162408	-2.521775	-2.763679
1	-0.488934	-2.000482	-2.954457
1	-1.742930	-0.815132	-2.500959
6	-0.641150	-3.577706	-0.617898

1	-0.469064	-3.741274	0.447628
1	0.282983	-3.773478	-1.172114
1	-1.385162	-4.307176	-0.966609
6	-5.170067	0.809921	0.372965
6	-4.758575	-0.061732	1.582907
1	-4.295387	0.579039	2.345211
1	-5.670473	-0.470522	2.034576
1	-5.841949	1.593073	0.744684
1	-5.759775	0.194571	-0.319882
1	-1.993236	-0.020732	1.637859
6	-3.550996	2.680454	-0.149822
6	-2.426811	3.310400	-0.853187
1	-3.562663	0.840871	-1.155107
1	-1.391715	1.600978	-1.592275
1	-2.408151	4.399472	-0.816886
1	-4.055412	3.303384	0.589645
79	0.513430	-0.603110	-0.066739
15	2.557549	0.519715	0.162613
8	3.105481	0.641832	1.672057
8	2.633142	2.037310	-0.325225
8	3.636452	-0.219842	-0.744023
6	3.078765	-0.469726	2.598535
1	3.361869	-0.057633	3.566643
1	2.072153	-0.897079	2.658771
1	3.796860	-1.234994	2.292916
6	1.891709	3.106620	0.319795
1	2.195034	4.019410	-0.191890
1	0.816377	2.949499	0.190054
1	2.158159	3.162444	1.377319
6	4.982435	0.306095	-0.959429
1	5.522782	-0.487723	-1.472823
1	4.926136	1.199623	-1.582357
1	5.456840	0.532798	-0.002149

[AuP(OMe)₃]⁺: ts5-PO

E(Gas Phase) = -1290.089785
G(Solv.=Dichlorometane) = -1289.988020
1 Imaginary Frequency = -323.8cm⁻¹

6	1.935258	2.146580	-0.340860
6	1.756177	0.843814	0.062441
6	0.267463	-1.757725	-1.558116
6	3.128835	-1.499386	-0.624984
6	2.678569	-0.025797	0.727060
6	4.141117	0.289169	1.017096
1	4.200448	0.787269	1.994657
1	4.543035	0.975843	0.265734
1	-0.770567	-1.917544	-1.830031
6	1.113475	2.797063	-1.428147
1	1.788509	3.284942	-2.145196
1	0.472456	3.592680	-1.025601
1	0.490363	2.083456	-1.973569
6	2.921335	3.105564	0.287946
1	3.354782	2.743385	1.219024
1	2.424656	4.062150	0.492346
1	3.736275	3.329929	-0.415502
6	4.618378	-1.673566	-0.339601
6	4.940874	-1.012731	1.009729

1	4.612595	-1.657242	1.835884
1	6.013968	-0.841542	1.140312
1	4.894549	-2.733568	-0.344470
1	5.193468	-1.188880	-1.135840
1	2.238855	-0.645714	1.508619
6	2.229329	-2.521608	-0.266712
6	0.884846	-2.615494	-0.662726
1	2.886476	-0.929553	-1.516235
1	0.847626	-1.132690	-2.228958
1	0.271966	-3.372328	-0.178048
1	2.575747	-3.250585	0.466110
79	-0.238475	0.229647	-0.047290
15	-2.592482	-0.196620	0.220117
8	-3.623137	1.033183	-0.019626
8	-3.079019	-0.705681	1.668667
8	-3.052051	-1.411106	-0.725810
6	-3.441353	1.957866	-1.112318
1	-4.137138	2.778045	-0.934744
1	-2.415742	2.342437	-1.128961
1	-3.675224	1.474651	-2.065405
6	-2.939430	0.130312	2.838435
1	-3.216161	-0.493471	3.688190
1	-1.902251	0.466313	2.950893
1	-3.610024	0.990045	2.768854
6	-4.391295	-1.980283	-0.668644
1	-4.471800	-2.634641	-1.536200
1	-4.505775	-2.551366	0.254076
1	-5.142147	-1.188678	-0.721250

[AuP(OMe)₃]⁺: 7-PO

E(Gas Phase) = -1290.096915
G(Solv.=Dichlorometane) = -1289.992920

6	2.010075	2.127056	-0.252057
6	1.782361	0.820373	0.053304
6	0.315576	-1.108138	-1.798665
6	3.049950	-1.356399	-0.581466
6	2.690060	-0.246820	0.573651
6	4.107054	0.095374	1.106667
1	4.057499	0.582065	2.086040
1	4.623918	0.766366	0.413969
1	-0.671164	-1.124102	-2.254528
6	1.100712	2.953047	-1.139630
1	1.704515	3.444426	-1.914516
1	0.618088	3.757812	-0.569761
1	0.326879	2.364501	-1.640678
6	3.175201	2.954394	0.262071
1	3.618654	2.570286	1.178319
1	2.837494	3.978956	0.454553
1	3.961991	3.023670	-0.502406
6	4.479145	-1.864539	-0.231793
6	4.826805	-1.253533	1.135065
1	4.434108	-1.875333	1.949990
1	5.905049	-1.154111	1.292613
1	4.534313	-2.957898	-0.231761
1	5.184293	-1.513496	-0.992402
1	2.182663	-0.798153	1.376611
6	2.023497	-2.422502	-0.613937

6	0.772324	-2.297358	-1.146988
1	3.063209	-0.808795	-1.527557
1	1.039136	-0.484332	-2.313317
1	0.052220	-3.099067	-0.999543
1	2.255900	-3.344515	-0.081783
79	-0.214932	0.273475	-0.048579
15	-2.600403	-0.233959	0.231128
8	-3.634061	0.981447	0.517208
8	-3.000292	-1.243726	1.420120
8	-3.106956	-1.027224	-1.068106
6	-3.535908	2.237310	-0.189873
1	-4.197750	2.929806	0.330133
1	-2.510092	2.621469	-0.164208
1	-3.865179	2.117641	-1.225861
6	-2.804124	-0.883419	2.806019
1	-3.064099	-1.768711	3.385777
1	-1.756407	-0.619108	2.990290
1	-3.458497	-0.051419	3.076052
6	-4.441692	-1.604925	-1.164311
1	-4.570122	-1.878434	-2.211072
1	-4.502367	-2.487949	-0.526290
1	-5.194341	-0.870221	-0.869936

[AuP(OMe)₃]⁺: ts9-PO

E(Gas Phase) = -1290.093128
G(Solv.=Dichlorometane) = -1289.989207
1 Imaginary Frequency = -141.9cm⁻¹

6	1.957234	2.103759	-0.084540
6	1.756365	0.762285	0.008886
6	1.032830	-0.185039	-2.126695
6	3.285102	-1.250874	-0.607198
6	2.593912	-0.361364	0.539504
6	3.821536	-0.066002	1.440873
1	3.531359	0.335279	2.417027
1	4.480504	0.659004	0.952511
1	0.157829	0.151929	-2.679619
6	1.143594	3.012931	-0.978894
1	1.820271	3.584602	-1.628894
1	0.597937	3.752450	-0.379171
1	0.427704	2.483107	-1.611037
6	3.008469	2.876564	0.691913
1	3.313228	2.395724	1.618762
1	2.627541	3.874186	0.934288
1	3.902325	3.023087	0.068962
6	4.435360	-2.012636	0.109653
6	4.525958	-1.424502	1.537037
1	3.996301	-2.067202	2.250247
1	5.556207	-1.331809	1.892634
1	4.244518	-3.090465	0.132446
1	5.372375	-1.871471	-0.437532
1	1.950205	-1.045557	1.110432
6	2.294127	-2.111054	-1.310322
6	1.228814	-1.603439	-1.979781
1	3.714448	-0.528695	-1.314167
1	1.899619	0.442324	-2.290229
1	0.446925	-2.264308	-2.346992
1	2.375361	-3.189665	-1.190139

79	-0.309884	0.243086	-0.119839	1	-4.254173	2.825101	0.859675
15	-2.578361	-0.339879	0.265643	1	-2.608146	2.688006	0.176659
8	-3.613114	0.868352	0.560620	1	-4.027804	2.148967	-0.780835
8	-2.882661	-1.305972	1.511545	6	-2.341365	-1.083292	2.839003
8	-3.126518	-1.188919	-0.973664	1	-2.428134	-2.046722	3.339949
6	-3.586995	2.092094	-0.205727	1	-1.314610	-0.711660	2.927302
1	-4.254543	2.783923	0.307748	1	-3.045485	-0.367116	3.267706
1	-2.574755	2.510097	-0.234215	6	-4.365423	-1.609064	-0.997785
1	-3.948504	1.912686	-1.222140	1	-4.579184	-1.795649	-2.049082
6	-2.641954	-0.885767	2.873686	1	-4.261781	-2.548250	-0.452867
1	-2.833434	-1.760801	3.494145	1	-5.147727	-0.989942	-0.553395
1	-1.601380	-0.566121	2.999840				
1	-3.323263	-0.075587	3.143129				
6	-4.438382	-1.825057	-0.966699				
1	-4.607375	-2.156993	-1.990349				
1	-4.425854	-2.676312	-0.284422				
1	-5.206798	-1.108081	-0.668854				

[AuP(OMe)₃]⁺: 10-PO

E(Gas Phase) = -1290.161137
G(Solv.=Dichlorometane) = -1290.053502

6	1.593167	1.903126	-0.388436
6	2.006480	0.611413	-0.715948
6	1.935744	0.063819	-2.150133
6	3.292251	-1.587306	-0.471226
6	2.737674	-0.329402	0.255434
6	3.993990	0.148944	1.026440
1	3.764998	0.780950	1.886518
1	4.639595	0.732851	0.359472
1	1.238903	0.629800	-2.769269
6	1.227553	2.949478	-1.428879
1	2.111652	3.576854	-1.610524
1	0.440585	3.613150	-1.057998
1	0.910501	2.543389	-2.389719
6	1.813527	2.502098	0.991663
1	1.834482	1.758286	1.789233
1	1.028818	3.229824	1.221078
1	2.768503	3.044260	1.009758
6	4.000825	-2.328005	0.664544
6	4.694535	-1.180229	1.457559
1	4.609630	-1.338304	2.536617
1	5.763558	-1.136757	1.230063
1	3.267271	-2.850049	1.292212
1	4.710801	-3.077099	0.302460
1	2.017985	-0.701914	0.999603
6	2.239261	-2.231677	-1.322890
6	1.580608	-1.413151	-2.153933
1	4.080671	-1.219861	-1.151885
1	2.933079	0.210117	-2.601070
1	0.817278	-1.762536	-2.843887
1	2.046389	-3.300674	-1.277905
79	-0.333237	0.526741	-0.115774
15	-2.501632	-0.207691	0.324416
8	-3.526312	0.923626	0.841891
8	-2.670634	-1.330476	1.450696
8	-3.088945	-0.899120	-0.982671
6	-3.601538	2.229043	0.222571