

Supporting Information: Computational Part

Site-selective gold(I) catalyzed synthesis of 1,3-dioxin-3 ones via cascade reaction.

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Computational methods

Geometries of the molecules were optimized by using the M06 meta-hybrid functional¹ in combination with the Def2-SVP² basis set. This method was applied previously in related reactions.³ Solvent effects were calculated with the PCM continuum solvation model⁴ with *p*-xylene parameters. The nature of minimum and transition structure of all stationary points on the potential energy surface was confirmed by frequency analysis at the same level of theory. The wave function stability was confirmed in all stationary points.⁵ The thermochemical corrections have been combined with single point energies calculated at the DLPNO-CCSD(T)/def2-TZVPP//B3LYP-D3/6-31+G(d) level to yield the $G_{298,\text{sol}}$ at higher level of theory. All calculations were performed using the ultrafine grid implemented in Gaussian 09 E.01.⁶

¹ (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.(b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.

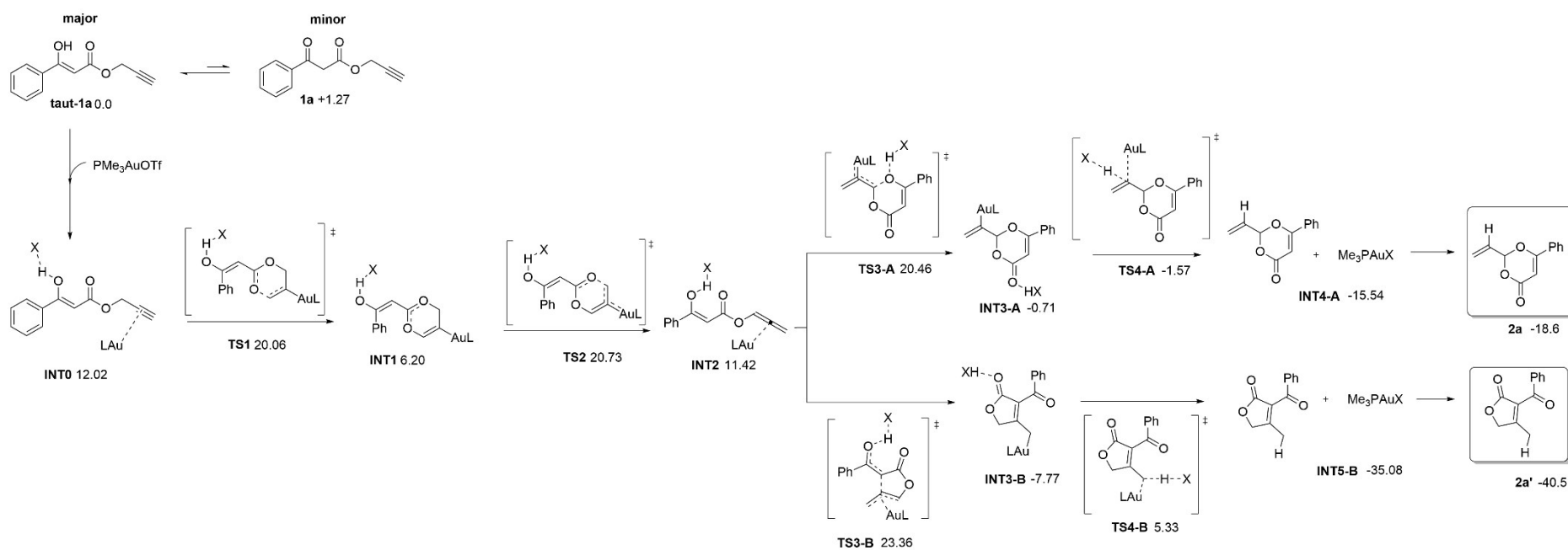
² Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

³ (a) Marin-Luna, M.; Bolaño, I; Silva, C.; Nieto, O. *Comput. Theor. Chem.* **2019**, *1148*, 33. (b) Virumbrales C.; Solas M.; S. Suárez-Pantiga S.; Fernández-Rodríguez M. A.; Marín-Luna M.; Silva López C.; Sanz R. *Org. Biomol. Chem.* **2019**, *17*, 9924. (c) Nieto Faza, O.; Silva Lopez, C. *Theor. Chem. Acc.*, **2011**, *128*, 647. (d) Nieto Faza, O.; Silva Lopez, C. Computational Approaches to Homogeneous Gold Catalysis, in *Homogeneous Gold Catalysis, Topics in Current Chemistry*, ed. L. M. Slaughter, Springer, Cham, 2015, p. 213.

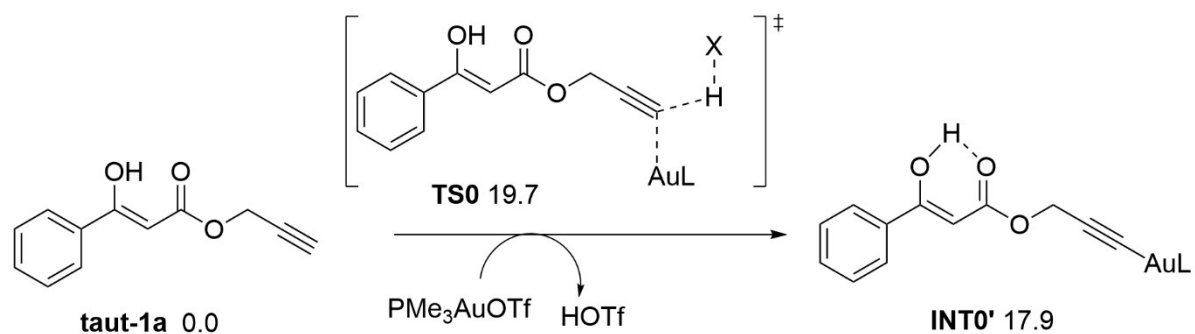
⁴ Tomasi, J.; Persico, M. *Chem. Rev.* **1994**, *94*, 2027.

⁵ Bauernschmitt, R.; Ahlrichs, R. *J. Chem. Phys.* **1996**, *104*, 9047.

⁶ Gaussian 09, Revision E.01, Frisch M. J., Trucks G. W., Schlegel H. B., Scuseria G. E. et al, Gaussian, Inc., Wallingford CT, 2013.

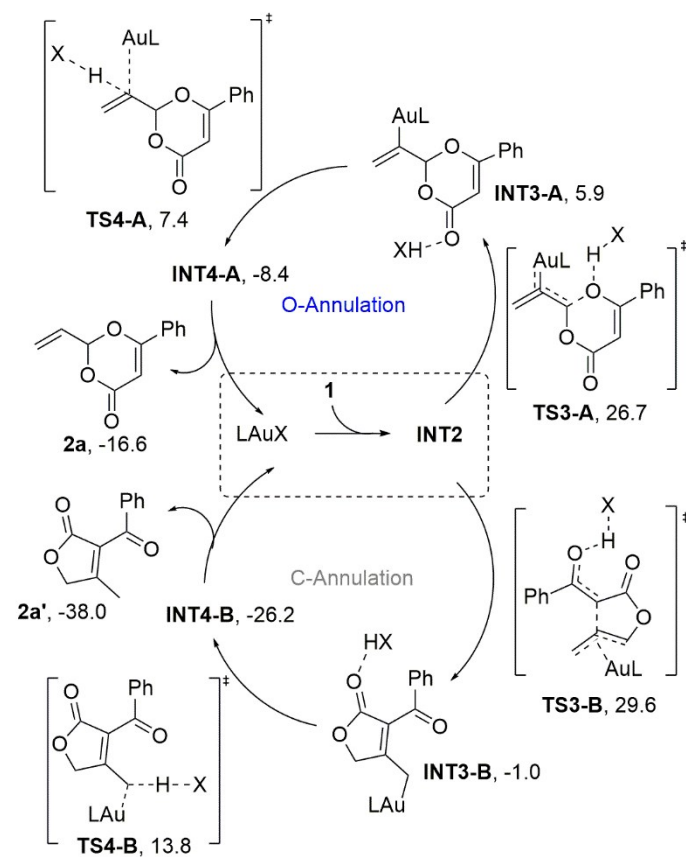
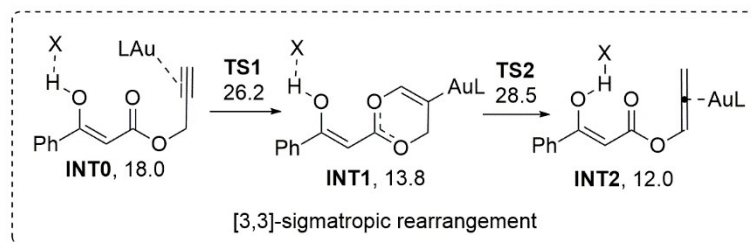


Scheme S1. Computed mechanism for the transformation of **1a** into **2** and **2a'** at the PCM(*p*-Xylene)/M06/def2-SVP theoretical level. Gibbs free energies are reported in kcal mol⁻¹ (1 atm and 298 K), relative to **taut-1a**. L refers to PMe₃ and X to OTf(-) anion.



Scheme S2. Computed mechanism for the transformation of **1a** into **INTO'** at the PCM(*p*-Xylene)/M06/def2-SVP theoretical level. Gibbs free energies are reported in kcal mol⁻¹ (1 atm and 298 K), relative to **taut-1a**. L refers to PMe₃ and X to OTf(-) anion.

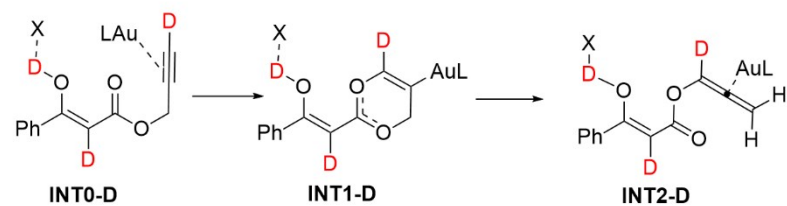
In order to validate the computational method here used, we performed single point energy calculations at a higher level of theory. The profile reaction computed at PCM(*p*-Xylene)/M06/def2-TZVP//PCM(*p*-Xylene)/M06/def2-SVP theoretical level is depicted in Scheme S3. As shown, these computational results provided the same conclusions that those we commented in the main text. The difference of the obtained relative energies by using both methods is insignificant and irrelevant from a kinetic point of view.



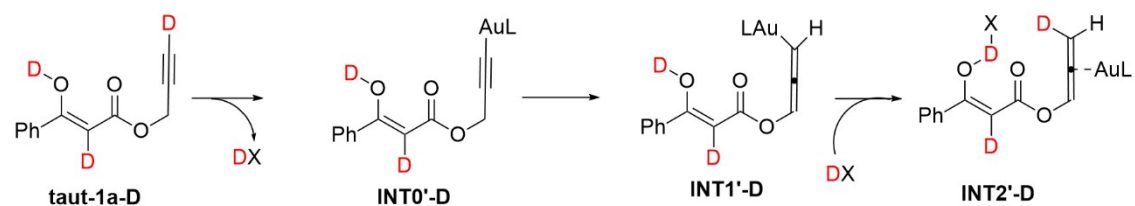
Scheme S3. Computed mechanism for the transformation of **1a** into **INT0'** at the PCM(*p*-Xylene)/M06/def2-TZVP//PCM(*p*-Xylene)/M06/def2-SVP theoretical level. Gibbs free energies are reported in kcal mol⁻¹ (1 atm and 298 K), relative to **taut-1a**. L refers to PMe₃ and X to OTf(-) anion.

The partial deuteration of the C_a-position could be explained via the transformations shown in Scheme S4 b and c.

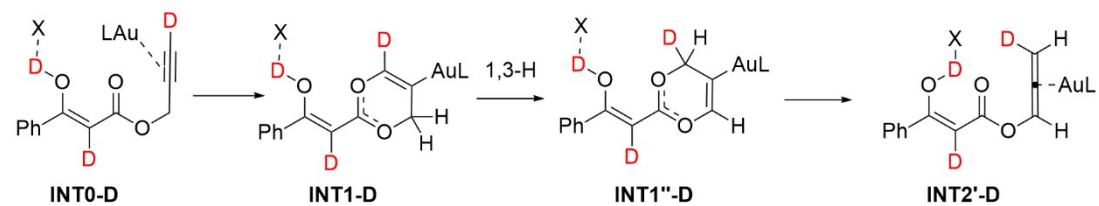
a) Proposed mechanism in this work



b) Participation of a propargylate/allenolate equilibria of INT0-D



c) Alternative involving a 1,3-H shift



Scheme S4. Alternative pathways for explaining deuterium-labelling results. L refers to PMe₃ and X to OTf(-) anion.

Computational data

Table S1. Imaginary number and value of frequencies, electronic ($E_{\text{SCF},298,\text{sol}}$), Gibbs free ($G_{298,\text{sol}}$), and enthalpies ($H_{298,\text{sol}}$) energies for systems shown in Scheme S1 and S2 (in Hartree) computed at PCM(DCM)/M06/def2-SVP level. Just the best conformer found is shown.

Filename	ImFreqs	$E_{\text{SCF},298,\text{sol}}$ PCM(<i>p</i> -Xylene)/ M06/def2-SVP	$G_{298,\text{sol}}$ PCM(<i>p</i> -Xylene)/ M06/def2-SVP	$H_{298,\text{sol}}$ PCM(<i>p</i> -Xylene)/ M06/def2-SVP	$G_{298,\text{sol}}$ PCM(<i>p</i> -Xylene)/M06/def2- TZVP//PCM(<i>p</i> - Xylene)/M06/def2-SVP
PMe₃AuOTf					
Pme3AuOTf	-	-1557.27802	-1557.18504	-1557.11715	-1558.312864
1a					
1a_01	-	-687.949353	-687.800691	-687.744237	-688.563650
1a_02	-	-687.947166	-687.800161	-687.74209	-688.563785
1a_03	-	-687.947065	-687.800006	-687.741898	-688.563445
1a_04	-	-687.936644	-687.788807	-687.731892	-688.551835
1a_05	-	-687.934829	-687.78768	-687.729982	-688.553719
taut-1a					
taut_1a_01	-	-687.952332	-687.802718	-687.746446	-688.563985
taut_1a_02	-	-687.952332	-687.802714	-687.746445	-688.563981
taut_1a_03	-	-687.95211	-687.802659	-687.746251	-688.564293
taut_1a_04	-	-687.95211	-687.802658	-687.746251	-688.564292
taut_1a_05	-	-687.945639	-687.796832	-687.739785	-688.558069
taut_1a_05	-	-687.944498	-687.794478	-687.738839	-688.556183
2a					
2a_01	-	-687.985575	-687.832458	-687.779338	-688.623391

2a_02	-	-687.985518	-687.832289	-687.77921	-688.624916
2a'					
2a'_01	-	-688.016682	-687.864624	-687.81035	-688.590727
2a'_02	-	-688.019659	-687.867288	-687.813352	-688.590808
TS0					
ts0_01	-666.45	-2245.218732	-2244.956398	-2244.855876	-2246.837636
INT0'					
Int0'_01	-	-1283.95991	-1283.72282	-1283.64111	-1284.746422
INT0					
int0_01	-	-2245.23785	-2244.9686	-2244.86974	-2246.848395
int0_02	-	-2245.23602	-2244.96399	-2244.86821	-2246.844747
int0_03	-	-2245.2216	-2244.95286	-2244.8536	-2246.839274
int0_04	-	-2245.21158	-2244.94802	-2244.84397	-2246.828372
int0_05	-	-2245.20006	-2244.9362	-2244.83357	-2246.828218
TS1					
ts1_01	-226.3	-2245.22452	-2244.95579	-2244.85714	-2246.835324
INT1					
int1_01	-	-2245.25226	-2244.97783	-2244.88229	-2246.854035
int1_02	-	-2245.24289	-2244.97302	-2244.87313	-2246.855136
int1_03	-	-2245.24724	-2244.97249	-2244.87741	-2246.849586
TS2					

ts2_01	-182.7	-2245.22595	-2244.95472	-2244.85948	-2246.831706
INT2					
int2_01	-	-2245.23913	-2244.96955	-2244.87181	-2246.849955
int2_02	-	-2245.22033	-2244.9557	-2244.85372	-2246.839163
int2_03	-	-2245.23201	-2244.96541	-2244.86427	-2246.849311
TS3-A					
ts3A_01	-342.47	-2245.21762	-2244.95514	-2244.85438	-2246.834304
TS3-B					
ts3b_01	-397.46	-2245.22147	-2244.95052	-2244.85633	-2246.830006
INT3-A					
Int3a_01	-	-2245.26281	-2244.98889	-2244.89417	-2246.863911
Int3a_02	-	-2245.25646	-2244.98762	-2244.88844	-2246.867718
Int3a_03	-	-2245.25467	-2244.98749	-2244.88648	-2246.867522
Int3a_04	-	-2245.25525	-2244.9861	-2244.88671	-2246.865886
Int3a_05	-	-2245.25387	-2244.98074	-2244.88488	-2246.856465
INT3-B					
int3b_01	-	-2245.27207	-2245.00013	-2244.90391	-2246.876854
int3b_02	-	-2245.26149	-2244.99737	-2244.89334	-2246.878753
int3b_03	-	-2245.26415	-2244.99655	-2244.89631	-2246.875193
TS4-A					
ts4a_01	-266.98	-2245.25947	-2244.99026	-2244.8956	-2246.865429

TS4-B					
ts4b_01	-1047.93	-2245.24178	-2244.97926	-2244.87935	-2246.855086
INT4-A					
Int4a_01	-	-2245.28623	-2245.01253	-2244.91679	-2246.890578
INT4-B					
Int4b_01	-	-2245.31418	-2245.04366	-2244.94513	-2246.918986

Cartesian Coordinates

Just the cartesian coordinates of the most stable conformer are shown.

PMe₃AuOTf

SCF = -1557.27801665

Num. Imaginary Freq = 0

				C	-3.655188	0.981227	-1.486329
				H	-3.446341	0.361615	-2.371003
				H	-4.739908	1.161541	-1.410572
				H	-3.130340	1.941090	-1.602832
Au	-0.818506	-0.273659	-0.009659	C	-4.088812	-1.352764	0.149842
P	-3.056630	0.137942	0.008778	H	-5.155586	-1.075295	0.154217
C	-3.580602	1.202066	1.386246	H	-3.889335	-2.024042	-0.698654
H	-4.667184	1.379766	1.337281	H	-3.845603	-1.885565	1.081202
H	-3.329403	0.719861	2.342578	S	2.140613	0.573622	-0.007302
H	-3.048278	2.163353	1.331953	O	2.085375	1.317363	-1.259550

O	2.050578	1.309339	1.247933
C	3.796067	-0.237634	0.012956
F	3.954067	-0.990869	-1.059787
F	4.729526	0.697804	0.022349
F	3.929240	-0.987788	1.091292
O	1.260210	-0.676704	-0.023003

1a

SCF = -687.949353105

Num. Imaginary Freq = 0

C	2.139651	0.879584	1.387975
C	1.129205	-0.059379	1.197950
C	1.091547	-0.825546	0.025498
C	2.079206	-0.636943	-0.950587
C	3.078273	0.309216	-0.765490
C	3.110320	1.067527	0.406457
H	2.166670	1.469467	2.308098
H	0.372030	-0.185576	1.977086
H	2.034803	-1.248794	-1.855720

H	3.840680	0.457837	-1.535284
H	3.900652	1.809157	0.555306
C	0.037604	-1.845958	-0.235583
C	-1.190335	-1.842038	0.664158
H	-1.866056	-2.620894	0.278607
H	-0.936853	-2.080737	1.708057
C	-1.895630	-0.513176	0.638547
O	0.132697	-2.643657	-1.141006
O	-2.233399	0.130304	1.594328
O	-2.081027	-0.122414	-0.633736
C	-2.557961	1.207819	-0.835726
H	-3.013072	1.214901	-1.837292
H	-3.340317	1.442774	-0.095238
C	-1.469565	2.170553	-0.752887
C	-0.548044	2.951844	-0.686036
H	0.269677	3.647003	-0.625973

taut-1a

SCF = -687.952332014

Num. Imaginary Freq = 0

C	-4.332268	0.795413	-0.320140
C	-2.988170	1.105834	-0.142119
C	-2.036294	0.088342	0.011328
C	-2.463616	-1.247341	-0.014113
C	-3.806939	-1.554771	-0.190438
C	-4.745829	-0.534569	-0.344850
H	-5.063345	1.599709	-0.440384
H	-2.658858	2.146770	-0.121586
H	-1.742949	-2.059517	0.110527
H	-4.125311	-2.600708	-0.205960
H	-5.802740	-0.779214	-0.483592
C	-0.619313	0.451330	0.195457
C	0.400898	-0.461635	0.273558
C	1.756735	-0.009833	0.449477
O	-0.399682	1.751995	0.276539
O	2.102861	1.164142	0.544347
O	2.644895	-1.014363	0.510781
C	4.013137	-0.650925	0.657302
H	4.112141	0.153856	1.405039

H	4.516576	-1.548049	1.048602
C	4.620365	-0.236116	-0.599647
C	5.133797	0.106041	-1.640429
H	5.587610	0.413053	-2.565124
H	0.578168	1.881702	0.392149
H	0.219107	-1.532426	0.194689

2a

SCF = -687.985574550

Num. Imaginary Freq = 0

C	-2.042546	-1.716569	-0.010909
C	-0.614257	-1.585234	0.244856
C	0.000999	-0.385002	0.081534
C	-2.061014	0.592033	0.414919
H	-0.050327	-2.504913	0.399356
O	-2.644485	-2.743758	-0.164469
C	1.447563	-0.149765	0.031257
C	1.950341	1.150497	0.180496
C	2.345028	-1.209906	-0.164870

C	3.321293	1.382108	0.144121
H	1.254918	1.979198	0.333231
C	3.713646	-0.974756	-0.197528
H	1.967566	-2.225509	-0.311932
C	4.205476	0.321592	-0.042686
H	3.703106	2.399554	0.264604
H	4.403117	-1.808540	-0.354645
H	5.283176	0.504894	-0.072537
O	-2.696025	-0.519424	-0.160916
O	-0.740831	0.729168	-0.058936
C	-2.855704	1.812408	0.109835
H	-3.916288	1.721467	0.370073
C	-2.360615	2.926317	-0.419728
H	-1.302379	3.011972	-0.684281
H	-1.992281	0.420618	1.514244
H	-3.001140	3.791030	-0.611337

2a'

SCF = -688.016681759

Num. Imaginary Freq = 0

C	2.983682	1.283375	0.035564
C	1.576280	1.074101	0.491522
C	1.212088	-0.172144	0.133773
C	2.360563	-0.823969	-0.544562
H	3.064891	2.130957	-0.670270
H	3.658725	1.500467	0.884113
C	0.836680	2.120631	1.233422
H	0.672184	3.005532	0.594441
H	-0.141079	1.769646	1.590441
H	1.424325	2.466668	2.099911
C	-0.020422	-0.939424	0.467182
C	-1.347297	-0.378653	0.093242
C	-2.492173	-0.974951	0.638749
C	-1.488986	0.685998	-0.805550
C	-3.754945	-0.501955	0.306985
H	-2.361222	-1.815532	1.325824
C	-2.755391	1.152978	-1.145575
H	-0.601104	1.140415	-1.256171
C	-3.887301	0.563273	-0.585712

H	-4.644901	-0.965889	0.741119
H	-2.860748	1.978393	-1.854910
H	-4.882091	0.933087	-0.850494
O	0.086430	-2.003284	1.041431
O	3.371054	0.089247	-0.597967
O	2.459310	-1.920875	-1.008244

TS0

SCF = -2245.21873229

Num. Imaginary Freq = 1

C	5.609158	-0.365122	3.116480
C	5.205084	-1.290419	2.160251
C	4.480579	-0.874350	1.033859
C	4.187980	0.487732	0.878778
C	4.587184	1.409834	1.838154
C	5.297013	0.984889	2.960797
H	6.169238	-0.701211	3.993821
H	5.439809	-2.350589	2.280079
H	3.665655	0.845939	-0.012011

H	4.326293	2.461939	1.695746
H	5.611033	1.710241	3.717116
C	4.029334	-1.876664	0.054859
C	3.083858	-1.613350	-0.913908
C	2.676889	-2.673600	-1.798440
O	4.579987	-3.064404	0.193455
O	3.140462	-3.809603	-1.767175
O	1.725501	-2.450756	-2.733659
C	1.077174	-1.204987	-2.857761
H	1.783886	-0.353344	-2.928325
H	0.530044	-1.236450	-3.814425
C	0.165071	-0.883114	-1.784422
C	-0.541428	-0.526737	-0.829734
P	-4.545773	-0.653992	1.046578
C	-4.535736	-1.172063	2.791708
H	-3.915163	-0.478564	3.378531
H	-5.561481	-1.176191	3.194835
H	-4.105212	-2.180842	2.877606
C	-5.401572	0.952812	1.051470
H	-5.523352	1.312026	0.018779

H	-6.392588	0.855821	1.524048
H	-4.801735	1.689247	1.606756
C	-5.713751	-1.791350	0.235745
H	-5.313307	-2.815794	0.261338
H	-6.688806	-1.767005	0.749091
H	-5.847916	-1.496758	-0.815856
Au	-2.424813	-0.592237	0.062752
H	2.643435	-0.617974	-0.957845
H	4.180300	-3.650806	-0.509393
H	0.024305	0.310358	-0.113888
O	0.656109	1.376672	0.566642
S	1.394685	2.287824	-0.382744
O	2.302960	3.209511	0.281718
O	1.876078	1.580104	-1.577457
C	0.027624	3.350835	-1.021756
F	-0.492479	4.067779	-0.041762
F	0.482515	4.163613	-1.956717
F	-0.928716	2.592290	-1.544064

INT0'

SCF = -1283.95990537

Num. Imaginary Freq = 0

C	4.916377	3.496366	0.026098
C	4.945809	2.162168	0.418687
C	3.915117	1.288664	0.046575
C	2.843093	1.784859	-0.709326
C	2.814629	3.119687	-1.096300
C	3.852695	3.978337	-0.734008
H	5.730862	4.165971	0.316527
H	5.775088	1.777554	1.016859
H	2.009202	1.128559	-0.976986
H	1.970336	3.495553	-1.681056
H	3.828348	5.027904	-1.041116
C	3.979025	-0.123426	0.466913
C	3.218793	-1.110185	-0.108834
C	3.302154	-2.461980	0.397845

O	4.835858	-0.366107	1.439536
O	4.056174	-2.786354	1.313394
O	2.544551	-3.428057	-0.134142
C	1.675771	-3.180968	-1.240979
H	2.257231	-2.745199	-2.075694
H	1.361925	-4.184042	-1.571890
C	0.520085	-2.357564	-0.922637
C	-0.432854	-1.631076	-0.662695
P	-3.816291	0.927390	0.416469
C	-5.453583	0.297095	-0.085274
H	-5.624541	-0.689476	0.371184
H	-6.250728	0.989323	0.231904
H	-5.485507	0.180742	-1.179081
C	-3.992058	1.205507	2.211272
H	-3.078614	1.677946	2.602934
H	-4.858570	1.853518	2.422306
H	-4.125445	0.239922	2.722054
C	-3.773181	2.613806	-0.280163
H	-3.766486	2.559184	-1.379252
H	-4.650235	3.193881	0.051022

H	-2.854427	3.124399	0.045547
Au	-1.997233	-0.447544	-0.179191
H	2.532307	-0.848350	-0.910654
H	4.771135	-1.345903	1.631080

INTO

SCF = -2245.23784696

Num. Imaginary Freq = 0

C	2.908642	2.078849	3.134274
C	1.703793	2.309801	2.477220
C	1.642908	2.307271	1.076947
C	2.818942	2.064163	0.351280
C	4.019785	1.822414	1.009343
C	4.069553	1.832316	2.404271
H	2.940365	2.089643	4.227423
H	0.786583	2.490224	3.042169
H	2.805333	2.085083	-0.742392
H	4.929406	1.643377	0.428895
H	5.017433	1.654790	2.920585

C	0.351703	2.577200	0.411862
C	0.145720	2.383788	-0.926415
C	-1.039468	2.872985	-1.615126
O	-0.586481	3.002242	1.235770
O	-1.762514	3.759706	-1.243529
O	-1.275646	2.311419	-2.854476
C	-1.375286	0.914209	-2.952991
H	-1.927749	0.476477	-2.101369
H	-1.964693	0.699743	-3.860964
C	-0.095721	0.211548	-3.110641
C	0.972293	-0.342399	-3.373266
H	1.857027	-0.720459	-3.864743
P	1.358188	-2.230812	0.700025
C	2.697990	-3.426673	0.385826
H	3.602970	-2.893804	0.057052
H	2.923827	-3.991953	1.304960
H	2.396595	-4.128562	-0.406259
C	1.935073	-1.234886	2.098931
H	1.127638	-0.539307	2.375268
H	2.176504	-1.894145	2.948896

H	2.827742	-0.657639	1.810069
C	-0.016230	-3.222090	1.349120
H	-0.419590	-3.874308	0.560679
H	0.331712	-3.831498	2.199084
H	-0.802720	-2.528864	1.678082
Au	0.781150	-1.035030	-1.232561
H	0.947028	1.962062	-1.533674
H	-1.469471	2.867777	0.827495
O	-2.554787	1.319035	0.309982
S	-2.107150	-0.032110	0.696428
O	-1.930102	-0.964750	-0.441976
O	-1.037339	-0.090490	1.706449
C	-3.574830	-0.726875	1.573199
F	-3.308983	-1.953550	2.007520
F	-4.613081	-0.785615	0.758436
F	-3.885652	0.028904	2.611497

TS1

SCF = -2245.22452409

Num. Imaginary Freq = 1

C	-0.402151	-1.283036	-2.006770	H	4.453852	0.914891	3.158335
C	0.425409	-1.994029	-0.990129	H	2.716631	1.022196	2.674163
C	0.168050	-2.991205	-0.276419	H	3.365438	-0.501492	3.370509
C	-2.379647	-2.107503	-0.924513	C	-3.635803	-1.711118	-0.349680
H	-0.423508	-1.909679	-2.916280	C	-4.091815	-0.428699	-0.168904
H	0.138868	-3.819106	0.415744	C	-5.438460	-0.168044	0.384597
O	-1.717226	-1.091134	-1.518607	C	-5.704303	1.070691	0.984730
O	-1.920765	-3.245059	-0.889839	C	-6.463159	-1.122592	0.318263
Au	2.181075	-1.274050	-0.003043	C	-6.958564	1.339411	1.522503
P	3.982584	-0.184463	1.044059	H	-4.909446	1.818367	1.030607
C	4.457201	1.332982	0.163914	C	-7.717358	-0.849591	0.851978
H	3.573157	1.985693	0.119824	H	-6.286743	-2.080357	-0.178960
H	5.281245	1.836981	0.694598	C	-7.967671	0.380674	1.459326
H	4.767501	1.090840	-0.863363	H	-7.149776	2.306895	1.995113
C	5.524617	-1.146023	1.195170	H	-8.509562	-1.600502	0.785871
H	5.342516	-2.053301	1.790595	H	-8.955034	0.593832	1.878889
H	5.873007	-1.449277	0.196389	O	-3.424130	0.676699	-0.415202
H	6.306562	-0.542059	1.683892	H	-0.010747	-0.286263	-2.245336
C	3.597945	0.364980	2.733724	H	-2.471309	0.550451	-0.630979
				H	-4.240394	-2.541141	0.017507

O	-0.789666	1.386587	-0.352673
S	0.630983	1.768796	-0.320249
O	1.278539	1.683817	1.000947
O	1.442612	1.243257	-1.438471
C	0.595261	3.582288	-0.652284
F	-0.106658	4.209317	0.276669
F	0.052215	3.825947	-1.833334
F	1.830677	4.068148	-0.647319

INT1

SCF = -2245.25226230

Num. Imaginary Freq = 0

C	0.246635	-1.924921	-1.388762
C	1.060352	-2.115698	-0.161449
C	0.420625	-2.548797	0.919480
C	-1.683616	-2.025790	0.052798
H	0.324942	-2.783356	-2.077892
H	0.808719	-2.738823	1.920436
O	-1.184477	-1.769340	-1.107820

O	-0.999044	-2.668829	0.952903
Au	2.812318	-1.005259	-0.004329
P	4.362512	0.756491	0.176509
C	6.147977	0.434575	0.379619
H	6.523940	-0.136613	-0.482520
H	6.703815	1.383638	0.456546
H	6.318583	-0.159964	1.289715
C	3.923296	1.839025	1.574523
H	4.567073	2.733748	1.595559
H	2.871052	2.135189	1.438752
H	4.020712	1.291987	2.524237
C	4.253183	1.868613	-1.262624
H	4.889617	2.757191	-1.117704
H	4.563441	1.339533	-2.176264
H	3.199130	2.173773	-1.363729
C	-3.012238	-1.672762	0.339965
C	-3.763393	-0.774730	-0.402010
C	-5.181689	-0.538387	-0.084501
C	-5.772172	0.675594	-0.465186
C	-5.956821	-1.497640	0.583422

C	-7.106666	0.928254	-0.170033
H	-5.164627	1.422369	-0.981593
C	-7.292635	-1.243987	0.869952
H	-5.519254	-2.461957	0.856622
C	-7.868686	-0.029679	0.497101
H	-7.556285	1.881323	-0.461223
H	-7.891711	-2.001699	1.381990
H	-8.919675	0.168892	0.725490
O	-3.323007	-0.048029	-1.390253
H	0.500755	-1.010752	-1.946238
H	-2.332228	0.077511	-1.458598
H	-3.414529	-2.065556	1.273794
O	-0.890390	1.001283	-1.533181
S	-0.314700	1.362894	-0.209569
O	1.066279	1.859916	-0.268280
O	-0.631037	0.400916	0.856457
C	-1.304748	2.846583	0.261713
F	-1.172750	3.805812	-0.639019
F	-2.589324	2.520950	0.348003
F	-0.908158	3.309515	1.436286

TS2

SCF = -2245.22594654

Num. Imaginary Freq = 1

C	0.678097	-2.322774	1.569333
C	1.066238	-2.274796	0.251408
C	0.375086	-2.621804	-0.849988
C	-1.766713	-2.264536	0.126814
H	0.674554	-1.413721	2.187278
H	0.800639	-2.685557	-1.856326
O	-1.447453	-2.438400	1.294994
O	-0.981152	-2.726783	-0.906083
Au	2.587444	-0.821908	-0.084987
P	4.018120	1.008289	-0.411892
C	4.373413	1.899918	1.132640
H	4.915553	1.245307	1.831202
H	4.978341	2.797496	0.923746
H	3.409550	2.188437	1.579011
C	3.257002	2.261704	-1.488570

H	3.916077	3.140153	-1.584164
H	3.063637	1.836865	-2.485064
H	2.301313	2.557748	-1.030579
C	5.652494	0.688284	-1.155334
H	6.215988	1.630390	-1.257425
H	6.222109	-0.007800	-0.521566
H	5.527876	0.231399	-2.148585
C	-2.941233	-1.607192	-0.348923
C	-3.690126	-0.757645	0.433969
C	-4.970570	-0.202164	-0.035216
C	-5.400323	1.034121	0.466530
C	-5.768909	-0.880273	-0.966377
C	-6.601699	1.585014	0.035245
H	-4.767450	1.560831	1.185245
C	-6.972366	-0.328917	-1.391079
H	-5.455459	-1.860039	-1.338972
C	-7.389670	0.905146	-0.892498
H	-6.925712	2.554117	0.424475
H	-7.594559	-0.869174	-2.109927
H	-8.336988	1.337431	-1.227413

O	-3.329667	-0.320836	1.617873
H	0.591291	-3.284399	2.090001
H	-3.202243	-1.740962	-1.399744
H	-2.347069	-0.356794	1.757738
O	-0.711182	0.249809	1.630703
S	-0.277040	1.582143	1.130864
O	1.184947	1.687945	0.968954
O	-0.956332	2.728890	1.722136
C	-0.893076	1.563111	-0.614370
F	-2.218992	1.565083	-0.633750
F	-0.468696	0.482250	-1.264137
F	-0.462740	2.632915	-1.267724

INT2

SCF = -2245.23913079

Num. Imaginary Freq = 0

C	0.570513	3.052470	0.974736
C	1.904789	2.538920	0.951265
C	2.475290	1.729377	-0.005481

C	-1.453396	2.838960	-0.187875	Au	-2.270800	0.485240	-0.060713
O	0.006333	3.608563	1.882025	P	-2.718571	-1.611543	0.916453
C	3.743638	1.018942	0.263480	C	-2.385244	-3.034098	-0.162569
C	4.594618	0.692217	-0.801077	H	-2.556678	-3.971657	0.390884
C	4.100835	0.629325	1.562159	H	-3.064988	-2.989011	-1.027127
C	5.779258	0.001939	-0.570748	H	-1.355112	-2.995039	-0.542234
H	4.328632	0.988038	-1.819419	C	-4.463795	-1.811849	1.402459
C	5.283147	-0.064025	1.789912	H	-4.619695	-2.802848	1.859381
H	3.424238	0.838731	2.395547	H	-4.740804	-1.029636	2.125052
C	6.125765	-0.378182	0.724039	H	-5.110570	-1.715113	0.517657
H	6.435526	-0.243493	-1.409900	C	-1.804381	-1.905958	2.462957
H	5.544053	-0.374028	2.805581	H	-2.034348	-2.912974	2.847892
H	7.053712	-0.928572	0.903478	H	-0.722645	-1.819749	2.292452
O	-0.133093	2.800740	-0.228085	H	-2.106475	-1.152758	3.206392
O	1.929567	1.576443	-1.185694	H	2.141413	0.695957	-1.613028
C	-2.202143	2.363839	-1.221608	H	2.459787	2.736265	1.869806
C	-2.812313	2.475698	-2.383599	O	2.155054	-0.850461	-2.097497
H	-2.813377	3.433136	-2.919129	S	1.034888	-1.673837	-1.575337
H	-1.901622	3.257015	0.728144	O	0.978617	-3.039077	-2.087564
H	-3.329024	1.635522	-2.857132	O	-0.249442	-0.957525	-1.477621

C	1.503471	-1.896615	0.208782
F	0.770739	-2.863707	0.759869
F	1.265625	-0.777813	0.896798
F	2.777518	-2.207859	0.345012

TS3-A

SCF = 5

Num. Imaginary Freq = 16.4893

C	0.470763	-2.856879	-1.679900
C	1.639666	-2.935231	-0.871071
C	2.135821	-1.935787	-0.049396
C	-0.456686	-1.057777	-0.427910
H	2.220523	-3.850600	-0.998209
O	0.002297	-3.631535	-2.457833
C	3.488737	-2.065131	0.537860
C	3.711481	-1.670571	1.863545
C	4.559124	-2.551308	-0.223427
C	4.978877	-1.780942	2.423940
H	2.878390	-1.286066	2.458905

C	5.828922	-2.645047	0.335450
H	4.394855	-2.823594	-1.270214
C	6.039385	-2.264247	1.659967
H	5.142604	-1.479546	3.462022
H	6.663776	-3.007199	-0.270594
H	7.039217	-2.337011	2.097072
O	-0.195793	-1.560106	-1.592040
O	1.458501	-0.878545	0.275583
C	-1.052468	0.244944	-0.368101
C	-0.366039	1.366638	-0.618633
H	0.718029	1.346458	-0.792194
H	-0.587380	-1.763978	0.408981
H	-0.846312	2.350422	-0.640213
Au	-3.105444	0.163371	0.039376
P	-5.426568	0.143736	0.496088
C	-6.121713	1.778174	0.908981
H	-7.203301	1.700823	1.106723
H	-5.616318	2.180867	1.799696
H	-5.954046	2.472826	0.072216
C	-5.910010	-0.910601	1.903536

H	-5.618999	-1.952489	1.701843
H	-5.389235	-0.575485	2.813105
H	-6.998928	-0.862124	2.067739
C	-6.470889	-0.446854	-0.877022
H	-7.534648	-0.433466	-0.588011
H	-6.323726	0.197750	-1.756593
H	-6.179741	-1.472734	-1.148462
H	2.128259	0.215332	0.632665
O	2.715454	1.111102	0.888610
S	3.847953	1.370706	-0.141141
O	5.162149	1.284964	0.461037
O	3.564060	0.712237	-1.407174
C	3.558630	3.173354	-0.421387
F	4.444228	3.608749	-1.296701
F	3.698397	3.837945	0.708242
F	2.343310	3.378289	-0.897572

TS3-B

SCF = -2245.22146594

Num. Imaginary Freq = 1

C	3.996689	-2.614470	0.829021
C	3.765691	-1.530856	-0.008098
C	3.406245	-0.283672	0.527112
C	3.316201	-0.142469	1.922396
C	3.544413	-1.230499	2.755645
C	3.878005	-2.469645	2.210202
H	4.273134	-3.580494	0.398841
H	3.864617	-1.656615	-1.087775
H	3.049872	0.822520	2.361899
H	3.460613	-1.111531	3.839109
H	4.054099	-3.325922	2.867291
C	3.118987	0.844034	-0.365986
C	3.090811	2.159263	0.084380
C	2.974651	3.254974	-0.906026
O	2.856943	0.630330	-1.628297
O	3.832419	4.003535	-1.261111
O	1.706451	3.396317	-1.416543
C	0.717319	2.770332	-0.737408
C	0.861424	2.067540	0.373985

C	0.393991	1.361816	1.464670
H	0.339325	1.906485	2.420879
P	-3.679377	0.012512	0.015441
C	-5.068653	1.192811	0.011025
H	-4.819871	2.052734	-0.628792
H	-5.982341	0.708673	-0.371241
H	-5.250091	1.559650	1.032365
C	-3.585835	-0.595924	-1.695773
H	-2.784745	-1.345296	-1.792623
H	-4.551942	-1.030855	-1.999625
H	-3.329716	0.241534	-2.362323
C	-4.299755	-1.402556	0.981296
H	-4.469105	-1.097649	2.024911
H	-5.244140	-1.773227	0.550034
H	-3.552676	-2.209660	0.967145
Au	-1.620836	0.840600	0.758630
H	0.749025	0.321602	1.567349
H	-0.268973	2.906131	-1.191360
H	3.582257	2.416550	1.025725
H	2.456329	-0.272490	-1.835992

O	1.647918	-1.622967	-2.144829
S	0.188835	-1.564222	-1.853490
O	-0.277201	-0.212464	-1.509828
O	-0.657604	-2.348899	-2.747983
C	0.067514	-2.485529	-0.252350
F	0.723449	-1.854001	0.716389
F	-1.209572	-2.581078	0.118099
F	0.564126	-3.702405	-0.366615

INT3-A

SCF = -2245.26281422

Num. Imaginary Freq = 0

C	1.776535	-1.429222	-0.932966
C	3.159551	-1.415341	-0.537380
C	3.741754	-0.218056	-0.232832
C	1.614215	0.605308	0.229111
H	3.732405	-2.334182	-0.654197
O	1.204134	-2.367555	-1.474362
C	5.178930	0.023330	-0.080402

C	5.625976	1.219151	0.500528	H	-5.432712	2.714506	-1.297286
C	6.120959	-0.925219	-0.506171	H	-4.175508	3.763675	-0.556381
C	6.986899	1.455196	0.659127	H	-3.870895	2.998800	-2.138380
H	4.894017	1.958977	0.832940	C	-4.622940	1.234715	1.187833
C	7.479236	-0.686072	-0.343561	H	-5.692558	1.167014	0.929010
H	5.789844	-1.850733	-0.984720	H	-4.322099	0.323538	1.725856
C	7.915066	0.504045	0.239922	H	-4.461262	2.099306	1.849263
H	7.326125	2.388651	1.116018	C	-4.126801	0.005204	-1.355162
H	8.205324	-1.429956	-0.681797	H	-5.217934	0.026078	-1.512206
H	8.985256	0.691277	0.364645	H	-3.614664	0.055103	-2.328109
O	1.093027	-0.289915	-0.745950	H	-3.848155	-0.945177	-0.874475
O	2.980972	0.866442	-0.064573	H	-0.310094	-2.233215	-1.472802
C	0.787311	1.841698	0.277128	O	-1.330856	-2.147365	-1.323834
C	1.388878	3.024576	0.463019	S	-1.852581	-3.189248	-0.280734
H	2.479757	3.131756	0.551404	O	-1.017888	-4.369421	-0.234731
H	1.599834	0.067825	1.204014	O	-3.294039	-3.262621	-0.385781
H	0.811176	3.953278	0.529678	C	-1.519070	-2.287919	1.302151
Au	-1.269472	1.608236	0.034462	F	-0.255904	-1.901319	1.347380
P	-3.607177	1.412802	-0.319749	F	-2.301012	-1.227363	1.401095
C	-4.348601	2.857736	-1.156922	F	-1.762060	-3.099375	2.308890

INT3-B

SCF = -2245.27206499

Num. Imaginary Freq = 0

C	5.308419	1.775370	1.921757
C	4.395493	2.344208	1.044446
C	3.188300	1.692597	0.752587
C	2.913150	0.459174	1.357629
C	3.830803	-0.111370	2.235045
C	5.026626	0.545332	2.518525
H	6.247552	2.289565	2.143564
H	4.593128	3.305131	0.561998
H	1.984018	-0.077120	1.137776
H	3.609741	-1.076550	2.699461
H	5.745733	0.095350	3.209059
C	2.263238	2.361380	-0.199504
C	0.987962	1.635638	-0.619992
C	-0.069282	2.622785	-1.033918
O	2.510073	3.445193	-0.682733

O	-0.683325	3.386841	-0.316223
O	-0.303248	2.513684	-2.331486
C	0.460472	1.440679	-2.829238
C	1.196801	0.830726	-1.888409
C	1.949501	-0.431619	-1.955301
H	2.941205	-0.356584	-1.475545
P	-0.808996	-2.917099	0.553411
C	-0.761625	-2.120625	2.199361
H	-0.893161	-1.033589	2.072979
H	-1.555298	-2.507878	2.859954
H	0.220657	-2.295429	2.666176
C	-2.556867	-2.742547	0.058238
H	-2.730069	-3.259610	-0.897498
H	-3.222097	-3.165628	0.829296
H	-2.787336	-1.675728	-0.081775
C	-0.636399	-4.696651	0.924582
H	0.363124	-4.894498	1.340055
H	-1.403042	-5.019778	1.648133
H	-0.745780	-5.279772	-0.002265
Au	0.739297	-1.798735	-0.858046

H 2.087624 -0.758999 -2.998664
H 0.287935 1.213244 -3.878813
H 0.562116 1.033757 0.201015
H -2.241441 3.212514 -0.489273
O -3.188285 2.840330 -0.526295
S -3.232004 1.303821 -0.225674
O -1.980412 0.646474 -0.573872
O -4.505841 0.780030 -0.650133
C -3.255977 1.307133 1.621835
F -2.110452 1.781006 2.072140
F -4.248953 2.036162 2.071554
F -3.402530 0.057649 2.028494

TS4-A

SCF = -2245.25947051

Num. Imaginary Freq = 1

C -3.017592 -2.796149 -0.940296
C -3.768066 -1.614494 -0.543911
C -3.122129 -0.435961 -0.330458

C -1.456176 -1.225422 -1.724833
H -4.812682 -1.758710 -0.268535
O -3.398877 -3.933520 -0.903649
C -3.651116 0.759493 0.330053
C -2.960419 1.975695 0.216821
C -4.833245 0.708505 1.083827
C -3.444471 3.116574 0.847166
H -2.044147 2.026858 -0.374726
C -5.316872 1.853183 1.704189
H -5.368732 -0.238031 1.200282
C -4.622531 3.058800 1.588996
H -2.889949 4.054044 0.752688
H -6.237840 1.804166 2.291518
H -5.002646 3.956791 2.084422
O -1.714010 -2.537070 -1.312752
O -1.847637 -0.302366 -0.734092
C -0.019902 -0.980334 -2.038896
C 0.843084 -2.002883 -2.319695
H 0.516346 -3.051111 -2.327614
H -2.065141 -1.008863 -2.633720

H	1.838884	-1.791507	-2.728034
Au	1.214113	-1.365043	-0.128103
P	1.901440	-1.004868	2.088417
C	3.140333	0.314366	2.253167
H	3.400383	0.459724	3.314316
H	4.046247	0.058802	1.683300
H	2.705367	1.237186	1.841461
C	2.601061	-2.432991	2.975307
H	3.514194	-2.777925	2.467690
H	2.846305	-2.151824	4.012503
H	1.874197	-3.258779	2.984536
C	0.491680	-0.453539	3.094467
H	0.818711	-0.232018	4.123545
H	0.077420	0.451328	2.623436
H	-0.282103	-1.235769	3.114022
H	0.246799	0.332619	-2.117996
O	0.219409	1.715972	-1.876414
S	0.673832	2.378356	-0.614428
O	0.675822	1.483509	0.556602
O	0.136099	3.717221	-0.416316

C	2.474632	2.619369	-0.942694
F	3.055959	1.439567	-1.150131
F	2.666980	3.377869	-2.003195
F	3.055333	3.187619	0.103921

TS4-B

SCF = 5

Num. Imaginary Freq = 15.3042

C	-2.126854	4.158078	-2.293078
C	-1.204688	3.349611	-1.643710
C	-1.593928	2.556492	-0.554455
C	-2.928731	2.583477	-0.130283
C	-3.852628	3.391252	-0.785150
C	-3.454530	4.178879	-1.862971
H	-1.814329	4.776080	-3.139451
H	-0.159860	3.315464	-1.963039
H	-3.269790	1.963039	0.701570
H	-4.893433	3.401066	-0.451498
H	-4.184774	4.813073	-2.374098

C	-0.552752	1.721701	0.090572
C	-0.895293	1.003059	1.394281
C	-0.810179	1.967209	2.577093
O	0.572407	1.638573	-0.364239
O	-1.327052	3.035470	2.709907
O	-0.014070	1.406621	3.515570
C	0.469877	0.196802	3.031123
C	0.030601	-0.107509	1.802399
C	0.254723	-1.326221	1.003271
H	0.006122	-1.324481	-0.076785
P	4.225728	-0.041712	-0.847746
C	4.176964	1.751750	-1.152898
H	4.031364	2.279750	-0.198345
H	5.111281	2.094032	-1.626777
H	3.319943	1.986195	-1.802150
C	5.719207	-0.301859	0.160960
H	5.868088	-1.377984	0.334855
H	6.603039	0.110508	-0.352995
H	5.598701	0.195708	1.134804
C	4.636531	-0.775436	-2.462329

H	3.818930	-0.583310	-3.172925
H	5.570892	-0.339454	-2.852338
H	4.757360	-1.863848	-2.356747
Au	2.230192	-0.769690	0.077178
H	0.705504	-2.212685	1.472628
H	1.124648	-0.342161	3.714347
H	-1.942124	0.648574	1.361686
H	-0.998790	-1.838933	1.053770
O	-2.228915	-2.106672	1.116413
S	-3.033040	-1.357472	0.058123
O	-2.165140	-0.751570	-0.953178
O	-4.098692	-0.549130	0.632709
C	-3.876943	-2.756529	-0.797435
F	-2.975713	-3.583238	-1.296857
F	-4.645099	-3.412346	0.049667
F	-4.618278	-2.280056	-1.779383

INT5-A

SCF = -2245.28622607

Num. Imaginary Freq = 0

C	-3.254845	-2.697692	-0.648068	C	-0.216252	-1.254434	-2.091501
C	-3.882247	-1.430331	-0.313463	C	0.596031	-2.344561	-2.213287
C	-3.139984	-0.290136	-0.262899	H	0.222320	-3.351694	-1.999725
C	-1.653445	-1.335210	-1.687252	H	-2.300915	-1.157116	-2.576945
H	-4.906954	-1.466331	0.056157	H	1.575883	-2.255251	-2.693411
O	-3.707944	-3.795004	-0.479520	Au	1.045079	-1.363897	-0.163455
C	-3.513616	0.993668	0.329440	P	1.952649	-1.069663	1.992751
C	-2.727515	2.123854	0.061422	C	3.301484	0.143513	2.072601
C	-4.624784	1.111843	1.178215	H	3.671012	0.226126	3.107687
C	-3.039772	3.348342	0.640265	H	4.126589	-0.154614	1.408890
H	-1.873128	2.036109	-0.612723	H	2.903721	1.112211	1.737088
C	-4.941956	2.341055	1.741277	C	2.606014	-2.570298	2.792158
H	-5.232490	0.233633	1.414618	H	3.439888	-2.975982	2.199932
C	-4.147859	3.459547	1.477496	H	2.963162	-2.337258	3.808644
H	-2.397593	4.208333	0.432461	H	1.816094	-3.334088	2.850796
H	-5.807760	2.427292	2.403488	C	0.682270	-0.431572	3.124060
H	-4.395252	4.422427	1.933749	H	1.116928	-0.242486	4.119091
O	-1.963971	-2.575979	-1.136282	H	0.293776	0.503817	2.693388
O	-1.895957	-0.293442	-0.776802	H	-0.139340	-1.157928	3.213266
				H	0.086480	-0.247157	-2.419994

O 0.274267 1.761630 -1.886275
S 0.776531 2.310769 -0.612419
O 0.751707 1.351075 0.520079
O 0.344954 3.668086 -0.284916
C 2.588358 2.471963 -0.939723
F 3.116919 1.276108 -1.205888
F 2.817228 3.266289 -1.968913
F 3.215448 2.964518 0.122490

INT5-B

SCF = -2245.31417690

Num. Imaginary Freq = 0

C -5.667699 -0.559641 -2.201364
C -4.314112 -0.701694 -1.928932
C -3.883503 -1.085031 -0.649723
C -4.833636 -1.311565 0.354905
C -6.189668 -1.158023 0.082401
C -6.607260 -0.787988 -1.194336
H -5.997226 -0.271081 -3.203187

H -3.559546 -0.527742 -2.701082
H -4.521309 -1.577930 1.367806
H -6.925088 -1.327677 0.873147
H -7.674154 -0.675406 -1.407226
C -2.421163 -1.212397 -0.425060
C -1.929403 -1.815654 0.892891
C -1.846011 -0.737649 1.969761
O -1.615854 -0.835577 -1.251450
O -2.677425 0.064576 2.296150
O -0.617513 -0.776359 2.515028
C 0.143920 -1.728085 1.837411
C -0.529317 -2.357705 0.871870
C -0.024759 -3.390794 -0.063042
H -0.223276 -3.093608 -1.105860
P -0.659894 2.601185 0.284263
C -2.377482 2.361808 -0.268351
H -2.837907 1.545505 0.311821
H -2.955891 3.285514 -0.103420
H -2.395984 2.094539 -1.335751
C -0.791667 2.936618 2.065394

H	0.207960	3.125898	2.483552
H	-1.437204	3.813895	2.235093
H	-1.230261	2.059125	2.566471
C	-0.146787	4.179928	-0.462372
H	-0.131166	4.082790	-1.558178
H	-0.845747	4.982671	-0.175316
H	0.867079	4.437151	-0.121231
Au	0.730513	0.872491	-0.240662
H	1.063132	-3.512808	0.045052
H	1.182108	-1.798121	2.162423
H	-2.652518	-2.578758	1.239186
H	-0.515027	-4.365074	0.104542
O	3.326306	-2.614976	0.160179
S	3.142793	-1.169646	0.147181
O	3.116501	-0.462572	1.428909
C	4.625934	-0.497616	-0.720313
F	5.711877	-0.771454	-0.020806
F	4.740233	-1.030963	-1.921967
F	4.514085	0.816709	-0.842864
O	2.036126	-0.733191	-0.796370