

## *Supporting Information: Computational Part*

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

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#### **Table of Contents**

<b>Computational methods</b> .....	S2
<b>Computational data</b> .....	S7
<b>Cartesian Coordinates</b> .....	S10

## Computational methods

Geometries of the molecules were optimized by using the M06 meta-hybrid functional<sup>1</sup> in combination with the Def2-SVP<sup>2</sup> basis set. This method was applied previously in related reactions.<sup>3</sup> Solvent effects were calculated with the PCM continuum solvation model<sup>4</sup> 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.<sup>5</sup> 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.<sup>6</sup>

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

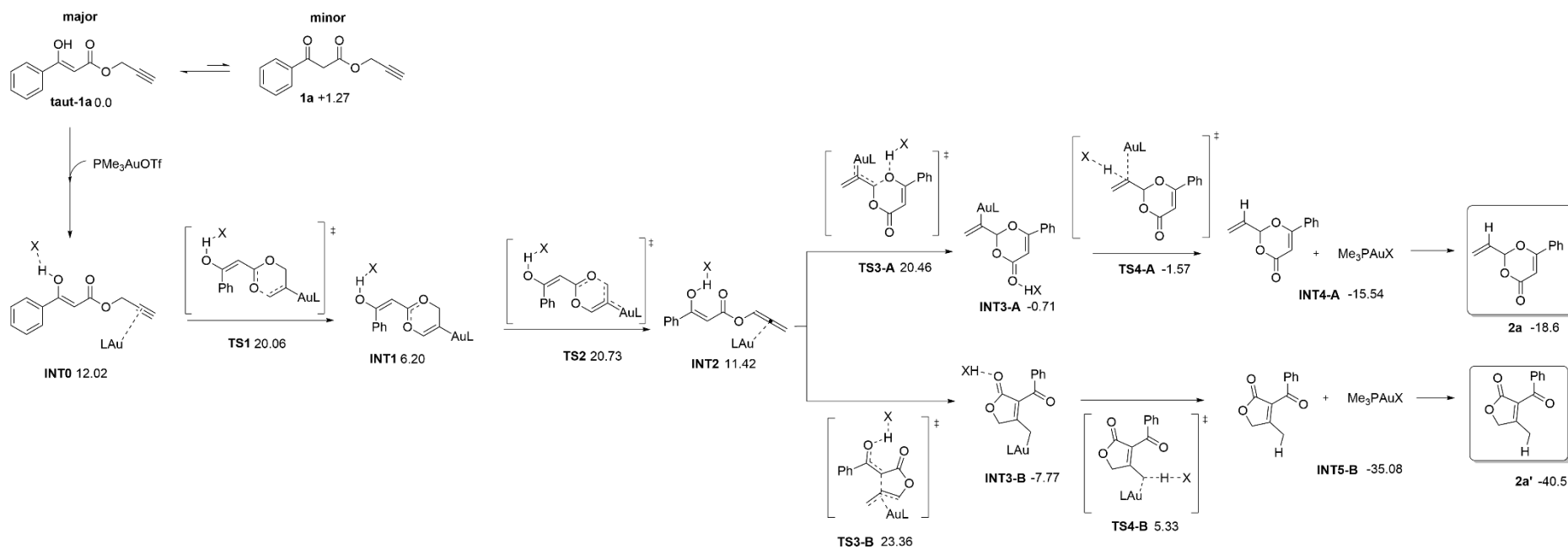
<sup>2</sup> Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

<sup>3</sup> (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.

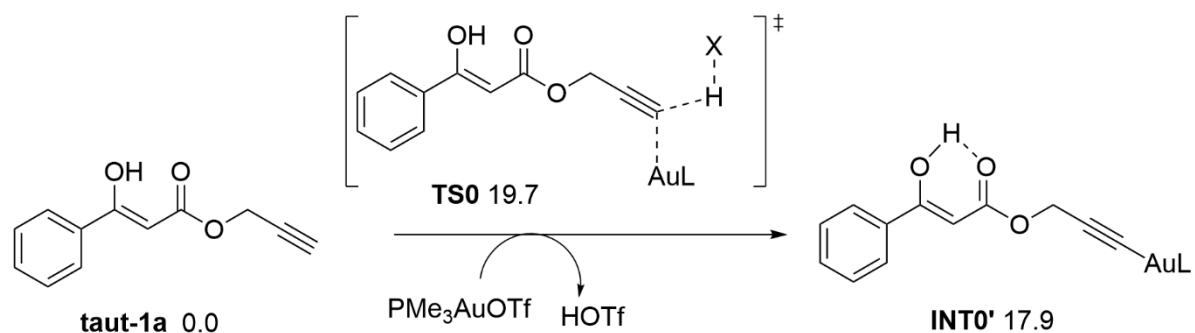
<sup>4</sup> Tomasi, J.; Persico, M. *Chem. Rev.* **1994**, *94*, 2027.

<sup>5</sup> Bauernschmitt, R.; Ahlrichs, R. *J. Chem. Phys.* **1996**, *104*, 9047.

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

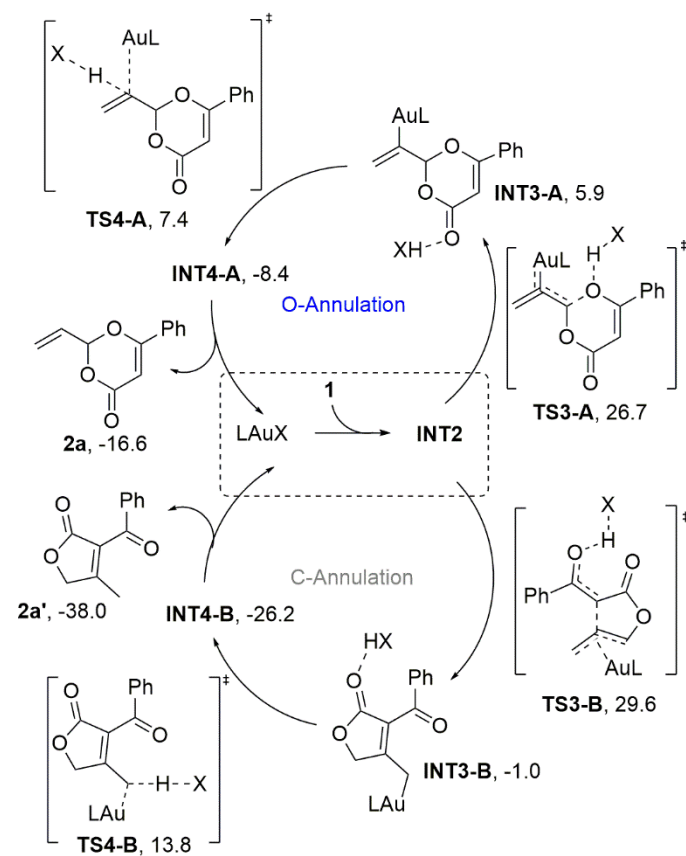
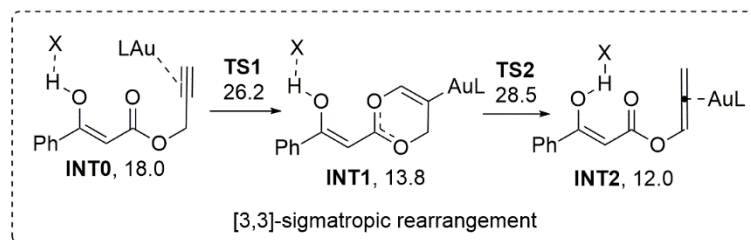


**Scheme S1.** Computed mechanism for the transformation of **1a** into **2** and **2a'** at the PCM(*p*-Xylene)/M06/def2-SVP theoretical level. Gibbs free energies are reported in kcal mol<sup>-1</sup> (1 atm and 298 K), relative to **taut-1a**. L refers to  $\text{PMe}_3$  and X to  $\text{OTf}^-$  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<sup>-1</sup> (1 atm and 298 K), relative to **taut-1a**. L refers to PMe<sub>3</sub> and X to OTf(-) anion.

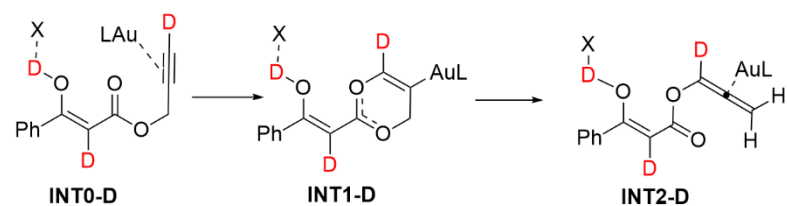
In order to validate the computational method here used, we performed single point energy calculations at a higher level of theory. The profile reaction computed at PCM(*p*-Xylene)/M06/def2-TZVP//PCM(*p*-Xylene)/M06/def2-SVP theoretical level is depicted in Scheme S3. As shown, these computational results 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.



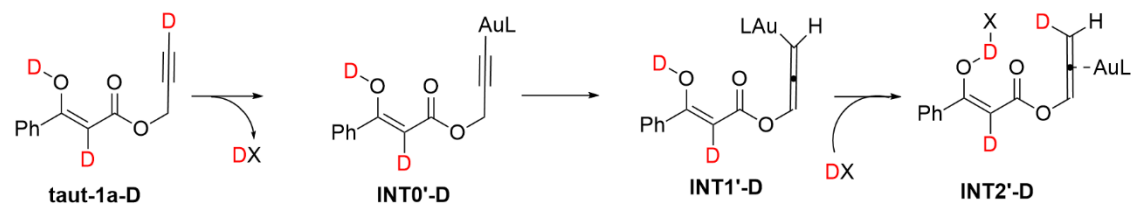
**Scheme S3.** Computed mechanism for the transformation of **1a** into **INT0'** at the PCM(*p*-Xylene)/M06/def2-TZVP//PCM(*p*-Xylene)/M06/def2-SVP theoretical level. Gibbs free energies are reported in kcal mol<sup>-1</sup> (1 atm and 298 K), relative to **taut-1a**. L refers to PMe<sub>3</sub> and X to OTf(-) anion.

The partial deuteration of the C<sub>a</sub>-position could be explained via the transformations shown in Scheme S4 b and c.

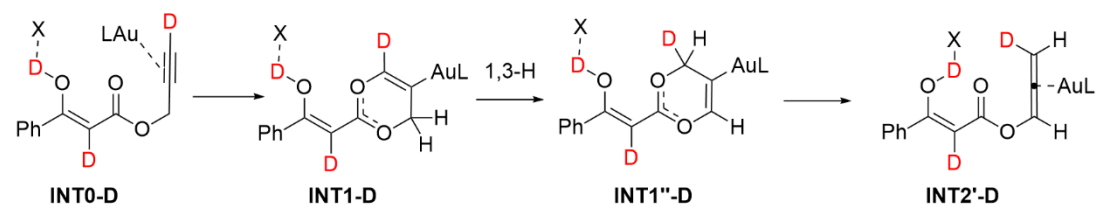
a) Proposed mechanism in this work



b) Participation of a propargylate/allenoate equilibria of **INT0-D**



c) Alternative involving a 1,3-H shift



**Scheme S4.** Alternative pathways for explaining deuterium-labelling results. L refers to PMe<sub>3</sub> 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
<b>PMe<sub>3</sub>AuOTf</b>					
Pme3AuOTf	-	-1557.27802	-1557.18504	-1557.11715	-1558.312864
<b>1a</b>					
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
<b>taut-1a</b>					
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
<b>2a</b>					
2a_01	-	-687.985575	-687.832458	-687.779338	-688.623391

2a_02	-	-687.985518	-687.832289	-687.77921	-688.624916
<b>2a'</b>					
2a'_01	-	-688.016682	-687.864624	-687.81035	-688.590727
2a'_02	-	-688.019659	-687.867288	-687.813352	-688.590808
<b>TS0</b>					
ts0_01	-666.45	-2245.218732	-2244.956398	-2244.855876	-2246.837636
<b>INT0'</b>					
Int0'_01	-	-1283.95991	-1283.72282	-1283.64111	-1284.746422
<b>INT0</b>					
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
<b>TS1</b>					
ts1_01	-226.3	-2245.22452	-2244.95579	-2244.85714	-2246.835324
<b>INT1</b>					
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
<b>TS2</b>					



ts2_01	-182.7	-2245.22595	-2244.95472	-2244.85948	-2246.831706
<b>INT2</b>					
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
<b>TS3-A</b>					
ts3A_01	-342.47	-2245.21762	-2244.95514	-2244.85438	-2246.834304
<b>TS3-B</b>					
ts3b_01	-397.46	-2245.22147	-2244.95052	-2244.85633	-2246.830006
<b>INT3-A</b>					
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
<b>INT3-B</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
<b>TS4-A</b>					
ts4a_01	-266.98	-2245.25947	-2244.99026	-2244.8956	-2246.865429

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

## Cartesian Coordinates

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

### **PMe<sub>3</sub>AuOTf**

SCF = -1557.27801665

Num. Imaginary Freq = 0

Au -0.818506 -0.273659 -0.009659  
P -3.056630 0.137942 0.008778  
C -3.580602 1.202066 1.386246  
H -4.667184 1.379766 1.337281  
H -3.329403 0.719861 2.342578  
H -3.048278 2.163353 1.331953

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  
C -4.088812 -1.352764 0.149842  
H -5.155586 -1.075295 0.154217  
H -3.889335 -2.024042 -0.698654  
H -3.845603 -1.885565 1.081202  
S 2.140613 0.573622 -0.007302  
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