Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

DFT Studies on the Mechanism of Acetylene Hydrochlorination over Gold-based Catalyst and Its Guidance for Catalyst Construction

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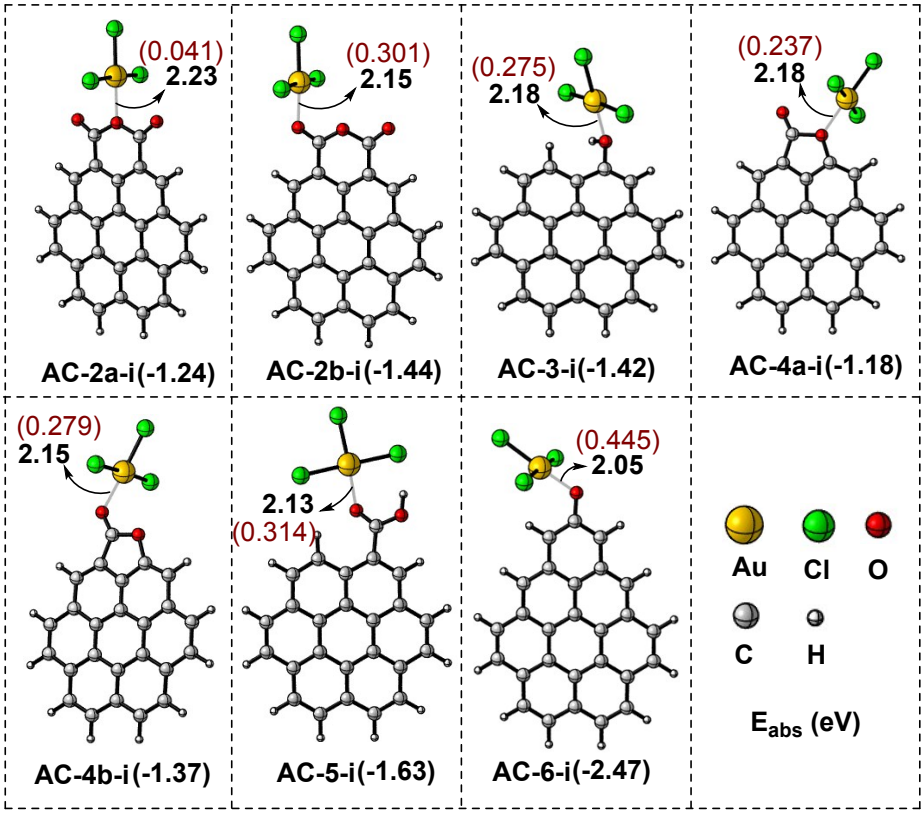

Fig. S1 Optimized geometries of possible models proposed for the AC site: $AuCl_3$/AC.

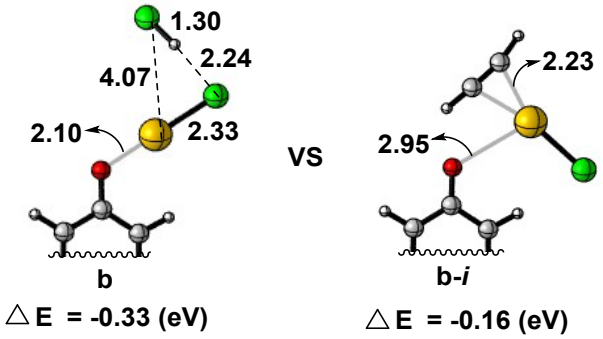

Fig. S2 Optimized geometries of **b** and **b-*i***.

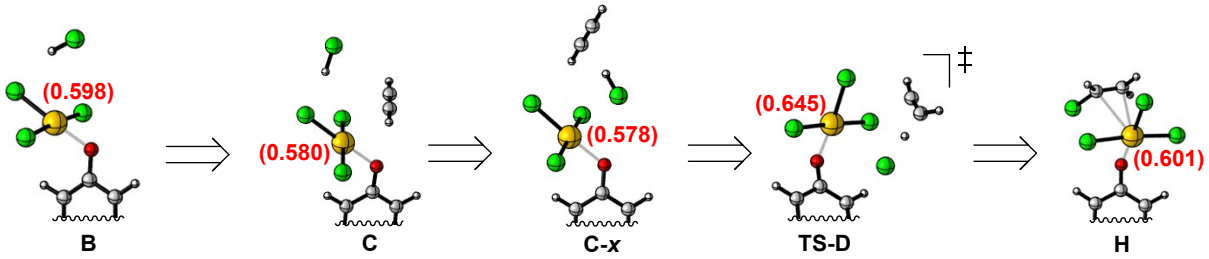

Fig. S3 The investigation of a charge transfer of the Au(III)-catalyzed acetylene hydrochlorination. Numbers in red are the NPA charges.

We also investigated the change of valence states of $AuCl_3$/AC-catalyzed acetylene hydrochlorination. NPA charges of the metal center in Fig. S3 indicate that there is not a clear process of the charge transfer, which causes the change of valence states in the process of acetylene hydrochlorination of HCl and C_2H_2 with the catalyst $AuCl_3$/AC.

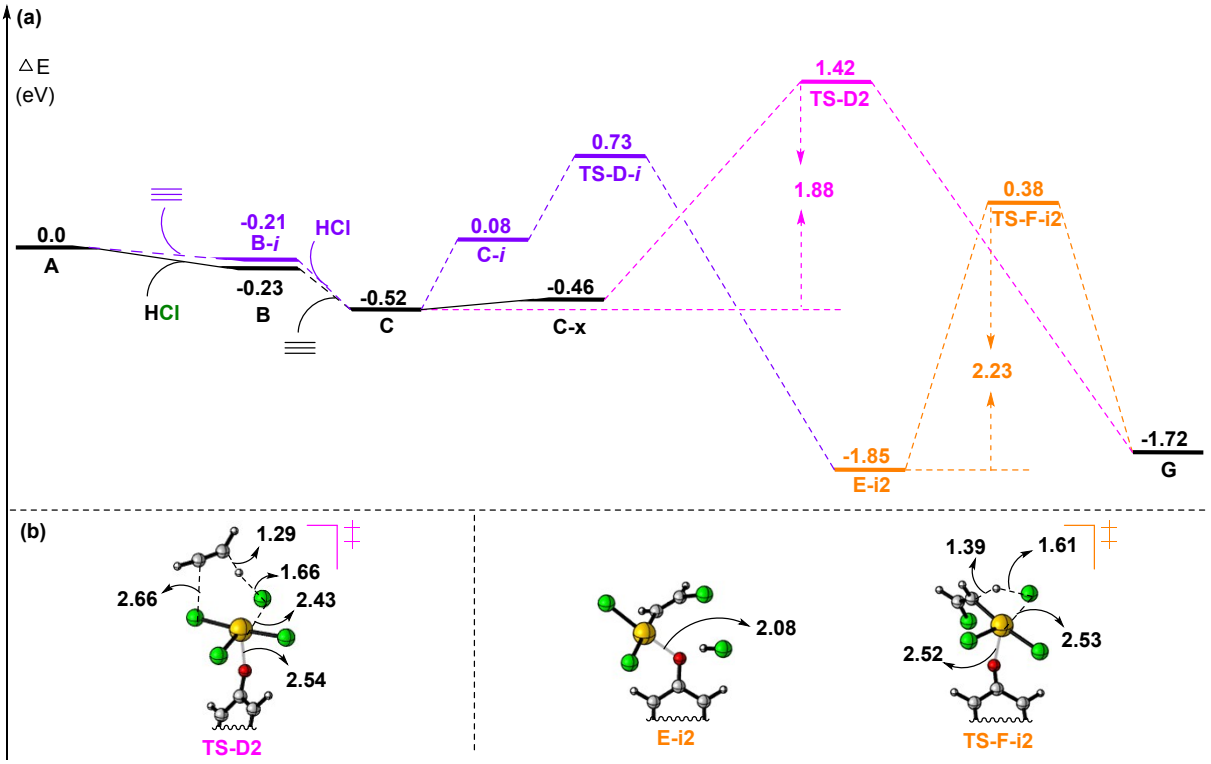

Fig. S4 The energy profiles of acetylene hydrochlorination of HCl and C_2H_2 with catalysts $AuCl_3$/AC along other possible pathways.

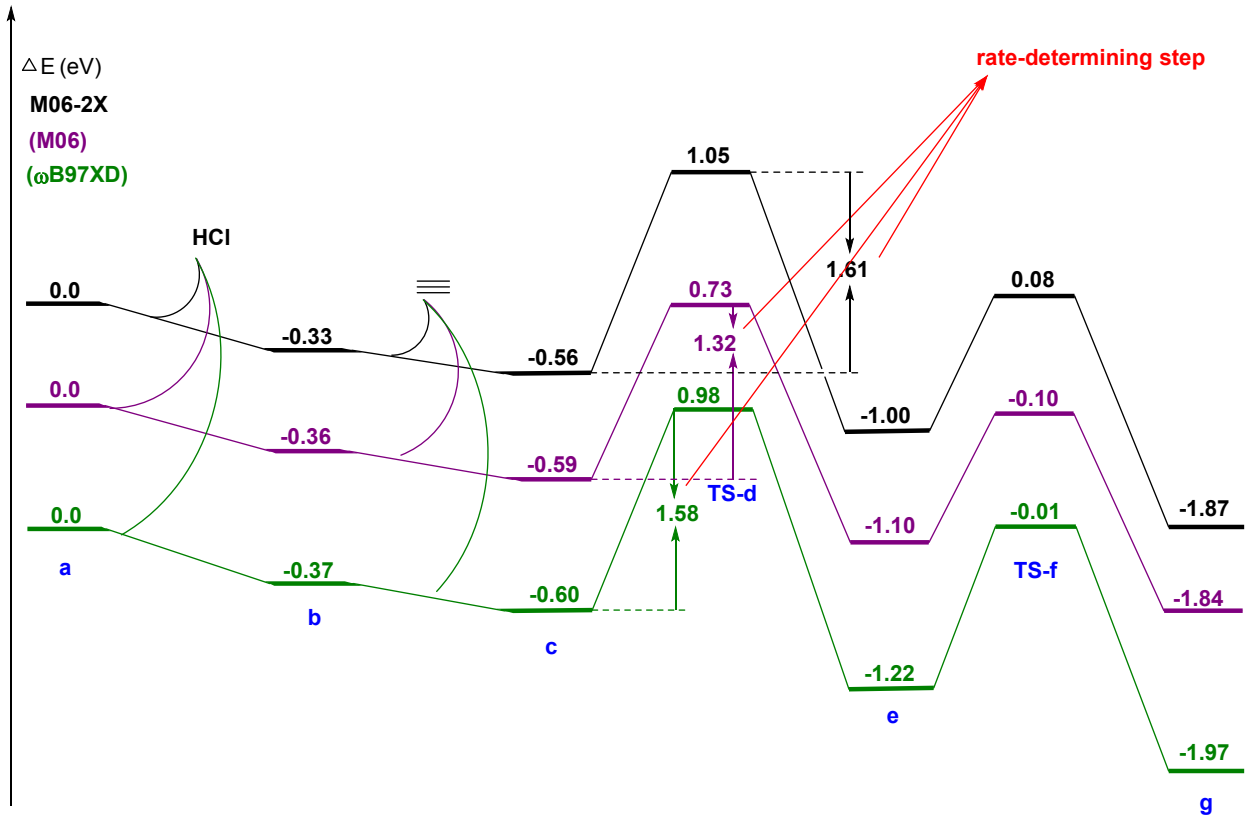

Fig. S5 Energy profiles of different DFT results for the Au(I)-catalyzed acetylene hydrochlorination. Values are given in eV.

To investigate whether this discrepancy is due to the employed functional, we recalculated the energy profile using the ωb97xd and m06 methods. Indeed, the calculations show that the energy profile change depending on the functional employed, which is shown in Fig. S5 The computation results indicate that when different functionals are taken into consideration, the fluctuation tendency of energies in this pathway is almost the same. Therefore, we can draw the conclusion that the M06-2X functional could provide accuracy in energetic information for this work and the use of other functionals will not affect the over conclusions.

The Cartesian coordinates (Å), SCF energies for the optimized structures.

1

Total SCF energy: -1073.09252177 a.u.

Atom	X	Y	Z
C	3.678672	-1.282267	0.000000
C	2.466172	0.830769	0.000000
C	1.240319	0.110773	0.000000
C	1.238905	-1.312585	0.000000
C	-2.459530	-2.023818	0.000000
C	-1.238173	-1.313137	0.000000
C	0.000636	-2.023554	0.000000
H	4.616611	-1.832047	0.000000
C	-1.240682	0.110050	0.000000
C	0.000000	0.813183	0.000000
C	-2.466788	0.828833	0.000000
C	-3.685169	0.079474	0.000000
C	-2.452641	2.235008	0.000000
C	-1.246775	2.933223	0.000000
H	-4.625410	0.623930	0.000000
H	-3.392109	2.780463	0.000000
C	-1.244653	-4.127211	0.000000
H	-1.236723	-5.213739	0.000000
C	2.460529	-2.022580	0.000000
C	0.001106	-3.438627	0.000000
C	3.685404	0.081478	0.000000
H	4.625159	0.626802	0.000000
C	2.451194	2.236056	0.000000
H	3.389926	2.782842	0.000000
C	-3.677680	-1.284722	0.000000
H	-4.615444	-1.834787	0.000000
C	-2.429347	-3.443462	0.000000
H	-3.372910	-3.983354	0.000000
C	1.246773	-4.126378	0.000000
H	1.239726	-5.212903	0.000000
C	2.431390	-3.441737	0.000000
H	3.375144	-3.981284	0.000000
C	-0.000443	2.219397	0.000000
C	-1.164767	4.343141	0.000000
H	-2.004504	5.023179	0.000000
C	1.162710	4.343738	0.000000
H	2.001751	5.024501	0.000000
C	1.244494	2.934168	0.000000
O	-0.001393	4.955142	0.000000

2

Total SCF energy: -1222.43785088 a.u.

Atom	X	Y	Z
C	1.661009	-3.679021	0.000084
C	-0.439816	-2.458697	0.000094
C	0.273063	-1.236768	-0.000047
C	1.696820	-1.235997	-0.000074
C	2.399399	2.459991	-0.000022
C	1.696721	1.236043	-0.000062
C	2.407456	0.000098	-0.000071
H	2.209287	-4.616896	0.000270
C	0.272889	1.236673	-0.000073
C	-0.430733	-0.000046	-0.000093
C	-0.440138	2.458478	0.000008
C	-1.835700	-0.000038	-0.000263
C	0.294169	3.680256	0.000060
C	-1.858442	2.427784	0.000084
C	-2.535143	1.232677	-0.000211
H	-0.256207	4.616663	0.000108
H	-2.427616	3.353230	0.000223
C	4.504780	1.247268	-0.000008
H	5.591344	1.241562	-0.000008
C	2.399608	-2.459878	-0.000007
C	3.818174	0.000181	-0.000040
C	0.294534	-3.680279	0.000071
H	-0.255594	-4.616835	0.000402
C	-1.858292	-2.428108	0.000491
H	-2.427099	-3.353807	0.000242
C	1.660528	3.679154	0.000053
H	2.208830	4.617017	0.000072
C	3.822526	2.432536	0.000007
H	4.361857	3.375611	0.000025
C	4.504955	-1.246999	0.000004
H	5.591518	-1.241015	0.000052
C	3.822895	-2.432230	0.000022
H	4.362181	-3.375334	0.000076
C	-2.535061	-1.233012	-0.000151
C	-4.015804	1.228352	-0.000279
O	-4.700987	2.211133	0.001798
O	-4.641005	0.000150	-0.002617
C	-4.015602	-1.228814	-0.000184
O	-4.701418	-2.211011	0.001091

3

Total SCF energy: -996.960052941 a.u.

Atom	X	Y	Z
C	1.790464	3.406515	0.007129
C	-0.539903	2.724670	-0.012754

C	-0.151297	1.367516	-0.001821
C	1.234833	1.027450	0.005950
C	1.042721	-2.724261	-0.009980
C	0.647550	-1.369299	-0.004013
C	1.634370	-0.340883	0.005433
H	2.548652	4.185387	0.012192
C	-0.736329	-1.029799	-0.005972
C	-1.139348	0.337380	-0.002368
C	-1.715286	-2.046512	-0.015299
C	-2.510417	0.680343	-0.005582
C	-1.290494	-3.406513	-0.023373
C	-3.087781	-1.689884	0.006270
C	-3.475792	-0.377486	0.021645
C	-2.874495	2.055648	-0.044319
H	-2.047110	-4.186508	-0.030307
H	-3.852836	-2.459889	0.027253
H	-3.920321	2.345370	-0.108859
C	3.378173	-2.051104	0.005539
H	4.435287	-2.303225	0.009370
C	2.211569	2.046636	0.011977
C	3.005809	-0.677071	0.010537
C	0.464511	3.733852	-0.006738
H	0.154195	4.775362	-0.014245
C	-1.925797	3.039679	-0.042899
H	-2.222972	4.084369	-0.076448
C	0.036517	-3.731350	-0.020760
H	0.345458	-4.773475	-0.026255
C	2.431390	-3.036741	-0.005035
H	2.728463	-4.082306	-0.009669
C	3.969902	0.370321	0.019279
H	5.024127	0.106099	0.024276
C	3.587618	1.682108	0.020014
H	4.333765	2.472477	0.025852
O	-4.811946	-0.112028	0.040439
H	-4.962069	0.785273	0.366177

4

Total SCF energy: -1109.08116734 a.u.

Atom	X	Y	Z
C	-1.555817	-3.598547	0.000152
C	0.645874	-2.540898	-0.000131
C	-0.023902	-1.293648	-0.000460
C	-1.434893	-1.175369	-0.000277
C	-1.819746	2.587784	0.000044
C	-1.231610	1.309367	-0.000262
C	-2.034292	0.124622	-0.000223
H	-2.158034	-4.503127	0.000333
C	0.182873	1.196055	-0.000480
C	0.731858	-0.101296	-0.000678
C	1.043362	2.327310	-0.000235

C	2.097663	-0.206218	-0.000730
C	0.408509	3.608334	0.000054
C	2.468200	2.155290	-0.000094
C	2.977062	0.874308	-0.000356
H	1.029744	4.499630	0.000186
H	3.113614	3.028999	0.000227
C	-4.014873	1.543362	0.000287
H	-5.098274	1.629167	0.000496
C	-2.225043	-2.340531	-0.000003
C	-3.438058	0.239749	0.000069
C	-0.185017	-3.698467	0.000129
H	0.282381	-4.679482	0.000338
C	2.091894	-2.606589	0.000120
H	2.588391	-3.571038	0.000624
C	-0.956084	3.727716	0.000163
H	-1.409066	4.715574	0.000390
C	-3.240358	2.674116	0.000292
H	-3.706884	3.655461	0.000521
C	-4.223725	-0.953479	0.000226
H	-5.306254	-0.858987	0.000408
C	-3.643891	-2.192789	0.000203
H	-4.263470	-3.085384	0.000360
C	2.785360	-1.428005	-0.000166
C	4.331244	0.238770	0.000276
O	5.428014	0.705018	0.000742
O	4.135525	-1.162078	0.000332

5

Total SCF energy: -1110.30591956 a.u.

Atom	X	Y	Z
C	2.318653	-3.375992	-0.022881
C	-0.023118	-2.736673	-0.043213
C	0.331438	-1.371973	-0.019452
C	1.711928	-1.007958	-0.002276
C	1.454277	2.737624	0.014714
C	1.084315	1.374164	0.007883
C	2.089525	0.365361	0.013284
H	3.092930	-4.138592	-0.023091
C	-0.294593	1.008541	-0.007602
C	-0.684837	-0.365895	-0.015142
C	-1.277518	2.019111	-0.021533
C	-2.057225	-0.732368	-0.022268
C	-0.882890	3.387349	-0.017108
C	-2.639400	1.640058	-0.034734
C	-3.034995	0.324847	-0.019963
C	-2.377247	-2.122776	-0.064836
H	-1.656480	4.150155	-0.028705
H	-3.406783	2.408304	-0.049022
H	-3.412865	-2.427199	-0.090203
C	3.800220	2.106661	0.039648
H	4.852280	2.378719	0.052379

C	2.709567	-2.007532	-0.002477
C	3.454364	0.726292	0.029006
C	0.999623	-3.727017	-0.044074
H	0.707390	-4.773449	-0.061970
C	-1.399700	-3.077609	-0.073014
H	-1.674113	-4.128782	-0.105101
C	0.436998	3.734083	0.001965
H	0.732909	4.779514	0.006318
C	2.836650	3.075831	0.032107
H	3.113970	4.126422	0.038539
C	4.438967	-0.301029	0.031361
H	5.487759	-0.017094	0.044188
C	4.078844	-1.618784	0.015942
H	4.838145	-2.396334	0.016560
C	-4.520500	0.152473	0.005484
O	-5.302587	1.031699	-0.270930
O	-4.955819	-1.057009	0.410753
H	-5.927962	-0.999914	0.396605

6

Total SCF energy: -1111.20351071 a.u.

Atom	X	Y	Z
C	-1.513979	3.682805	0.000248
C	0.588552	2.456463	0.000119
C	-0.128903	1.229801	0.000072
C	-1.548569	1.232171	0.000113
C	-2.252977	-2.458211	-0.000071
C	-1.548673	-1.232123	-0.000023
C	-2.262886	0.000073	0.000066
H	-2.064535	4.619148	0.000317
C	-0.129087	-1.229806	-0.000064
C	0.587074	-0.000026	-0.000016
C	0.588280	-2.456524	-0.000153
C	1.984460	-0.000122	-0.000056
C	-0.151450	-3.683061	-0.000200
C	1.990091	-2.429410	-0.000191
C	2.717829	1.225939	-0.000010
H	0.399022	-4.619772	-0.000268
H	2.534828	-3.371738	-0.000260
C	-4.358394	-1.246108	0.000056
H	-5.445092	-1.242230	0.000087
C	-2.252778	2.458292	0.000202
C	-3.672353	0.000127	0.000106
C	-0.151139	3.683130	0.000209
H	0.399539	4.619740	0.000245
C	1.990309	2.429263	0.000078
H	2.535363	3.371410	0.000114
C	-1.514388	-3.682652	-0.000161
H	-2.064988	-4.618982	-0.000197
C	-3.673959	-2.432659	-0.000029

H	-4.212688	-3.375954	-0.000067
C	-4.358262	1.246310	0.000196
H	-5.444955	1.242655	0.000228
C	-3.673647	2.432864	0.000242
H	-4.212341	3.376175	0.000312
C	2.717658	-1.226259	-0.000146
C	4.124687	-1.205458	-0.000187
H	4.668523	-2.147960	-0.000256
C	4.928538	0.000025	-0.000145
C	4.124866	1.205409	-0.000052
H	4.668053	2.148312	-0.000015
O	6.166734	-0.000289	-0.000183

A-1

Total SCF energy: -1668.93878991 a.u.

Atom	X	Y	Z
C	-1.876976	-2.467299	-0.000052
C	0.226710	-1.248434	-0.000019
C	-0.486350	-0.000078	-0.000023
C	-1.888857	-0.000038	-0.000033
C	-1.876833	2.467224	-0.000062
C	-2.593123	1.241566	-0.000042
C	0.226797	1.248241	-0.000019
C	-4.725470	2.459992	-0.000009
C	-2.593197	-1.241584	-0.000037
C	-4.015980	1.238651	-0.000019
C	-0.468778	-2.452995	-0.000047
H	0.076827	-3.392184	-0.000052
C	1.635439	-1.179883	0.000035
H	2.319305	-2.016102	0.000086
C	-3.987331	3.678471	-0.000055
H	-4.537578	4.615795	-0.000062
C	-4.726270	0.000061	-0.000007
C	-4.016045	-1.238591	-0.000022
O	2.252417	-0.000169	0.000073
Au	4.555437	0.000011	0.000030
Cl	6.825133	0.000051	-0.000067
C	-3.987563	-3.678416	-0.000095
H	-4.537894	-4.615688	-0.000032
C	-4.725611	-2.459876	-0.000003
C	-6.140161	0.000091	0.000035
C	-6.828843	-1.245709	0.000122
H	-7.915211	-1.237739	0.000271
C	-6.828765	1.245931	0.000048
H	-7.915135	1.238038	0.000142
C	-0.468629	2.452830	-0.000047
H	0.077012	3.392001	-0.000053
C	-2.622860	3.686121	-0.000086
H	-2.077567	4.625561	-0.000127
C	-2.623089	-3.686150	-0.000113

H	-2.077832	-4.625612	-0.000099
C	-6.145687	2.430668	0.000057
H	-6.685300	3.374057	0.000083
C	-6.145834	-2.430475	0.000081
H	-6.685504	-3.373833	0.000105
C	1.635517	1.179614	0.000046
H	2.319460	2.015763	0.000124

A-**2a**

Total SCF energy: -1818.30097944 a.u.

Atom	X	Y	Z
C	-4.101862	3.686768	0.004454
C	-2.008501	2.458665	-0.036289
C	-2.722296	1.236524	-0.022142
C	-4.145247	1.241881	0.007338
C	-4.865352	-2.449887	0.027950
C	-4.156442	-1.228884	0.009845
C	-4.861156	0.009594	0.024596
H	-4.647224	4.626071	0.014699
C	-2.733477	-1.236788	-0.021075
C	-2.021707	-0.003226	-0.035437
C	-2.030500	-2.464887	-0.035131
C	-0.616048	-0.009761	-0.059459
C	-2.769700	-3.683812	-0.018083
C	-0.615047	-2.444578	-0.062158
C	0.070399	-1.251882	-0.072263
H	-2.224656	-4.623085	-0.028800
H	-0.054558	-3.375385	-0.072479
C	-6.963927	-1.227554	0.077241
H	-8.050023	-1.216397	0.105585
C	-4.843052	2.469030	0.021832
C	-6.271338	0.016195	0.057430
C	-2.736522	3.684129	-0.023205
H	-2.182943	4.618471	-0.036034
C	-0.593400	2.425511	-0.059938
H	-0.024267	3.351147	-0.068714
C	-4.134982	-3.674045	0.012517
H	-4.688596	-4.608545	0.027449
C	-6.287616	-2.416179	0.062989
H	-6.830478	-3.356865	0.080009
C	-6.952567	1.266089	0.071613
H	-8.038786	1.265415	0.098017
C	-6.265537	2.448417	0.054364
H	-6.799918	3.393969	0.065885
C	0.080872	1.226507	-0.070027
C	1.539192	-1.276701	-0.091938
O	2.247522	-2.236320	-0.107879
O	2.175438	-0.021829	-0.085959
C	1.549436	1.238242	-0.083416
O	2.265505	2.192361	-0.087578

Cl 6.744277 0.048967 0.147652

Au 4.457206 -0.007812 0.014000

A-**2b**

Total SCF energy: -1818.307858 a.u.

Atom X Y Z

C 3.212601 -3.846313 -0.034613

C 1.498341 -2.127426 -0.068390

C 2.500388 -1.126737 -0.039051

C 3.875037 -1.492409 -0.005408

C 5.505674 1.897571 0.058554

C 4.511526 0.895763 0.024728

C 4.879216 -0.481068 0.027546

H 3.501953 -4.893232 -0.032711

C 3.137411 1.263846 -0.009855

C 2.139168 0.249913 -0.040351

C 2.764572 2.629065 -0.011391

C 0.782671 0.612304 -0.067922

C 3.788294 3.620994 0.021288

C 1.388694 2.965788 -0.041880

C 0.425913 1.983692 -0.067177

H 3.498790 4.667720 0.019982

H 1.079246 4.007407 -0.042976

C 7.226277 0.183100 0.100057

H 8.273985 -0.102910 0.131407

C 4.238757 -2.856483 -0.002038

C 6.241541 -0.844777 0.064551

C 1.892669 -3.497804 -0.066196

H 1.120899 -4.261614 -0.090439

C 0.138127 -1.737064 -0.094844

H -0.645132 -2.489815 -0.113616

C 5.106988 3.266430 0.055048

H 5.878085 4.031093 0.081921

C 6.872980 1.504414 0.097073

H 7.636326 2.276646 0.126048

C 6.583521 -2.226671 0.067242

H 7.634276 -2.501622 0.097125

C 5.619793 -3.196805 0.035109

H 5.897773 -4.246775 0.038213

C -0.207287 -0.403821 -0.093956

C -0.996843 2.363802 -0.093170

O -1.438989 3.469624 -0.106310

O -1.923627 1.305144 -0.099926

C -1.614530 -0.000909 -0.104727

O -2.532463 -0.810524 -0.112965

Cl -6.912167 0.048536 0.174667

Au -4.661743 -0.336916 0.014025

A-3

Total SCF energy: -1592.82363914 a.u.

Atom	X	Y	Z
C	-3.607446	3.605437	0.017834
C	-1.459349	2.605890	-0.512949
C	-2.009650	1.317557	-0.335895
C	-3.380834	1.173210	0.028070
C	-3.670040	-2.567777	0.235065
C	-3.121150	-1.281375	0.043341
C	-3.936742	-0.125429	0.215716
H	-4.234078	4.482085	0.157808
C	-1.751366	-1.139253	-0.323933
C	-1.196329	0.161179	-0.518333
C	-0.946304	-2.286380	-0.492229
C	0.159069	0.314657	-0.885763
C	-1.520061	-3.572544	-0.289398
C	0.411913	-2.122884	-0.881658
C	0.918505	-0.874473	-1.071693
C	0.698358	1.621323	-1.048896
H	-0.892582	-4.449869	-0.418601
H	1.049743	-2.987677	-1.037944
H	1.748998	1.751753	-1.294768
C	-5.824258	-1.575615	0.761692
H	-6.869577	-1.677666	1.040078
C	-4.187021	2.317894	0.204349
C	-5.293866	-0.267198	0.576049
C	-2.292754	3.745223	-0.326024
H	-1.860902	4.732749	-0.461735
C	-0.087634	2.725822	-0.865886
H	0.336606	3.718922	-0.983045
C	-2.834488	-3.706405	0.060873
H	-3.262853	-4.693268	0.212686
C	-5.041994	-2.683977	0.598107
H	-5.458792	-3.676546	0.744790
C	-6.086642	0.902953	0.744019
H	-7.130960	0.787712	1.021027
C	-5.553419	2.148668	0.565258
H	-6.169187	3.034011	0.698476
Au	3.710009	-0.098577	0.092856
Cl	5.225522	0.620218	1.637821
O	2.269255	-0.771732	-1.449465
H	2.345934	-0.223499	-2.247961

A-4a

Total SCF energy: -1704.944904 a.u.

Atom	X	Y	Z
C	-2.390165	3.792886	-0.049441
C	-0.777814	1.963342	-0.073267

C	-1.876623	1.070482	-0.046212
C	-3.222111	1.512035	-0.017459
C	-5.044910	-1.801692	0.053313
C	-4.004463	-0.854201	0.018678
C	-4.280188	0.549497	0.015240
H	-2.593418	4.860242	-0.050751
C	-2.658894	-1.302834	-0.011240
C	-1.646634	-0.323091	-0.042806
C	-2.311318	-2.682175	-0.006237
C	-0.347165	-0.761013	-0.066650
C	-3.395304	-3.613946	0.028356
C	-0.936514	-3.083537	-0.032243
C	0.035133	-2.103707	-0.061518
H	-3.171760	-4.676974	0.032750
H	-0.683597	-4.139761	-0.026259
C	-6.656585	0.016987	0.083241
H	-7.686882	0.361328	0.110539
C	-3.494871	2.893142	-0.018965
C	-5.617241	0.991564	0.047602
C	-1.088896	3.352797	-0.074406
H	-0.275734	4.072800	-0.095165
C	0.579952	1.463286	-0.096329
H	1.419806	2.152192	-0.113847
C	-4.696557	-3.188943	0.056092
H	-5.499953	-3.919997	0.082762
C	-6.385815	-1.326779	0.086006
H	-7.198403	-2.047259	0.114212
C	-5.875104	2.396478	0.045282
H	-6.908085	2.732301	0.072039
C	-4.858530	3.311420	0.013121
H	-5.080392	4.374927	0.012849
C	0.744917	0.110418	-0.091696
C	1.515433	-2.086942	-0.084920
O	2.368382	-2.909137	-0.086030
O	1.890009	-0.679874	-0.107034
Au	3.960897	0.079844	0.010784
Cl	6.049530	0.991870	0.147777

A-4b

Total SCF energy: -1704.9499791 a.u.

Atom	X	Y	Z
C	-3.956064	3.705347	-0.005236
C	-1.848786	2.474791	-0.044884
C	-2.616061	1.284242	-0.030541
C	-4.031314	1.279263	-0.000253
C	-4.716086	-2.442233	0.029829
C	-4.028213	-1.214501	0.007861
C	-4.731615	0.031401	0.019421
H	-4.483380	4.655300	0.004570
C	-2.610450	-1.215714	-0.023555

C	-1.962384	0.033762	-0.041586
C	-1.841856	-2.414089	-0.032072
C	-0.593622	0.029072	-0.065440
C	-2.577488	-3.641132	-0.010455
C	-0.411175	-2.359896	-0.057904
C	0.198657	-1.119223	-0.073584
H	-2.030356	-4.579558	-0.016924
H	0.162184	-3.282434	-0.062331
C	-6.818241	-1.223601	0.076491
H	-7.904520	-1.222346	0.105215
C	-4.724056	2.504605	0.013066
C	-6.139519	0.029349	0.054180
C	-2.581890	3.695973	-0.032037
H	-2.037059	4.635766	-0.042870
C	-0.401473	2.424825	-0.067720
H	0.175814	3.343152	-0.074870
C	-3.946216	-3.648749	0.018421
H	-4.477525	-4.596346	0.034840
C	-6.137961	-2.414215	0.064640
H	-6.682911	-3.353792	0.082674
C	-6.826420	1.282109	0.067377
H	-7.912544	1.275240	0.096036
C	-6.150221	2.471403	0.047347
H	-6.696456	3.410414	0.058761
C	0.181255	1.190942	-0.076043
C	1.571884	-0.575316	-0.088297
O	2.642399	-1.158564	-0.094473
O	1.517155	0.794940	-0.091141
Au	4.581552	-0.159576	0.006264
Cl	6.639038	0.836450	0.135928

A-5

Total SCF energy: -1706.17892163 a.u.

Atom	X	Y	Z
C	4.427975	3.629718	0.009276
C	2.225145	2.629202	0.203261
C	2.786782	1.338593	0.117815
C	4.199782	1.196015	-0.020467
C	4.528491	-2.543405	-0.108156
C	3.952431	-1.254965	-0.037007
C	4.783447	-0.100146	-0.100938
H	5.070190	4.504945	-0.033531
C	2.540312	-1.111164	0.098063
C	1.943930	0.185590	0.168463
C	1.731746	-2.266591	0.162111
C	0.537978	0.334421	0.284750
C	2.333147	-3.556340	0.092361
C	0.333851	-2.110426	0.277537
C	-0.258529	-0.866476	0.321464
C	0.003971	1.652146	0.387948

H	1.692856	-4.432424	0.141840
H	-0.286382	-2.999812	0.308325
H	-1.061640	1.789838	0.497662
C	6.734759	-1.550403	-0.314869
H	7.811038	-1.653802	-0.423569
C	5.025281	2.340352	-0.078752
C	6.180715	-0.241829	-0.241013
C	3.077051	3.768744	0.147450
H	2.628186	4.755633	0.216919
C	0.819714	2.748671	0.349245
H	0.387514	3.742184	0.431768
C	3.684402	-3.688991	-0.039038
H	4.138685	-4.674151	-0.095319
C	5.939289	-2.660068	-0.249209
H	6.375397	-3.653436	-0.305859
C	6.989712	0.927399	-0.301343
H	8.064574	0.811858	-0.410404
C	6.431456	2.172083	-0.222893
H	7.057606	3.058800	-0.267648
C	-1.731606	-0.838471	0.340737
Au	-4.559117	0.160010	-0.110911
O	-2.404595	0.159856	0.055664
Cl	-6.829135	0.108123	-0.300860
O	-2.303370	-1.989253	0.661613
H	-3.276177	-1.895263	0.597461

A-6

Total SCF energy: -1707.10273686 a.u.

Atom	X	Y	Z
C	-2.695697	-2.620831	0.000005
C	-2.546705	1.135417	0.000020
C	-2.137786	-0.225598	0.000015
C	-3.111460	-1.259383	-0.000000
C	-0.773514	-0.547328	0.000025
C	-0.347715	-1.905646	0.000027
C	0.211746	0.478974	0.000036
C	-0.211504	1.821259	0.000038
C	1.579039	0.138354	0.000047
C	2.043024	-1.205822	0.000049
H	0.539149	2.609316	0.000051
H	2.325413	0.931934	0.000053
C	-4.903439	0.427627	-0.000023
C	-4.493694	-0.935235	-0.000021
C	-1.567097	2.167520	0.000032
C	-3.927288	1.463383	0.000011
C	-5.460530	-1.967202	-0.000032
O	3.281079	-1.544786	0.000069
Cl	6.512817	1.476615	-0.000079
Au	4.834755	-0.106207	-0.000005
C	-4.330021	2.819343	0.000013

C	-2.004248	3.532500	0.000055
H	-1.253155	4.317346	0.000065
C	-3.698989	-3.645809	-0.000005
H	-3.379023	-4.683885	-0.000002
C	-1.328180	-2.916073	0.000018
H	-1.010927	-3.956925	0.000019
C	1.030596	-2.203295	0.000037
H	1.358754	-3.239799	0.000035
C	-6.275841	0.751500	-0.000035
C	-6.836412	-1.616845	-0.000067
H	-7.577621	-2.410729	-0.000082
C	-7.229070	-0.303491	-0.000009
H	-8.285873	-0.050983	-0.000014
C	-6.656594	2.122120	-0.000037
H	-7.714918	2.368316	-0.000046
C	-5.718070	3.120791	-0.000005
H	-6.026743	4.161983	0.000010
C	-3.330340	3.843205	0.000015
H	-3.652093	4.880379	0.000007
C	-5.023544	-3.330459	-0.000021
H	-5.775108	-4.114593	-0.000035

A-**2a**-***i***

Total SCF energy: -2738.67151711 a.u.

Atom	X	Y	Z
C	4.557537	3.680759	0.000097
C	2.458156	2.462864	0.000071
C	3.164790	1.236561	0.000037
C	4.588164	1.235149	0.000032
C	5.292310	-2.459141	-0.000074
C	4.588158	-1.235147	-0.000033
C	5.298736	0.000000	-0.000006
H	5.108258	4.616945	0.000123
C	3.164785	-1.236552	-0.000019
C	2.457145	0.000006	0.000015
C	2.458146	-2.462854	-0.000038
C	1.050732	0.000010	0.000029
C	3.192025	-3.684982	-0.000067
C	1.043377	-2.437794	-0.000050
C	0.362450	-1.242452	-0.000011
H	2.642288	-4.621524	-0.000069
H	0.478934	-3.366192	-0.000100
C	7.396621	-1.246385	-0.000064
H	8.483053	-1.240194	-0.000081
C	5.292321	2.459140	0.000068
C	6.709272	-0.000003	-0.000015

C	3.192041	3.684990	0.000094
H	2.642308	4.621534	0.000111
C	1.043387	2.437812	0.000107
H	0.478949	3.366213	0.000167
C	4.557522	-3.680757	-0.000087
H	5.108239	-4.616945	-0.000114
C	6.714995	-2.431956	-0.000094
H	7.254196	-3.374850	-0.000135
C	7.396627	1.246375	0.000025
H	8.483058	1.240181	0.000022
C	6.715005	2.431949	0.000068
H	7.254211	3.374841	0.000103
C	0.362457	1.242474	0.000089
C	-1.103472	-1.267189	-0.000089
O	-1.830990	-2.211226	-0.000313
O	-1.723614	0.000019	0.000172
C	-1.103469	1.267217	0.000195
O	-1.830970	2.211269	0.000343
Cl	-6.209409	0.000131	-0.000179
Au	-3.955270	-0.000009	-0.000006
Cl	-3.880231	-0.000531	2.316404
Cl	-3.879860	0.000379	-2.316393

A-**2b**-***i***

Total SCF energy: -2738.67854732 a.u.

Atom	X	Y	Z
C	-3.707855	-3.835580	0.092997
C	-1.973821	-2.137422	0.069777
C	-2.963554	-1.124383	0.037851
C	-4.342596	-1.473484	0.035040
C	-5.934056	1.934106	-0.054472
C	-4.951379	0.921225	-0.024136
C	-5.335027	-0.450896	0.004188
H	-4.010206	-4.878579	0.113259
C	-3.572707	1.272939	-0.024051
C	-2.586264	0.247907	0.006874
C	-3.184220	2.633752	-0.055211
C	-1.225397	0.593897	0.003961
C	-4.196816	3.637482	-0.083871
C	-1.804499	2.954064	-0.061025
C	-0.852382	1.960565	-0.033809
H	-3.895080	4.680495	-0.106715
H	-1.483097	3.991655	- 0.089019
C	-7.675136	0.240846	-0.029259
H	-8.726669	-0.032317	-0.031323
C	-4.722226	-2.833353	0.061695
C	-6.702111	-0.798152	0.001370

C	-2.383737	-3.503093	0.097633
H	-1.620303	-4.275221	0.122411
C	-0.609491	-1.765350	0.071291
H	0.164235	-2.527735	0.096132
C	-5.519813	3.298186	-0.083260
H	-6.282617	4.071314	-0.106352
C	-7.306417	1.557584	-0.056075
H	-8.060976	2.338659	-0.080175
C	-7.060261	-2.175706	0.028193
H	-8.114591	-2.438114	0.025221
C	-6.107589	-3.157133	0.056801
H	-6.398641	-4.203373	0.076462
C	-0.249448	-0.435499	0.038616
C	0.572655	2.324269	-0.051997
O	1.038811	3.417334	-0.091763
O	1.487785	1.243759	-0.021680
C	1.154864	-0.045321	0.032838
O	2.065869	-0.874557	0.072831
Cl	6.320795	0.250907	-0.060080
Au	4.123754	-0.267550	0.007337
Cl	4.058206	-0.577000	-2.292088
Cl	4.053194	0.036013	2.307088

A-**3**-***i***

Total SCF energy: -2513.20021716 a.u.

Atom	X	Y	Z
C	-4.009232	3.642292	0.377483
C	-1.863975	2.670895	-0.214411
C	-2.437004	1.380452	-0.195225
C	-3.819312	1.220616	0.115377
C	-4.168624	-2.514131	-0.108827
C	-3.595904	-1.224026	-0.140212
C	-4.399301	-0.080449	0.139422
H	-4.625590	4.508107	0.603186
C	-2.214166	-1.066273	-0.450548
C	-1.635712	0.238075	-0.484780
C	-1.421349	-2.203288	-0.720983
C	-0.268638	0.408947	-0.799202
C	-2.018934	-3.493974	-0.679035
C	-0.048435	-2.024229	-1.038378
C	0.475078	-0.768531	-1.085833
C	0.291768	1.716709	-0.815197
H	-1.400015	-4.361951	-0.887044
H	0.589496	-2.877799	-1.244967
H	1.341691	1.866621	-1.052794
C	-6.323159	-1.548600	0.463236
H	-7.378170	-1.663258	0.696537

C	-4.612651	2.352318	0.401357
C	-5.768387	-0.237370	0.443642
C	-2.684786	3.796655	0.081505
H	-2.235178	4.785548	0.067689
C	-0.485022	2.806250	-0.527514
H	-0.046411	3.800131	-0.536700
C	-3.345193	-3.641899	-0.384825
H	-3.792434	-4.631621	-0.355685
C	-5.552497	-2.645561	0.198618
H	-5.987605	-3.640923	0.219898
C	-6.547887	0.919846	0.724578
H	-7.601331	0.792342	0.958196
C	-5.990511	2.168004	0.705718
H	-6.595718	3.042890	0.926395
Cl	4.917918	0.449867	1.599526
O	1.842140	-0.656484	-1.396630
H	1.999890	0.007796	-2.098885
Au	3.314200	-0.130777	0.117815
Cl	4.061595	1.375511	-1.506050
Cl	2.422571	-1.665436	1.584996

A-4a-*i*

Total SCF energy: -2625.31260298 a.u.

Atom	X	Y	Z
C	-2.945708	3.786338	-0.204075
C	-1.277362	2.007886	-0.205689
C	-2.346057	1.082044	-0.129876
C	-3.704208	1.482285	-0.090323
C	-5.421804	-1.880969	0.116389
C	-4.411674	-0.903784	0.033621
C	-4.731326	0.489695	-0.010620
H	-3.182739	4.846279	-0.232462
C	-3.053633	-1.311291	-0.004111
C	-2.071817	-0.303321	-0.087387
C	-2.666100	-2.679357	0.040413
C	-0.760006	-0.702525	-0.124495
C	-3.719493	-3.642424	0.124414
C	-1.281863	-3.040742	0.006284
C	-0.340525	-2.034651	-0.078102
H	-3.462493	-4.697199	0.160387
H	-0.996655	-4.087838	0.047104
C	-7.088992	-0.113513	0.108630
H	-8.129083	0.199937	0.137232
C	-4.020459	2.853809	-0.128372
C	-6.081000	0.890713	0.026941

C	-1.631949	3.386608	-0.240999
H	-0.842672	4.130713	-0.298719
C	0.094623	1.549650	-0.244285
H	0.909821	2.265142	-0.296846
C	-5.032241	-3.256502	0.160159
H	-5.812674	-4.009567	0.225628
C	-6.776161	-1.447366	0.152599
H	-7.564936	-2.191485	0.217321
C	-6.382928	2.286182	-0.015594
H	-7.425467	2.590873	0.013082
C	-5.395914	3.230484	-0.088976
H	-5.650666	4.286192	-0.118205
C	0.300461	0.204009	-0.204653
C	1.133589	-1.986398	-0.115186
O	2.021512	-2.766264	-0.059701
O	1.464563	-0.561353	-0.237699
Cl	5.645273	0.787751	0.333957
Au	3.524945	0.088152	0.039377
Cl	3.021490	0.425542	2.278838
Cl	3.890509	-0.234307	-2.222579

A-**4b**-***i***

Total SCF energy: -2625.31962816 a.u.

Atom	X	Y	Z
C	-4.370412	3.715085	-0.105191
C	-2.275404	2.465431	-0.040490
C	-3.054480	1.282403	-0.016410
C	-4.469743	1.290547	-0.039281
C	-5.191000	-2.423800	0.043492
C	-4.491139	-1.202600	0.026841
C	-5.181924	0.049572	-0.018170
H	-4.888622	4.669425	-0.139831
C	-3.073627	-1.216854	0.053390
C	-2.414358	0.026183	0.030957
C	-2.316110	-2.422631	0.096507
C	-1.045717	0.009051	0.051653
C	-3.063867	-3.642673	0.112353
C	-0.886306	-2.382894	0.119405
C	-0.264802	-1.147099	0.096745
H	-2.525648	-4.585631	0.144707
H	-0.321100	-3.309763	0.151357
C	-7.280815	-1.185526	-0.026135
H	-8.367226	-1.174003	-0.047148
C	-5.150345	2.521947	-0.084411
C	-6.589881	0.060498	-0.044311

C	-2.996227	3.693029	-0.085154
H	-2.442438	4.627322	-0.103681
C	-0.828741	2.402334	-0.022713
H	-0.241708	3.314135	-0.044611
C	-4.432535	-3.637323	0.086775
H	-4.973064	-4.579628	0.098983
C	-6.612543	-2.382507	0.015306
H	-7.167069	-3.316450	0.027109
C	-7.264559	1.319006	-0.089286
H	-8.350887	1.321891	-0.109000
C	-6.577039	2.501818	-0.108240
H	-7.114702	3.445160	-0.143101
C	-0.261560	1.162645	0.021245
C	1.105103	-0.611828	0.092620
O	2.175967	-1.211214	0.122171
O	1.072969	0.747415	0.043507
Cl	6.003137	0.952938	-0.137138
Au	4.022077	-0.124723	0.001184
Cl	3.976194	-0.459455	-2.294363
Cl	3.937437	0.194056	2.298635

A-**5**-***i***

Total SCF energy: -2626.55384463 a.u.

Atom	X	Y	Z
C	4.628375	3.691077	0.111388
C	2.490239	2.543905	0.030166
C	3.143741	1.294546	0.018444
C	4.569714	1.248152	0.048828
C	5.159805	-2.458250	-0.053694
C	4.492968	-1.212556	-0.025163
C	5.245343	-0.004544	0.028088
H	5.210829	4.607496	0.147400
C	3.068040	-1.164836	-0.053849
C	2.380035	0.087309	-0.027151
C	2.339636	-2.373191	-0.113481
C	0.961914	0.140880	-0.050343
C	3.031289	-3.618536	-0.140282
C	0.931371	-2.313467	-0.142716
C	0.252161	-1.113309	-0.105195
C	0.332604	1.419291	-0.056038
H	2.450177	-4.535215	-0.184645
H	0.371849	-3.241933	-0.183866
H	-0.744661	1.494250	-0.091836
C	7.302023	-1.318174	0.028654
H	8.388051	-1.347798	0.049885

C	5.317296	2.445489	0.096398
C	6.655884	-0.051171	0.055789
C	3.264388	3.738321	0.078190
H	2.744429	4.692160	0.087427
C	1.073203	2.568191	-0.016241
H	0.566026	3.529321	-0.022362
C	4.394228	-3.658660	-0.111212
H	4.919115	-4.609480	-0.132823
C	6.581774	-2.478820	-0.024849
H	7.088404	-3.439582	-0.047419
C	7.385288	1.169457	0.106999
H	8.470708	1.127310	0.129098
C	6.738634	2.372953	0.126416
H	7.304218	3.299855	0.164079
C	-1.215929	-1.206581	-0.095612
O	-1.935858	-0.271802	0.317335
Cl	-6.193148	0.648183	-0.186250
O	-1.706828	-2.340707	-0.527482
H	-2.671322	-2.413344	-0.316820
Au	-4.009928	0.116517	0.062604
Cl	-3.418926	2.301650	-0.374983
Cl	-4.582994	-2.123518	0.493950

A-**6**-***i***

Total SCF energy: -2627.4822261 a.u.

Atom	X	Y	Z
C	-3.154785	-2.618262	0.084480
C	-3.058599	1.137617	-0.077205
C	-2.631809	-0.216072	-0.020961
C	-3.589320	-1.262993	0.028116
C	-1.262047	-0.518579	-0.014904
C	-0.820143	-1.869109	0.039565
C	-0.294114	0.520524	-0.065522
C	-0.734093	1.856290	-0.119257
C	1.079052	0.200206	-0.063772
C	1.544860	-1.132428	-0.009170
H	0.006062	2.653106	-0.155067
H	1.803461	1.010130	-0.104835
C	-5.404339	0.397263	-0.036399
C	-4.975861	-0.958398	0.020485
C	-2.093691	2.183051	-0.126185
C	-4.443516	1.445872	-0.084922
C	-5.928136	-2.003080	0.069926
O	2.796103	-1.486082	-0.014320
Cl	6.004331	1.431986	0.098667
C	-4.865377	2.794984	-0.140988
C	-2.550212	3.540805	-0.182298

H	-1.810420	4.335231	-0.219944
C	-4.143757	-3.656413	0.134591
H	-3.809069	-4.688846	0.178210
C	-1.784467	-2.894424	0.089242
H	-1.451107	-3.929246	0.131729
C	0.562190	-2.146210	0.044701
H	0.911256	-3.174460	0.088266
C	-6.781249	0.701783	-0.044745
C	-7.308417	-1.672219	0.061076
H	-8.038632	-2.475129	0.100025
C	-7.719263	-0.365319	0.005172
H	-8.779512	-0.127866	-0.001298
C	-7.181367	2.065551	-0.102044
H	-8.243062	2.296533	-0.108561
C	-6.257283	3.076710	-0.148036
H	-6.580908	4.112387	-0.190851
C	-3.880460	3.832160	-0.189487
H	-4.217301	4.863586	-0.232225
C	-5.472152	-3.359274	0.127559
H	-6.212769	-4.152637	0.166734
Au	4.282998	-0.073571	0.032227
Cl	3.701923	0.398550	2.246036
Cl	4.681185	-0.507139	-2.212803

AuCl

Total SCF energy: -595.8242693 a.u.

Atom	X	Y	Z
Cl	0.000000	0.000000	-1.886351
Au	-0.000000	-0.000000	0.405924

$AuCl_3$

Total SCF energy: -1516.18794814 a.u.

Atom	X	Y	Z
Au	0.000000	0.000000	0.239705
Cl	0.000000	0.000000	-2.015924
Cl	-0.000000	-2.269904	0.451000
Cl	0.000000	2.269904	0.451000

C_2H_2

Total SCF energy: -77.3162132508 a.u.

Atom	X	Y	Z
C	0.000000	0.000000	0.601094
H	0.000000	0.000000	1.667606
C	0.000000	0.000000	-0.601094

H 0.000000 0.000000 -1.667606

HCl

Total SCF energy: -460.796271022 a.u.

Atom	X	Y	Z
Cl	0.000000	0.000000	0.071253
H	0.000000	0.000000	-1.211309

Product

Total SCF energy: -538.1652367 a.u.

Atom	X	Y	Z
C	0.00000	0.761891	0.000000
H	-0.778510	1.515601	0.000000
C	1.295696	1.032604	0.000000
H	1.625491	2.065719	0.000000
H	2.046190	0.249777	0.000000
Cl	-0.627491	-0.858710	0.000000

a

Total SCF energy: -1707.10273686 a.u.

Atom	X	Y	Z
C	-2.695697	-2.620831	0.000005
C	-2.546705	1.135417	0.000020
C	-2.137786	-0.225598	0.000015
C	-3.111460	-1.259383	-0.000000
C	-0.773514	-0.547328	0.000025
C	-0.347715	-1.905646	0.000027
C	0.211746	0.478974	0.000036
C	-0.211504	1.821259	0.000038
C	1.579039	0.138354	0.000047
C	2.043024	-1.205822	0.000049
H	0.539149	2.609316	0.000051
H	2.325413	0.931934	0.000053
C	-4.903439	0.427627	-0.000023
C	-4.493694	-0.935235	-0.000021
C	-1.567097	2.167520	0.000032
C	-3.927288	1.463383	0.000011
C	-5.460530	-1.967202	-0.000032
O	3.281079	-1.544786	0.000069
Cl	6.512817	1.476615	-0.000079
Au	4.834755	-0.106207	-0.000005
C	-4.330021	2.819343	0.000013

C	-2.004248	3.532500	0.000055
H	-1.253155	4.317346	0.000065
C	-3.698989	-3.645809	-0.000005
H	-3.379023	-4.683885	-0.000002
C	-1.328180	-2.916073	0.000018
H	-1.010927	-3.956925	0.000019
C	1.030596	-2.203295	0.000037
H	1.358754	-3.239799	0.000035
C	-6.275841	0.751500	-0.000035
C	-6.836412	-1.616845	-0.000067
H	-7.577621	-2.410729	-0.000082
C	-7.229070	-0.303491	-0.000009
H	-8.285873	-0.050983	-0.000014
C	-6.656594	2.122120	-0.000037
H	-7.714918	2.368316	-0.000046
C	-5.718070	3.120791	-0.000005
H	-6.026743	4.161983	0.000010
C	-3.330340	3.843205	0.000015
H	-3.652093	4.880379	0.000007
C	-5.023544	-3.330459	-0.000021
H	-5.775108	-4.114593	-0.000035

b

Total SCF eergy: -2167.91127343 a.u.

Atom	X	Y	Z
C	-3.136298	-2.640976	-0.035785
C	-3.112395	1.117961	0.029327
C	-2.658672	-0.228129	-0.003824
C	-3.597014	-1.294006	-0.002596
C	-1.284504	-0.503990	-0.037926
C	-0.814445	-1.847077	-0.071892
C	-0.334462	0.554526	-0.039897
C	-0.802140	1.881750	-0.006100
C	1.043044	0.259074	-0.075729
C	1.548869	-1.067322	-0.112383
H	-0.078433	2.694494	-0.007169
H	1.762107	1.077294	-0.076590
C	-5.443569	0.331750	0.063141
C	-4.988835	-1.016382	0.030758
C	-2.167684	2.182418	0.028131
C	-4.502761	1.399499	0.062605
C	-5.920789	-2.080250	0.031489
O	2.798006	-1.369582	-0.148272
Cl	5.978043	1.716052	-0.168718
C	-4.950402	2.740983	0.094968
C	-2.650202	3.531928	0.061972

H	-1.925969	4.341530	0.061329
C	-4.104857	-3.698957	-0.033751
H	-3.750752	-4.725557	-0.058557
C	-1.760659	-2.890344	-0.069305
H	-1.408933	-3.919743	-0.094330
C	0.571932	-2.098769	-0.107200
H	0.935074	-3.123174	-0.132703
C	-6.825701	0.609644	0.095172
C	-7.307132	-1.775993	0.064086
H	-8.021599	-2.593874	0.064303
C	-7.743065	-0.476581	0.094763
H	-8.807456	-0.259621	0.119303
C	-7.251819	1.966363	0.126708
H	-8.317522	2.176799	0.151104
C	-6.347138	2.995877	0.126736
H	-6.689920	4.026004	0.150899
C	-3.985506	3.797758	0.094137
H	-4.341545	4.823332	0.119391
C	-5.438767	-3.428033	-0.001338
H	-6.163701	-4.236735	-0.000103
Au	4.313587	0.090318	-0.156627
Cl	8.140739	-0.922249	0.779997
H	7.421797	0.109831	0.433499

c

Total SCF energy: -2245.23561727 a.u.

Atom	X	Y	Z
C	-3.46920700	-2.61790100	0.01201200
C	-3.40082600	1.14076800	0.00120100
C	-2.96350300	-0.21123400	-0.00323800
C	-3.91434200	-1.26546700	0.01652700
C	-1.59258900	-0.50409100	-0.02693600
C	-1.13744300	-1.85241000	-0.03199100
C	-0.63085400	0.54343800	-0.04649000
C	-1.08192600	1.87700000	-0.04196200
C	0.74264300	0.23269100	-0.06954200
C	1.23515300	-1.09969500	-0.07465500
H	-0.34785500	2.68029000	-0.05725400
H	1.47179400	1.04219600	-0.08409100
C	-5.74129500	0.38322600	0.04419000
C	-5.30287000	-0.97058600	0.04029600
C	-2.44367700	2.19412300	-0.01867300
C	-4.78773100	1.43947700	0.02472300
C	-6.24749400	-2.02289100	0.06026300
O	2.48557900	-1.40459000	-0.09477600
Cl	5.47653600	1.92498900	-0.11133900
C	-5.21913100	2.78673000	0.02888200
C	-2.90976800	3.54972100	-0.01406000

H	-2.17563500	4.35020900	-0.02967200
C	-4.45058300	-3.66395900	0.03298800
H	-4.10900600	-4.69509900	0.03012800
C	-2.09615200	-2.88391300	-0.01211500
H	-1.75717100	-3.91789500	-0.01539800
C	0.24745400	-2.11938300	-0.05573700
H	0.59582100	-3.14924800	-0.05930800
C	-7.12008300	0.67820300	0.06698100
C	-7.63018400	-1.70156600	0.08330200
H	-8.35444800	-2.51068700	0.09880100
C	-8.05051800	-0.39666100	0.08633600
H	-9.11226800	-0.16654300	0.10383200
C	-7.52975000	2.04036900	0.07020800
H	-8.59289200	2.26406200	0.08765400
C	-6.61279100	3.05883300	0.05207300
H	-6.94333300	4.09322600	0.05499300
C	-4.24182500	3.83192800	0.00895100
H	-4.58576200	4.86190200	0.01222700
C	-5.78128900	-3.37661000	0.05631100
H	-6.51574100	-4.17655800	0.07264800
Au	3.99629100	0.11060100	-0.09781400
C	5.21977400	-2.69783500	-0.03762200
H	4.19785800	-3.00566300	-0.10952100
C	6.34897400	-2.28493200	0.04923700
H	7.33978700	-1.88900600	0.13079900
Cl	8.59721500	0.49634600	0.47395200
H	7.41446000	1.03115100	0.27650700

c-*x*

Total SCF energy: -2245.23050243 a.u.

Atom	X	Y	Z
Au	4.065328	-0.500141	-0.000097
Cl	5.637019	-2.214633	0.000147
Cl	5.581017	2.605565	-0.000055
H	6.653668	1.877088	0.000177
C	8.210351	0.186780	0.000367
H	7.574449	-0.682790	0.000555
C	8.904476	1.172950	0.000199
H	9.526808	2.040255	0.000054
C	-2.590663	-2.242848	0.000050
C	-3.796270	1.316914	0.000052
C	-2.926838	0.193372	0.000050
C	-3.466372	-1.121278	0.000043
C	-1.538135	0.381485	0.000043
C	-0.654328	-0.734266	0.000025
C	-0.985161	1.693466	0.000049
C	-1.862438	2.794254	0.000077
C	0.412885	1.860069	0.000004
C	1.327160	0.771472	-0.000089
H	-1.445944	3.799564	0.000102

H	0.838707	2.860451	0.000029
C	-5.743490	-0.188025	0.000011
C	-4.872222	-1.313611	0.000026
C	-3.251165	2.632089	0.000075
C	-5.202929	1.128652	0.000030
C	-5.405377	-2.623709	0.000011
O	2.587260	1.006425	-0.000182
C	-6.065123	2.250017	0.000014
C	-4.149330	3.749694	0.000076
H	-3.729925	4.751760	0.000107
C	-3.159337	-3.558971	0.000048
H	-2.488919	-4.413540	0.000064
C	-1.207415	-2.028756	0.000042
H	-0.537852	-2.886461	0.000042
C	0.740507	-0.523578	-0.000024
H	1.410481	-1.382504	-0.000020
C	-7.140566	-0.377231	-0.000022
C	-6.815890	-2.789260	-0.000021
H	-7.223067	-3.796045	-0.000033
C	-7.653052	-1.704307	-0.000038
H	-8.730187	-1.847010	-0.000065
C	-7.986902	0.765474	-0.000041
H	-9.063176	0.616123	-0.000070
C	-7.468258	2.034524	-0.000024
H	-8.128937	2.896305	-0.000040
C	-5.498216	3.564637	0.000041
H	-6.170034	4.417782	0.000035
C	-4.509561	-3.739386	0.000027
H	-4.929720	-4.740854	0.000023

e

Total SCF nergy: -2245.25203907 a.u.

Atom	X	Y	Z
Au	4.410570	-0.030612	0.010416
Cl	5.359121	-0.975884	-1.892003
Cl	3.401142	0.975379	1.879505
H	6.085242	1.433844	2.221569
C	6.005088	1.160393	0.116775
H	6.440870	1.342127	-0.860805
C	6.519869	1.622298	1.246498
H	7.421778	2.230448	1.205056
C	-3.189546	-2.621878	0.182014
C	-3.121868	1.116563	-0.197060
C	-2.684318	-0.230402	-0.079789
C	-3.634849	-1.276010	0.065181
C	-1.315246	-0.526909	-0.107568
C	-0.859125	-1.869521	0.015083
C	-0.353627	0.510526	-0.259975
C	-0.803948	1.836819	-0.376882
C	1.020397	0.196529	-0.286469

C	1.516117	-1.127848	-0.132593
H	-0.070291	2.632740	-0.486401
H	1.736893	1.002759	-0.417411
C	-5.461246	0.372038	-0.020537
C	-5.022719	-0.977196	0.093520
C	-2.165942	2.159615	-0.344427
C	-4.508202	1.419668	-0.164976
C	-5.966277	-2.020586	0.236764
O	2.759856	-1.438807	-0.133066
C	-4.939281	2.761771	-0.276742
C	-2.631606	3.510002	-0.455150
H	-1.897840	4.303118	-0.565770
C	-4.169068	-3.658732	0.325217
H	-3.826658	-4.685889	0.413514
C	-1.815193	-2.891187	0.155560
H	-1.475392	-3.920782	0.248145
C	0.526866	-2.137314	0.002527
H	0.879333	-3.160973	0.101212
C	-6.838813	0.671157	0.010171
C	-7.348577	-1.694975	0.263610
H	-8.072494	-2.497007	0.373679
C	-7.768765	-0.395072	0.154200
H	-8.829710	-0.161505	0.176691
C	-7.248214	2.028534	-0.103710
H	-8.310600	2.255367	-0.079193
C	-6.332293	3.038285	-0.241572
H	-6.662767	4.069324	-0.326287
C	-3.962746	3.797259	-0.421615
H	-4.306487	4.824028	-0.504989
C	-5.499706	-3.368556	0.350998
H	-6.233185	-4.161850	0.460834

g

Total SCF energy: -2245.28397497 a.u.

Atom	X	Y	Z
C	3.199624	-2.807646	-0.016322
C	2.761278	0.926764	0.009098
C	2.460242	-0.463136	-0.001983
C	3.510016	-1.417795	-0.004755
C	1.125612	-0.890145	-0.011563
C	0.804040	-2.277011	-0.024959
C	0.066545	0.058031	-0.009733
C	0.379438	1.431018	0.004501
C	-1.269398	-0.385148	-0.023320
C	-1.629381	-1.760334	-0.037374
H	-0.432657	2.156718	0.002812
H	-2.068291	0.355254	-0.017910
C	5.165486	0.403357	0.013059
C	4.862803	-0.987617	0.003059
C	1.704673	1.880028	0.011560

C	4.111694	1.360479	0.015800
C	5.906475	-1.941450	-0.000183
O	-2.843454	-2.189336	-0.049035
Cl	-6.221864	0.673321	0.003749
Au	-4.470585	-0.845315	-0.029856
C	4.407469	2.744408	0.024320
C	2.032841	3.275288	0.019163
H	1.219548	3.995881	0.017795
C	4.279660	-3.751489	-0.018632
H	4.041585	-4.811287	-0.027126
C	1.859552	-3.208359	-0.026264
H	1.625123	-4.270873	-0.035959
C	-0.548515	-2.678885	-0.037115
H	-0.795722	-3.737550	-0.046912
C	6.508322	0.832435	0.019492
C	7.250472	-1.485454	0.006825
H	8.051739	-2.218656	0.004164
C	7.540304	-0.145180	0.016290
H	8.574206	0.189068	0.021160
C	6.781215	2.229149	0.028312
H	7.817038	2.557442	0.032910
C	5.768489	3.152125	0.030507
H	5.994823	4.214268	0.036732
C	3.331494	3.687491	0.025373
H	3.571649	4.746553	0.030156
C	5.575582	-3.334862	-0.010768
H	6.385906	-4.057987	-0.012949
C	-3.258020	2.434585	1.395043
H	-3.984191	1.726190	1.783703
H	-2.453984	2.779246	2.038002
C	-3.407709	2.860327	0.149071
H	-4.211846	2.541204	-0.506276
Cl	-2.313010	4.013928	-0.583773

TS-d

Imaginary frequency: -891.7139 cm^{-1}

Total SCF energy: -2245.1766815 a.u.

Atom	X	Y	Z
Au	-4.397228	0.016524	0.032144
Cl	-3.638383	2.287486	0.333292
Cl	-6.118441	-1.745904	-0.229792
H	-7.205411	-0.464930	-0.089553
C	-6.778869	1.491459	0.179335
H	-6.009812	2.240649	0.297405
C	-7.722598	0.685039	0.049453
H	-8.802852	0.696897	0.025233
C	3.391340	-2.671233	0.040905
C	3.268288	1.081944	-0.079780
C	2.850494	-0.277245	-0.050437
C	3.818065	-1.315476	0.011263

C	1.486836	-0.591062	-0.082148
C	1.045574	-1.945746	-0.048589
C	0.508293	0.441107	-0.145598
C	0.937144	1.779349	-0.174206
C	-0.860766	0.114278	-0.175624
C	-1.353114	-1.227935	-0.122051
H	0.187385	2.567593	-0.217863
H	-1.591076	0.919616	-0.225782
C	5.620957	0.361196	0.014443
C	5.202166	-0.999157	0.043400
C	2.296499	2.118426	-0.141250
C	4.650998	1.402115	-0.046608
C	6.161417	-2.035483	0.105530
O	-2.587277	-1.520805	-0.128035
C	5.062106	2.754815	-0.073452
C	2.742035	3.479232	-0.167308
H	1.995682	4.267182	-0.214429
C	4.386711	-3.700506	0.103741
H	4.059961	-4.736381	0.126718
C	2.019064	-2.958014	0.010409
H	1.696738	-3.997161	0.035164
C	-0.337693	-2.231568	-0.070922
H	-0.669707	-3.266820	-0.044149
C	6.994639	0.677327	0.046477
C	7.539726	-1.692308	0.136972
H	8.275224	-2.490171	0.185530
C	7.941099	-0.382543	0.108010
H	8.999000	-0.135578	0.132458
C	7.383838	2.045519	0.017575
H	8.443372	2.285587	0.042423
C	6.452218	3.048260	-0.039529
H	6.766930	4.087588	-0.059947
C	4.069961	3.783168	-0.134506
H	4.398189	4.818249	-0.154329
C	5.714028	-3.394115	0.134892
H	6.458890	-4.183198	0.184159

TS-f

Imaginary frequency: -388.3319 cm^{-1}

Total SCF energy: -2245.2121255 a.u.

Atom	X	Y	Z
C	3.242399	-2.656753	0.010838
C	3.146435	1.090860	-0.238045
C	2.721310	-0.265238	-0.193762
C	3.676921	-1.304452	-0.035533
C	1.360700	-0.576047	-0.307653
C	0.913149	-1.926840	-0.255827
C	0.396786	0.457105	-0.478681
C	0.831814	1.791585	-0.515071
C	-0.968087	0.129383	-0.599289

C	-1.464105	-1.204496	-0.495205
H	0.091183	2.581151	-0.623538
H	-1.687059	0.926976	-0.759758
C	5.484197	0.365990	0.031128
C	5.057719	-0.991530	0.074909
C	2.186372	2.128313	-0.394120
C	4.525636	1.407807	-0.123127
C	6.005922	-2.028394	0.230019
O	-2.708643	-1.494801	-0.561862
C	4.944275	2.757860	-0.162128
C	2.638712	3.486697	-0.425283
H	1.900488	4.275191	-0.539084
C	4.225809	-3.686533	0.169930
H	3.892669	-4.719966	0.206295
C	1.872746	-2.939751	-0.098815
H	1.543011	-3.975969	-0.057314
C	-0.471057	-2.206701	-0.346798
H	-0.812496	-3.237835	-0.297629
C	6.854448	0.678778	0.142061
C	7.381214	-1.688554	0.338142
H	8.108645	-2.486228	0.457187
C	7.790026	-0.381636	0.295190
H	8.845439	-0.137311	0.379912
C	7.251387	2.044185	0.098641
H	8.308340	2.281288	0.185515
C	6.330573	3.047966	-0.047134
H	6.651158	4.085247	-0.076266
C	3.963095	3.787290	-0.314508
H	4.296806	4.820487	-0.339234
C	5.550483	-3.383607	0.274056
H	6.286721	-4.172828	0.394864
Au	-4.335003	-0.080888	0.136364
Cl	-2.976102	1.328980	1.599233
Cl	-6.534705	-0.927013	-0.590696
H	-6.014988	1.975757	-1.592876
C	-6.194405	0.965670	0.267108
H	-6.550796	0.900759	1.287860
C	-6.310951	2.010428	-0.550452
H	-6.702182	2.942063	-0.152495

A

Total SCF energy: -2627.4822261 a.u.

Atom	X	Y	Z
C	-3.154785	-2.618262	0.084480
C	-3.058599	1.137617	-0.077205
C	-2.631809	-0.216072	-0.020961
C	-3.589320	-1.262993	0.028116
C	-1.262047	-0.518579	-0.014904
C	-0.820143	-1.869109	0.039565
C	-0.294114	0.520524	-0.065522

C	-0.734093	1.856290	-0.119257
C	1.079052	0.200206	-0.063772
C	1.544860	-1.132428	-0.009170
H	0.006062	2.653106	-0.155067
H	1.803461	1.010130	-0.104835
C	-5.404339	0.397263	-0.036399
C	-4.975861	-0.958398	0.020485
C	-2.093691	2.183051	-0.126185
C	-4.443516	1.445872	-0.084922
C	-5.928136	-2.003080	0.069926
O	2.796103	-1.486082	-0.014320
Cl	6.004331	1.431986	0.098667
C	-4.865377	2.794984	-0.140988
C	-2.550212	3.540805	-0.182298
H	-1.810420	4.335231	-0.219944
C	-4.143757	-3.656413	0.134591
H	-3.809069	-4.688846	0.178210
C	-1.784467	-2.894424	0.089242
H	-1.451107	-3.929246	0.131729
C	0.562190	-2.146210	0.044701
H	0.911256	-3.174460	0.088266
C	-6.781249	0.701783	-0.044745
C	-7.308417	-1.672219	0.061076
H	-8.038632	-2.475129	0.100025
C	-7.719263	-0.365319	0.005172
H	-8.779512	-0.127866	-0.001298
C	-7.181367	2.065551	-0.102044
H	-8.243062	2.296533	-0.108561
C	-6.257283	3.076710	-0.148036
H	-6.580908	4.112387	-0.190851
C	-3.880460	3.832160	-0.189487
H	-4.217301	4.863586	-0.232225
C	-5.472152	-3.359274	0.127559
H	-6.212769	-4.152637	0.166734
Au	4.282998	-0.073571	0.032227
Cl	3.701923	0.398550	2.246036
Cl	4.681185	-0.507139	-2.212803

B

Total SCF energy: -3088.2869115 a.u.

Atom	X	Y	Z
C	-3.456485	2.650883	-0.067969
C	-3.526672	-1.107450	0.057244
C	-3.040335	0.226456	0.016320
C	-3.950470	1.315177	-0.025927
C	-1.658433	0.468481	0.019612
C	-1.158386	1.799096	-0.019615
C	-0.737060	-0.612241	0.064912
C	-1.236210	-1.928034	0.101444
C	0.649240	-0.351095	0.075620

C	1.169127	0.960336	0.039051
H	-0.532191	-2.757073	0.131526
H	1.338715	-1.190969	0.111414
C	-5.837156	-0.263780	0.016932
C	-5.348862	1.072155	-0.025295
C	-2.608717	-2.194939	0.098670
C	-4.923839	-1.354254	0.057344
C	-6.253951	2.158627	-0.066114
O	2.434090	1.270232	0.059839
Cl	5.564604	-1.734251	-0.043292
C	-5.405451	-2.683867	0.098662
C	-3.125581	-3.531882	0.138531
H	-2.422035	-4.358786	0.169237
C	-4.398223	3.732245	-0.110865
H	-4.018137	4.749203	-0.144124
C	-2.076069	2.866780	-0.064687
H	-1.697217	3.886197	-0.096429
C	0.233563	2.016656	-0.013603
H	0.627813	3.028838	-0.046070
C	-7.226155	-0.507267	0.018852
C	-7.647342	1.888845	-0.063013
H	-8.341435	2.723370	-0.093940
C	-8.115836	0.600802	-0.021741
H	-9.185528	0.410141	-0.019736
C	-7.686506	-1.852447	0.061284
H	-8.757334	-2.036482	0.062722
C	-6.808193	-2.903964	0.099429
H	-7.176924	-3.924820	0.131146
C	-4.467447	-3.763979	0.138772
H	-4.849422	-4.779990	0.169851
C	-5.738373	3.494021	-0.109526
H	-6.443261	4.319459	-0.141952
Au	3.873321	-0.171883	0.014477
Cl	3.273705	-0.645477	-2.192435
Cl	4.297210	0.259094	2.255105
Cl	7.179122	1.526027	-0.307012
H	6.921888	0.283931	-0.052242

C

Total SCF energy: -3165.6139139 a.u.

Atom	X	Y	Z
C	3.734642	2.637589	0.020206
C	3.793774	-1.122155	-0.060056
C	3.311692	0.213139	-0.011285
C	4.224197	1.300494	-0.029544
C	1.931761	0.457635	0.051621
C	1.435940	1.789707	0.098103
C	1.007574	-0.621655	0.065982
C	1.502855	-1.938779	0.022238
C	-0.377366	-0.358202	0.118748

C	-0.893795	0.955143	0.158103
H	0.797137	-2.766799	0.037658
H	-1.069782	-1.196532	0.130176
C	6.104377	-0.282314	-0.148986
C	5.620473	1.054967	-0.098619
C	2.873504	-2.208217	-0.040559
C	5.188783	-1.371468	-0.128660
C	6.527725	2.140142	-0.118919
O	-2.157030	1.266247	0.193954
Cl	-5.261787	-1.773511	0.208901
C	5.665994	-2.702413	-0.178593
C	3.386025	-3.546501	-0.089746
H	2.680903	-4.372476	-0.073305
C	4.678642	3.717662	0.000044
H	4.301872	4.735679	0.038447
C	2.356145	2.856005	0.083259
H	1.980617	3.876517	0.119400
C	0.045642	2.009919	0.153729
H	-0.345163	3.023360	0.189307
C	7.491114	-0.528319	-0.219160
C	7.918743	1.867840	-0.190016
H	8.614387	2.701494	-0.205883
C	8.383014	0.578489	-0.238540
H	9.450990	0.385955	-0.293173
C	7.947082	-1.874833	-0.268513
H	9.016217	-2.060763	-0.322901
C	7.066681	-2.925060	-0.248837
H	7.432084	-3.946907	-0.286847
C	4.725843	-3.781100	-0.156473
H	5.104458	-4.798138	-0.194297
C	6.016623	3.477012	-0.067114
H	6.723130	4.301565	-0.083097
Au	-3.596373	-0.182992	0.205044
Cl	-3.037264	-0.663119	2.429431
Cl	-3.942247	0.218587	-2.062907
C	-5.702527	2.195737	0.442780
H	-5.954987	2.399019	-0.576446
C	-5.417259	1.937224	1.585116
H	-5.149890	1.678021	2.586990
Cl	-7.688788	0.172720	-1.788779
H	-6.688156	-0.429270	-1.226971

C-*x*

Total SCF energy: -3165.6116633 a.u.

Atom	X	Y	Z
C	-3.592657	2.643111	0.162435
C	-3.854052	-1.108130	0.136310
C	-3.301925	0.199918	0.189503
C	-4.151878	1.334927	0.110750
C	-1.915611	0.370465	0.315107

C	-1.350645	1.674625	0.364758
C	-1.053437	-0.758199	0.386460
C	-1.617287	-2.046408	0.334774
C	0.339757	-0.566602	0.500726
C	0.925233	0.718851	0.527850
H	-0.958982	-2.911278	0.382590
H	0.989717	-1.435882	0.558811
C	-6.108484	-0.145202	-0.077918
C	-5.554432	1.164582	-0.023481
C	-2.996935	-2.242178	0.211806
C	-5.256067	-1.282157	0.002880
C	-6.398152	2.296833	-0.105838
O	2.201311	0.953588	0.640086
Cl	5.320583	-1.824771	-0.549093
C	-5.803080	-2.585610	-0.052389
C	-3.579474	-3.551049	0.153608
H	-2.922176	-4.413899	0.209388
C	-4.472442	3.772117	0.078877
H	-4.042093	4.768623	0.119463
C	-2.207549	2.787363	0.288745
H	-1.778611	3.786641	0.324688
C	0.048901	1.820440	0.464255
H	0.493514	2.811862	0.487701
C	-7.501240	-0.316337	-0.214867
C	-7.797209	2.099427	-0.242987
H	-8.444119	2.969401	-0.305474
C	-8.329173	0.837004	-0.295370
H	-9.402101	0.701271	-0.400978
C	-8.027797	-1.636698	-0.267663
H	-9.101588	-1.765640	-0.373030
C	-7.208901	-2.732827	-0.188499
H	-7.627471	-3.733974	-0.231106
C	-4.925689	-3.713312	0.027604
H	-5.357101	-4.708882	-0.017388
C	-5.817284	3.604094	-0.049797
H	-6.475420	4.465563	-0.112786
Au	3.635422	-0.397650	0.073487
Cl	2.466283	-0.842593	-1.902481
Cl	4.688030	-0.003859	2.114481
Cl	5.110297	2.225276	-1.312658
H	6.195015	1.719850	-0.809678
C	8.473621	1.300085	-0.280580
H	9.099757	1.916140	-0.887144
C	7.774603	0.596524	0.404648
H	7.130245	-0.016944	1.004280

G

Total SCF energy: -3165.6580369 a.u.

Atom	X	Y	Z
C	-3.076684	-2.384250	-0.549076
C	-3.776051	1.282656	-0.082397
C	-3.077417	0.066890	-0.312363
C	-3.781015	-1.167429	-0.325075
C	-1.689755	0.084956	-0.522835
C	-0.982080	-1.129538	-0.747096
C	-0.975942	1.316417	-0.504703
C	-1.683460	2.509338	-0.272609
C	0.421922	1.310970	-0.707642
C	1.134826	0.118671	-0.941484
H	-1.135865	3.449185	-0.252623
H	0.991934	2.235892	-0.683610
C	-5.885187	0.030383	0.115331
C	-5.184174	-1.187274	-0.111727
C	-3.066283	2.516518	-0.062887
C	-5.179374	1.266023	0.130726
C	-5.882324	-2.417498	-0.123207
O	2.427200	0.149895	-1.178838
C	-5.872909	2.477598	0.360310
C	-3.794870	3.728363	0.173714
H	-3.248015	4.666640	0.189257
C	-3.810043	-3.615919	-0.554208
H	-3.267699	-4.541520	-0.723893
C	-1.694034	-2.341872	-0.754940
H	-1.151045	-3.269631	-0.922810
C	0.414479	-1.089942	-0.953441
H	0.977700	-2.007919	-1.115643
C	-7.279077	0.012109	0.327708
C	-7.285607	-2.410284	0.092418
H	-7.820728	-3.355163	0.083564
C	-7.959182	-1.236543	0.309576
H	-9.033182	-1.246801	0.473835
C	-7.954399	1.242954	0.554182
H	-9.028472	1.225183	0.717340
C	-7.276457	2.434030	0.570217
H	-7.807206	3.364954	0.745878
C	-5.141338	3.707481	0.375613
H	-5.684345	4.630670	0.554685
C	-5.156236	-3.629634	-0.350175
H	-5.703895	-4.567283	-0.354754
Au	3.575852	-0.432736	0.419045
C	6.243044	0.227311	-1.150422
H	6.643141	-0.482357	-0.432292
C	5.944836	1.456716	-0.750300
H	6.065317	1.813264	0.266712
Cl	5.277595	2.658595	-1.815507
H	6.074342	-0.106564	-2.168877

Cl	4.922784	-1.044539	2.184263
Cl	3.086274	1.626850	1.425847
Cl	3.833752	-2.528954	-0.585770

TS-D

Imaginary frequency: -661.8275 cm^{-1}

Total SCF energy: -3165.57156817 a.u.

Atom	X	Y	Z
C	2.683036	2.335684	-0.586511
C	3.702074	-1.258632	-0.144492
C	2.906441	-0.109623	-0.400516
C	3.485008	1.187350	-0.340289
C	1.545555	-0.254769	-0.709828
C	0.745288	0.892773	-0.968502
C	0.955952	-1.548715	-0.767097
C	1.753731	-2.670901	-0.509378
C	-0.424081	-1.668452	-1.073332
C	-1.225361	-0.549731	-1.321503
H	1.300840	-3.659460	-0.545474
H	-0.892041	-2.647379	-1.119519
C	5.662389	0.184496	0.221904
C	4.862885	1.335482	-0.029443
C	3.115951	-2.552236	-0.198677
C	5.080293	-1.113370	0.165949
C	5.436431	2.626433	0.033785
O	-2.498029	-0.675532	-1.653263
Cl	-5.552499	-0.437028	1.442312
C	5.869877	-2.257625	0.422370
C	3.938837	-3.693407	0.067976
H	3.485623	-4.679796	0.028570
C	3.289285	3.630863	-0.509983
H	2.669912	4.503990	-0.693667
C	1.326789	2.165802	-0.893537
H	0.700596	3.039393	-1.060671
C	-0.626286	0.725918	-1.270253
H	-1.249937	1.586598	-1.490464
C	7.030763	0.330145	0.529516
C	6.817190	2.747464	0.344960
H	7.256401	3.739541	0.393938
C	7.585868	1.638700	0.582562
H	8.640684	1.747401	0.819892
C	7.805684	-0.836004	0.780407
H	8.859663	-0.719256	1.017402
C	7.245907	-2.085349	0.730182
H	7.850697	-2.965365	0.928580
C	5.260843	-3.550198	0.365424
H	5.876108	-4.421812	0.568419
C	4.612001	3.768436	-0.214083
H	5.063339	4.754568	-0.157334
Au	-3.860855	-0.513324	-0.131527

Cl	-3.082223	-2.503646	0.748383
Cl	-4.567556	1.548096	-1.103132
Cl	-1.813463	1.678287	1.247893
H	-3.276106	2.455469	1.403060
C	-4.372521	3.057212	1.650941
H	-4.304753	3.606945	2.580394
C	-5.313880	2.853304	0.855376
H	-6.257396	2.772674	0.357240

TS-D2

Imaginary frequency: -554.5577 cm^{-1}

Total SCF energy: -3165.54265057 a.u.

Atom	X	Y	Z
Au	3.900819	-0.284024	0.124367
Cl	4.294400	1.751497	1.286939
Cl	3.690836	-2.348615	-0.907053
Cl	5.628168	0.383703	-1.456557
H	6.635824	0.785102	-0.201299
C	7.475196	0.966976	0.760537
H	8.469540	0.692596	0.439852
C	6.885867	1.372945	1.774102
H	6.448790	1.710092	2.690583
Cl	2.441732	-0.984497	1.766879
C	-2.887793	-2.221595	-0.282507
C	-4.070407	1.344195	-0.215568
C	-3.214449	0.214853	-0.329300
C	-3.747700	-1.095054	-0.175325
C	-1.851431	0.390693	-0.590611
C	-0.980786	-0.732902	-0.700277
C	-1.300339	1.696711	-0.747833
C	-2.161749	2.798981	-0.629004
C	0.078465	1.849125	-1.007062
C	0.992986	0.756206	-1.129952
H	-1.752040	3.800601	-0.743416
H	0.493102	2.848212	-1.120095
C	-5.988319	-0.143313	0.198888
C	-5.131513	-1.275356	0.086717
C	-3.531338	2.650195	-0.366415
C	-5.454227	1.168231	0.048712
C	-5.656990	-2.579514	0.236449
O	2.222158	0.919451	-1.361540
C	-6.300135	2.295031	0.162112
C	-4.411573	3.773334	-0.245049
H	-3.996805	4.770822	-0.360089
C	-3.447183	-3.530432	-0.123525
H	-2.786543	-4.389117	-0.203701
C	-1.524040	-2.018690	-0.539893
H	-0.862920	-2.879947	-0.614167
C	0.390046	-0.537867	-0.965124
H	1.044231	-1.404479	-1.045779

C	-7.362183	-0.320224	0.460200
C	-7.045609	-2.732651	0.497030
H	-7.447767	-3.735136	0.611266
C	-7.867592	-1.642274	0.605381
H	-8.927289	-1.775947	0.805637
C	-8.193709	0.828858	0.568790
H	-9.252351	0.687910	0.769419
C	-7.681521	2.091377	0.425494
H	-8.329890	2.958739	0.510601
C	-5.739636	3.601840	0.008365
H	-6.398113	4.461097	0.097420
C	-4.776691	-3.700688	0.123872
H	-5.190959	-4.697665	0.242336

B-*i*

Total SCF energy: -2704.80599944 a.u.

Atom	X	Y	Z
C	3.325889	2.634933	-0.009897
C	3.366778	-1.124896	0.040089
C	2.890855	0.213578	0.027781
C	3.809701	1.295472	0.002950
C	1.511334	0.466351	0.041269
C	1.020377	1.801064	0.029650
C	0.581189	-0.607807	0.069007
C	1.069661	-1.927512	0.078511
C	-0.802877	-0.337138	0.087811
C	-1.317511	0.979455	0.075335
H	0.358881	-2.751186	0.095437
H	-1.498486	-1.172414	0.110396
C	5.684130	-0.299096	0.004927
C	5.206372	1.041306	-0.008084
C	2.440496	-2.205330	0.064529
C	4.762034	-1.382853	0.028411
C	6.119827	2.120894	-0.031963
O	-2.578189	1.289491	0.098375
Cl	-5.671182	-1.763930	0.005373
C	5.232856	-2.716738	0.040609
C	2.946381	-3.546614	0.075321
H	2.236157	-4.368207	0.093130
C	4.276018	3.709199	-0.035171
H	3.904075	4.729680	-0.045642
C	1.946344	2.861288	0.003043
H	1.575963	3.884279	-0.006896
C	-0.370855	2.028319	0.042907
H	-0.756317	3.044380	0.031303
C	7.071127	-0.553683	-0.005214
C	7.511215	1.839948	-0.041628
H	8.211689	2.669571	-0.059721
C	7.969584	0.547827	-0.028521
H	9.037706	0.348661	-0.036000

C	7.520675	-1.903223	0.007994
H	8.590006	-2.095727	0.000216
C	6.634047	-2.947986	0.029773
H	6.994523	-3.972249	0.039307
C	4.286442	-3.789669	0.063916
H	4.660179	-4.809177	0.072587
C	5.614453	3.460612	-0.045573
H	6.325513	4.281233	-0.064713
Au	-4.027357	-0.167846	0.053361
Cl	-4.418967	0.236358	2.313430
Cl	-3.435362	-0.626725	-2.170831
C	-5.796884	2.007714	-1.392398
H	-5.569911	1.748216	-2.403933
C	-6.030969	2.263257	-0.238433
H	-6.221661	2.457887	0.794777

C-***i***

Total SCF energy: -3165.5917844 a.u.

Atom	X	Y	Z
C	-3.71444	-2.64077	-0.02057
C	-3.52006	1.09838	-0.33169
C	-3.1375	-0.2713	-0.31646
C	-4.1052	-1.27412	-0.03917
C	-1.80914	-0.6308	-0.57418
C	-1.40531	-1.99731	-0.55567
C	-0.83241	0.36591	-0.85874
C	-1.22601	1.71536	-0.86337
C	0.49782	-0.0122	-1.1243
C	0.95656	-1.36837	-1.08785
H	-0.47717	2.47863	-1.06606
H	1.2304	0.75689	-1.36273
C	-5.83742	0.45867	0.20134
C	-5.45392	-0.91223	0.21799
C	-2.54788	2.10013	-0.60426
C	-4.86707	1.46437	-0.07223
C	-6.41363	-1.91383	0.49068
O	2.17141	-1.6774	-1.29028
Cl	2.57501	1.19259	1.35971
C	-5.24271	2.82767	-0.08588
C	-2.956	3.47328	-0.60604
H	-2.20868	4.23519	-0.80838
C	-4.7085	-3.63409	0.25983
H	-4.40834	-4.67811	0.27388
C	-2.37685	-2.97328	-0.2762
H	-2.08064	-4.02022	-0.25645
C	-0.05574	-2.3318	-0.80576
H	0.24794	-3.37573	-0.78012
C	-7.17583	0.82017	0.45759
C	-7.75636	-1.52526	0.74414
H	-8.49258	-2.29635	0.95184

C	-8.12367	-0.20539	0.72798
H	-9.15445	0.07624	0.92544
C	-7.52962	2.19806	0.43776
H	-8.5618	2.47284	0.63766
C	-6.59753	3.16726	0.17556
H	-6.88404	4.21486	0.16604
C	-4.2499	3.82077	-0.35828
H	-4.54938	4.86473	-0.36197
C	-6.00254	-3.28408	0.50337
H	-6.74781	-4.04594	0.71269
Au	3.89335	-0.16424	0.01993
Cl	4.02284	-1.7349	1.72991
Cl	3.90117	1.4979	-1.63526
C	5.83411	-1.03841	-0.9931
H	6.70208	-0.48478	-0.69229
C	4.91136	-1.72386	-1.40611
H	4.08396	-2.31509	-1.76673
Cl	6.2131	2.08931	1.55604
H	4.92062	2.11016	1.57961

E-*i*

Total SCF energy: -3165.66253771 a.u.

Atom	X	Y	Z
C	-2.270990	2.027632	0.378410
C	-3.845997	-1.356710	-0.079771
C	-2.865827	-0.344446	0.087541
C	-3.258264	1.015849	0.215158
C	-1.506021	-0.685465	0.122365
C	-0.518002	0.322642	0.288846
C	-1.094631	-2.038960	-0.015422
C	-2.079580	-3.029027	-0.177163
C	0.286232	-2.346569	-0.011521
C	1.281927	-1.364835	0.127994
H	-1.771772	-4.067105	-0.284763
H	0.611501	-3.376062	-0.135686
C	-5.617994	0.348756	0.006934
C	-4.633165	1.363546	0.173120
C	-3.443292	-2.715197	-0.211488
C	-5.223295	-1.012411	-0.119505
C	-5.020850	2.718595	0.293749
O	2.537512	-1.729833	0.110902
C	-6.198342	-2.022247	-0.288763
C	-4.454836	-3.717626	-0.380961
H	-4.145231	-4.753935	-0.481992
C	-2.692245	3.391792	0.495287
H	-1.932503	4.158660	0.613787
C	-0.919680	1.664873	0.415718
H	-0.155416	2.432206	0.523139
C	0.845321	-0.031841	0.310285
H	1.581383	0.752655	0.466651

C	-6.984696	0.692910	-0.035900
C	-6.404244	3.040122	0.248437
H	-6.701872	4.080387	0.341086
C	-7.350496	2.062205	0.090050
H	-8.404576	2.324132	0.057312
C	-7.946925	-0.339743	-0.205108
H	-8.999296	-0.071186	-0.237270
C	-7.568065	-1.651769	-0.327641
H	-8.316291	-2.427881	-0.458202
C	-5.774239	-3.383607	-0.417570
H	-6.531643	-4.150753	-0.548201
C	-4.013654	3.721322	0.454951
H	-4.324992	4.757919	0.542770
Au	4.012420	-0.369410	-0.336075
C	5.023313	-1.015462	1.248677
H	5.998184	-1.442981	1.035040
C	4.584033	-0.935994	2.492398
H	5.152032	-1.308433	3.338284
Cl	3.070365	-0.219631	2.967250
Cl	2.312261	3.323714	-0.450507
H	2.562965	2.341425	-1.294257
Cl	5.792547	1.017417	-0.766630
Cl	2.712079	0.437497	-2.273032

E-*i*2

Total SCF energy: -3165.65493537 a.u.

Atom	X	Y	Z
C	3.313836	2.558547	-0.193500
C	3.583509	-1.192240	-0.192834
C	3.029066	0.115178	-0.228119
C	3.877267	1.252175	-0.162182
C	1.640032	0.283627	-0.323240
C	1.071415	1.585653	-0.347555
C	0.780850	-0.846614	-0.389656
C	1.345034	-2.133941	-0.355939
C	-0.616737	-0.658110	-0.464028
C	-1.202102	0.624264	-0.432732
H	0.685713	-2.998638	-0.389074
H	-1.259566	-1.529959	-0.532103
C	5.840082	-0.225134	-0.020779
C	5.282825	1.083997	-0.059586
C	2.727332	-2.327706	-0.255617
C	4.988435	-1.363862	-0.086969
C	6.125676	2.217589	0.008987
O	-2.498479	0.849163	-0.452824
C	5.538404	-2.666293	-0.043348
C	3.312839	-3.635393	-0.207978
H	2.655919	-4.499246	-0.250132

C	4.192414	3.688810	-0.123814
H	3.758972	4.684526	-0.147296
C	1.924536	2.700107	-0.285529
H	1.490965	3.697885	-0.298072
C	-0.333128	1.728029	-0.408161
H	-0.772040	2.722037	-0.414129
C	7.235638	-0.394008	0.087636
C	7.528014	2.022211	0.115233
H	8.174418	2.893266	0.166883
C	8.063131	0.760864	0.153334
H	9.138212	0.626728	0.236659
C	7.765234	-1.713544	0.128878
H	8.841073	-1.840648	0.213566
C	6.946891	-2.811042	0.065586
H	7.367800	-3.811531	0.100378
C	4.661504	-3.795331	-0.106549
H	5.095164	-4.790226	-0.068170
C	5.540662	3.523255	-0.027677
H	6.197791	4.386172	0.025173
Au	-3.888176	-0.638775	-0.030307
C	-4.928924	-0.056775	-1.630926
H	-5.064878	-0.807015	-2.403740
C	-5.454893	1.148658	-1.767163
H	-6.008368	1.449330	-2.650795
Cl	-5.360323	2.399416	-0.565317
Cl	-2.622964	3.064473	1.738905
H	-2.801786	2.110446	0.859080
Cl	-5.520749	-2.214242	0.288465
Cl	-2.555888	-1.335589	1.884653

TS-**D**-***i***

Imaginary frequency: -322.1096 cm^{-1}

Total SCF energy: -3165.5677853 a.u.

Atom	X	Y	Z
C	-2.639166	2.082683	-0.301219
C	-4.305661	-1.273213	-0.002341
C	-3.295290	-0.282551	-0.132302
C	-3.652867	1.093788	-0.170345
C	-1.951001	-0.659708	-0.224992
C	-0.929618	0.324008	-0.361213
C	-1.572633	-2.033516	-0.191283
C	-2.587005	-2.997313	-0.060924
C	-0.208944	-2.385918	-0.284040
C	0.851966	-1.438191	-0.417820
H	-2.312288	-4.050003	-0.033718
H	0.070558	-3.436768	-0.258939
C	-6.028696	0.484011	0.048187
C	-5.016391	1.477605	-0.079967
C	-3.940670	-2.646570	0.034122
C	-5.670495	-0.893329	0.087665

C	-5.367362	2.847061	-0.118409
O	2.067217	-1.781345	-0.496544
C	-6.671824	-1.882988	0.216228
C	-4.976797	-3.627523	0.166174
H	-4.696406	-4.676764	0.194617
C	-3.023827	3.462051	-0.335389
H	-2.246407	4.214166	-0.434396
C	-1.300227	1.680085	-0.395380
H	-0.521029	2.433417	-0.495245
C	0.418317	-0.070356	-0.460616
H	1.178533	0.698213	-0.582057
C	-7.383536	0.863092	0.134922
C	-6.739735	3.204556	-0.028418
H	-7.007722	4.256710	-0.057790
C	-7.711842	2.246954	0.092772
H	-8.757137	2.536482	0.159458
C	-8.373198	-0.150572	0.262783
H	-9.416543	0.145736	0.329205
C	-8.030010	-1.476535	0.303068
H	-8.797607	-2.238426	0.402885
C	-6.285876	-3.260073	0.253704
H	-7.062486	-4.012633	0.354382
C	-4.333798	3.827229	-0.247371
H	-4.615157	4.875877	-0.274235
Au	3.972306	-0.124299	0.068700
Cl	5.328178	-0.845622	-1.771359
Cl	2.861335	0.518347	2.011170
C	5.271482	-2.452718	0.155733
H	5.933371	-3.027032	-0.457190
C	4.508927	-1.954766	1.004623
H	4.029354	-2.088549	1.960821
Cl	3.554403	1.975463	-0.924645
Cl	6.718507	1.968795	0.910770
H	5.684515	2.307539	0.208615

TS-F-*i*

Imaginary frequency: -156.4655 cm^{-1}

Total SCF nergy: -3165.60721213 a.u.

Atom	X	Y	Z
C	-2.349216	2.187071	-0.110622
C	-3.762991	-1.285093	0.252265
C	-2.836502	-0.213404	0.200556
C	-3.284510	1.114023	-0.050827
C	-1.470071	-0.462205	0.394719
C	-0.540313	0.610017	0.341368
C	-0.997417	-1.782786	0.633661
C	-1.930464	-2.833134	0.676109
C	0.393221	-2.001428	0.804216
C	1.312894	-0.947005	0.773233
H	-1.577076	-3.846795	0.853413

H	0.774442	-3.007438	0.957867
C	-5.600304	0.290640	-0.190148
C	-4.666905	1.364915	-0.247245
C	-3.299848	-2.610054	0.494169
C	-5.147656	-1.035515	0.059001
C	-5.114371	2.683728	-0.500737
O	2.599127	-1.169729	0.991113
C	-6.071116	-2.104492	0.112658
C	-4.260621	-3.674197	0.541654
H	-3.905713	-4.684244	0.725527
C	-2.830853	3.510790	-0.372113
H	-2.109617	4.321358	-0.420310
C	-0.989348	1.920867	0.087234
H	-0.247614	2.720087	0.043873
C	0.826037	0.355052	0.544930
H	1.519251	1.198250	0.504646
C	-6.974498	0.539554	-0.384841
C	-6.504460	2.908627	-0.693089
H	-6.847045	3.920534	-0.887991
C	-7.400410	1.874262	-0.636589
H	-8.460049	2.062554	-0.786471
C	-7.884256	-0.550435	-0.324195
H	-8.942409	-0.354371	-0.474333
C	-7.449042	-1.828522	-0.083673
H	-8.158305	-2.649817	-0.041498
C	-5.587399	-3.429901	0.360286
H	-6.305991	-4.243302	0.399303
C	-4.160050	3.746835	-0.558458
H	-4.517483	4.752904	-0.756598
Au	3.875035	-0.430627	-0.425334
C	4.711178	1.106409	0.871362
H	5.709697	1.294323	0.485245
C	4.668605	0.857164	2.212993
H	5.559561	0.791211	2.832967
Cl	3.240296	0.750949	3.114188
Cl	2.591268	3.201122	0.212528
H	3.855286	1.861505	0.512385
Cl	5.389394	0.287448	-2.006032
Cl	3.010594	-2.041288	-1.880849

TS-F-*i*2

Imaginary frequency: -1020.5056 cm^{-1}

Total SCF energy: -3165.58068371 a.u.

Atom	X	Y	Z
C	3.035865	-2.450306	0.541272
C	3.672615	1.240125	0.230677
C	2.995654	0.005310	0.426873
C	3.718508	-1.217423	0.357609
C	1.619600	-0.007311	0.681596
C	0.928643	-1.238724	0.874732

C	0.879366	1.208930	0.746877
C	1.562858	2.416217	0.540826
C	-0.508779	1.170828	1.009530
C	-1.237918	-0.033523	1.229956
H	1.004610	3.349536	0.577756
H	-1.070835	2.101278	1.035736
C	5.794889	0.031509	-0.084534
C	5.115899	-1.206145	0.103811
C	2.942548	2.457300	0.287905
C	5.069773	1.255648	-0.022657
C	5.830385	-2.424176	0.036105
O	-2.485732	-0.052267	1.466031
C	5.738426	2.486075	-0.215703
C	3.644905	3.688223	0.084249
H	3.083762	4.617621	0.124521
C	3.784531	-3.668645	0.463265
H	3.259307	-4.609659	0.600343
C	1.655936	-2.435886	0.791876
H	1.132170	-3.380377	0.924320
C	-0.458643	-1.228675	1.132862
H	-0.986257	-2.171039	1.256791
C	7.182173	0.044767	-0.334976
C	7.228224	-2.385102	-0.216752
H	7.775198	-3.322117	-0.268196
C	7.879899	-1.193480	-0.395017
H	8.949019	-1.179772	-0.589055
C	7.833712	1.295622	-0.522159
H	8.903030	1.301604	-0.715373
C	7.137597	2.473856	-0.465198
H	7.648791	3.420810	-0.612507
C	4.986651	3.700910	-0.155636
H	5.508494	4.641186	-0.308231
C	5.125799	-3.654520	0.222370
H	5.684063	-4.584524	0.165942
Au	-3.792118	-0.097284	-0.693562
C	-5.353766	1.107382	-0.072402
H	-5.785336	1.696953	-0.877378
C	-5.633235	1.514853	1.189399
H	-6.309001	2.348721	1.370504
Cl	-5.110038	0.757714	2.609065
Cl	-5.592700	-1.749423	-0.022282
H	-5.888501	-0.164530	0.055421
Cl	-2.773340	1.779102	-1.618485
Cl	-2.199097	-1.592331	-1.584650

$C_2H_2Cl_2$

Total SCF energy: -997.761837371 a.u.

Atom	X	Y	Z
C	-0.366381	0.552102	0.000000
H	-1.449360	0.555599	0.000000

C 0.366381 -0.552102 0.000000

H 1.449360 -0.555599 0.000000

Cl -0.366381 -2.119400 0.000000

Cl 0.366381 2.119400 0.000000

G-*ii*

Total SCF nergy: -3165.6924576 a.u.

Atom X Y Z

C 3.577596 -2.728053 -0.357445

C 3.304806 1.011302 -0.078953

C 2.947440 -0.355205 -0.241365

C 3.945825 -1.362840 -0.194189

C 1.607146 -0.707803 -0.447638

C 1.227048 -2.069824 -0.607160

C 0.600916 0.294515 -0.502603

C 0.967857 1.643428 -0.339607

C -0.742024 -0.071844 -0.709661

C -1.162845 -1.423050 -0.842044

H 0.188652 2.403484 -0.376813

H -1.491928 0.716184 -0.763649

C 5.663857 0.358846 0.179652

C 5.304374 -1.008252 0.015080

C 2.299466 2.018241 -0.127454

C 4.661313 1.368966 0.132668

C 6.296833 -2.014366 0.061792

O -2.392560 -1.784789 -0.998484

Cl -5.345331 -1.843447 2.927994

C 5.014498 2.728771 0.298064

C 2.686462 3.387366 0.043627

H 1.915074 4.151254 0.005919

C 4.606278 -3.726233 -0.306221

H 4.324531 -4.767859 -0.431643

C 2.231663 -3.053832 -0.559240

H 1.953166 -4.098646 -0.681720

C -0.133783 -2.395218 -0.800341

H -0.426436 -3.435470 -0.920003

C 7.012222 0.712748 0.389890

C 7.647634 -1.633838 0.274587

H 8.409147 -2.407421 0.311839

C 7.992298 -0.316246 0.433078

H 9.030565 -0.040661 0.596818

C 7.342912 2.086916 0.553589

H 8.382949 2.355630 0.717518

C 6.379622 3.060285 0.510042

H 6.648947 4.104491 0.638443

C 3.990204 3.726251 0.247705

H 4.273714 4.766545 0.377015

C 5.908412 -3.382253 -0.105597

H 6.679154 -4.146585 -0.067230

Au -3.926649 -0.351335 -0.869565

Cl	-2.364917	1.147134	2.124597
Cl	-5.527712	1.348007	-0.647122
C	-3.201186	-0.287923	2.622340
H	-2.573122	-1.053836	3.060185
C	-4.510517	-0.406202	2.446913
H	-5.132694	0.353251	1.984593
Cl	-2.636498	3.332863	-0.816628
H	-3.768138	2.667974	-0.715096

TS-**F**-***ii***

Imaginary frequency: -386.259 cm^{-1}

Total SCF energy: -3165.6239912 a.u.

Atom	X	Y	Z
C	-2.710506	-2.279019	-0.541801
C	-3.732334	1.330320	-0.286762
C	-2.932694	0.171062	-0.470380
C	-3.517847	-1.120451	-0.371963
C	-1.564182	0.300448	-0.740467
C	-0.754877	-0.854749	-0.920265
C	-0.960084	1.585478	-0.821458
C	-1.764684	2.719901	-0.637129
C	0.434138	1.683638	-1.037237
C	1.267894	0.556285	-1.183645
H	-1.307644	3.705892	-0.691086
H	0.906357	2.662396	-1.070169
C	-5.708073	-0.091418	0.079612
C	-4.904249	-1.253159	-0.096894
C	-3.137394	2.618559	-0.373337
C	-5.119860	1.201541	-0.014218
C	-5.482963	-2.539392	0.005480
O	2.549840	0.690386	-1.349381
Cl	6.280719	-0.939562	0.403932
C	-5.913096	2.357191	0.168802
C	-3.965383	3.771951	-0.182273
H	-3.507748	4.755008	-0.247615
C	-3.322289	-3.569163	-0.425828
H	-2.699163	-4.450553	-0.547613
C	-1.345640	-2.124431	-0.813704
H	-0.718000	-3.006463	-0.923703
C	0.624299	-0.706134	-1.173857
H	1.233237	-1.590567	-1.335153
C	-7.085120	-0.221355	0.352687
C	-6.872686	-2.644753	0.280215
H	-7.315668	-3.633118	0.360304
C	-7.645251	-1.525603	0.446821
H	-8.706782	-1.622312	0.658113
C	-7.863530	0.955947	0.528746
H	-8.924570	0.851836	0.738785
C	-7.298362	2.201067	0.441188
H	-7.906267	3.090262	0.581329

C	-5.297062	3.645045	0.076204
H	-5.915506	4.526218	0.220491
C	-4.653797	-3.692345	-0.165426
H	-5.108634	-4.674554	-0.077419
Au	3.928326	-0.475467	-0.136883
Cl	2.350449	-1.973109	1.142852
C	5.627731	0.525075	-0.926120
H	5.862414	0.146448	-1.913433
C	5.779860	1.812825	-0.610401
H	6.075385	2.533909	-1.363529
Cl	5.535451	2.464789	0.965248
Cl	0.251711	0.467741	2.298634
H	1.092789	-0.479335	1.918610