Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Computational Part

Scandium Catalysed Stereoselective Thio-allylation of Allenyl-Imidates

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Table of Contents

Computational methods

Geometries of the molecules were optimized by using the M06 meta-hybrid functional.[1] The SDD[2] basis set and its associated effective core potential (ECP) were used to describe the Sc atom while the Def2-SVP[3] basis set were used in the rest of atoms. Solvent effects were calculated with the PCM continuum solvation model[4] for acetonitrile. This method was applied previously in similar reactions involving group III metals.[5] The nature of minimum and transition structures of all stationary points was confirmed by frequency analysis at the same level of theory. The wave function stability was confirmed in all stationary points.[6] All calculations were performed using the ultrafine grid implemented in Gaussian 09 E.01.[7]

Computed transition structures γ-*E*-TS2 and γ-*Z*-TS2

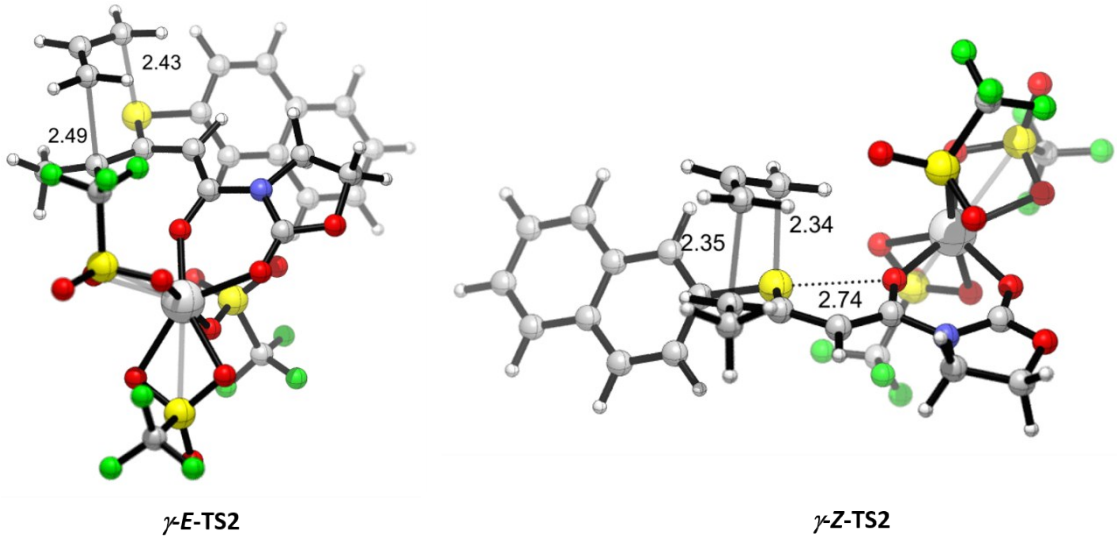

Figure S2. Computed transition structures **γ-*E*-TS2** and **γ-*Z*-TS2** at the PCM(acetonitrile)/M06/Def2-SVP/SDD(Sc) theoretical level. Distances are shown in Angstrom.

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

[2] (a) M. Kaupp, P. V. R. Schleyer, H. Stoll, H. Preuss, *Chem. Phys.* 1991, **94**, 1360 (b) A. Bergner, M. Dolg, H. Kuechle, H. Stoll, H. Preuss, H. *Mol. Phys.* 1993, **80**, 1431. (c) M. Dolg, H. Stoll, H. Preuss, R. M. Pitzer, *J. Phys. Chem.* 1993, **97**, 5852.

[3] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297.

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

[5] (a) H. Liu, C. Zeng, S-L You, *J. Org. Chem.* 2014, **79**, 1047. (b) M. Alajarin, D. Bañon, A. Egea, M. Marin-Luna, A. Vidal, *Org. Chem. Front.*, 2018, **5**, 2020

[6] R. Bauernschmitdd, R. Ahlrichs, *J. Chem. Phys.* 1996, **104**, 9047.

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

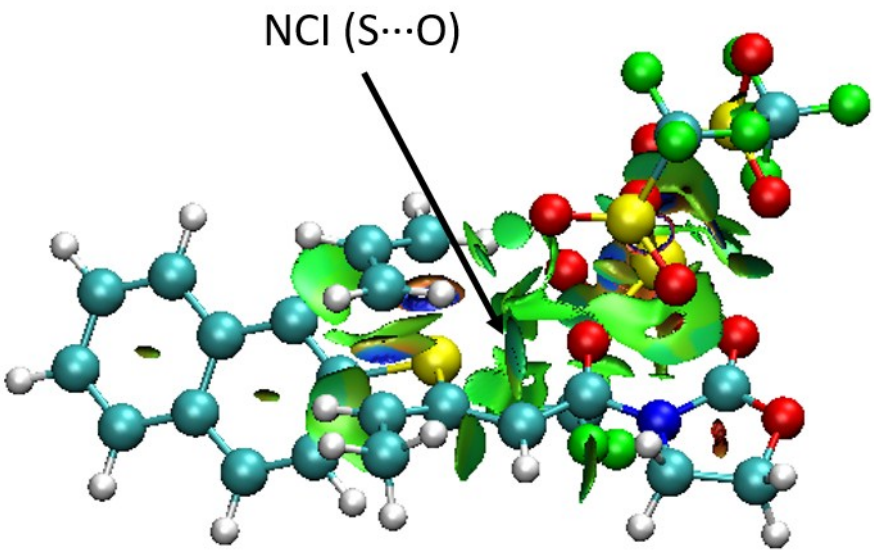

Figure S3. Representation of non-covalent interactions at the transition structure **γ-*Z*-TS2**. The picture was plotted with the CYLview program.[8]

Solvent study

The solvent in which the reaction is conducted highly influences on the **γ-*Z*-FP: γ-*E*-FP** product ratios and their yields as well. We performed a theoretical approach to rationalize this solvent-dependence. Single point energy calculations in different solvents were run over the optimized structures in acetonitrile which are involved in the rate-determining step (**INT1**, **γ-*E*-TS2, γ-*Z*-TS2, γ-*E*-INT2, γ-*Z*-INT2**). A comparison of the associated electronic energy barriers of that step is depicted in Figure S3. In all studied solvents (acetonitrile, dichloromethane, diethyl ether, toluene), the energy barriers for the **γ-*Z*-TS2** are lower than those for the **γ-*E*-TS2**, in agreeement with the **γ-*Z*-FP: γ-*E*-FP** experimentally molar distribution. Furthermore, the computed energy barriers in non-polar solvents (toluene, diethyl ether) are notably higher than those in polar solutions (acetonitrile, dichloromethane).

[8] *CYLVIEW: CYLview,1.0b;Legault, C. Y., Université de Sherbrooke, 2009 7*

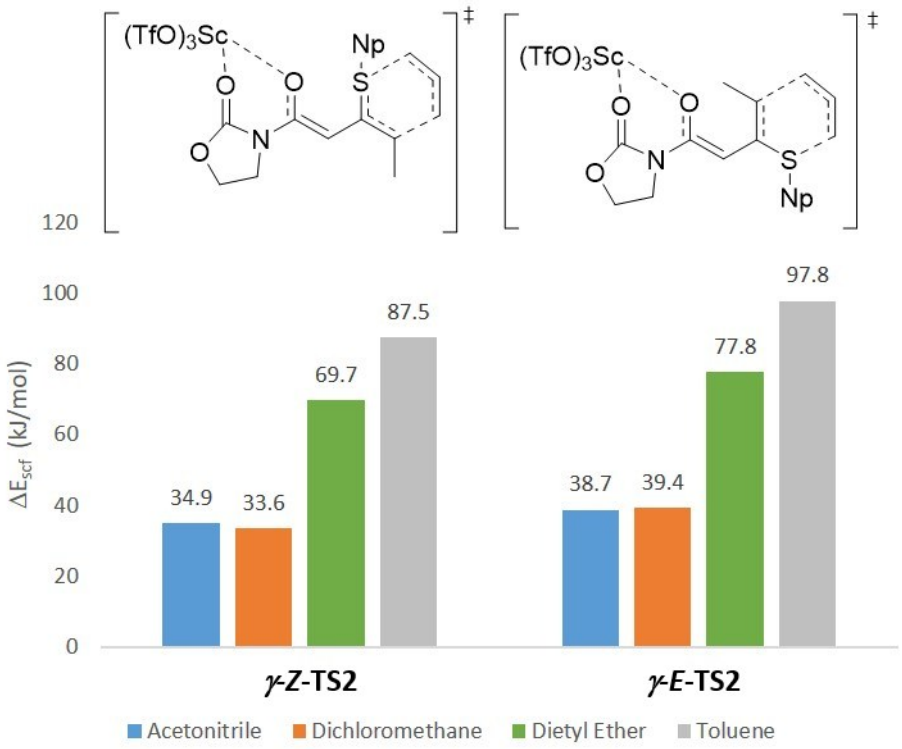

Figure S4. Electronic energy barriers of transition structures **γ-*E*-TS2** and **γ-*Z*-TS2** computed at the PCM(solvent)/M06/Def2-SVP/SDD(Sc)//PCM(acetonitrile)/M06/Def2-SVP/SDD(Sc) theoretical level.

Computational data

Table S2. Number of imaginary frequencies, electronic, free and enthalpies energies (in Hartrees) of all computed conformers for systems shown in **Scheme 3**. Free energies and enthalpy energies in solution at 298.15 K ($G_{298,sol}$ and $H_{298,sol}$) have been calculated at the PCM(acetonitrile)/M06/Def2-SVP/SDD(Sc) level. Note that the filenames are used in our calculations and do not follow any guide.

Filename	ImFreqs	Freq	$E_{SCF,298,sol}$ PCM/M06/Def2-SVP /SDD(Sc)	$G_{298,sol}$ PCM/M06/Def2-SVP /SDD(Sc)	$H_{298,sol}$ PCM/M06/Def2-SVP /SDD(Sc)
2a					
thioether_03	0	-	-899.8826984	-899.7148010	-899.6612070
thioether_04	0	-	-899.8818703	-899.7144870	-899.6606220
thioether_01	0	-	-899.8813970	-899.7134510	-899.6597860
thioether_02	0	-	-899.8813970	-899.7134490	-899.6597860
4g					
aleno_methyl	0	-	-589.8709014	-589.7483180	-589.6964190
$Sc(OTf)_3$					
scotf3	0	-	-2928.9965728	-2928.9656180	-2928.8802410
γ-*E*-FP					
product_E_5	0	-	-1489.8103528	-1489.4919650	-1489.4097070
product_E_6	0	-	-1489.8094048	-1489.4916920	-1489.4087520
product_E_2	0	-	-1489.8108209	-1489.4915610	-1489.4101260
product_E_7	0	-	-1489.8087588	-1489.4915420	-1489.4086600
product_E_01	0	-	-1489.8089643	-1489.4912610	-1489.4083890
product_E_3	0	-	-1489.8096485	-1489.4908320	-1489.4088420

product_E_4	0	-	-1489.8096894	-1489.4905140	-1489.4089160
product_E_1	0	-	-1489.8099057	-1489.4887910	-1489.4091730
γ-*Z*-FP					
product_Z_3	0	-	-1489.8158158	-1489.4976770	-1489.4152110
product_Z_11	0	-	-1489.8156143	-1489.4971320	-1489.4150260
product_Z_9	0	-	-1489.8156143	-1489.4971310	-1489.4150250
product_Z_10	0	-	-1489.8156143	-1489.4971230	-1489.4150270
product_Z_8	0	-	-1489.8156143	-1489.4971120	-1489.4150270
product_Z_1	0	-	-1489.8158236	-1489.4968470	-1489.4151870
product_z_01	0	-	-1489.8137901	-1489.4966700	-1489.4133010
product_Z_2	0	-	-1489.8169062	-1489.4966450	-1489.4162090
product_Z_7	0	-	-1489.8161849	-1489.4964820	-1489.4154060
product_Z_12	0	-	-1489.8157196	-1489.4961200	-1489.4160180
product_Z_6	0	-	-1489.8152167	-1489.4959140	-1489.4145070
product_Z_13	0	-	-1489.8084126	-1489.4913600	-1489.4083380
α-FP					
product_b_02	0	-	-1489.8167373	-1489.4963030	-1489.4162450
product_b_03	0	-	-1489.8141896	-1489.4943660	-1489.4133750
product_b_05	0	-	-1489.8144806	-1489.4937550	-1489.4141030
product_b_01	0	-	-1489.8100018	-1489.4932430	-1489.4102060
product_b_04	0	-	-1489.8083949	-1489.4895580	-1489.4077360
product_b_06	0	-	-1489.7987037	-1489.4793800	-1489.3982620
INT0					
rc_04	0	-	-4418.8491012	-4418.4725500	-4418.3315770

rc_03	0	-	-4418.8481142	-4418.4706350	-4418.3306840
rc_01	0	-	-4418.8478400	-4418.4698090	-4418.3300440
rc_02	0	-	-4418.8373263	-4418.4625820	-4418.3195080
TS1					
ts1_23	1	-244.71	-4418.8358130	-4418.4602560	-4418.3198970
ts1_18	1	-234.43	-4418.8353362	-4418.4586200	-4418.3194780
ts1_17	1	-215.97	-4418.8319948	-4418.4534620	-4418.3154220
ts1_10	1	-247.46	-4418.8290279	-4418.4517860	-4418.3130700
INT1					
int1_03	0	-	-4418.8523185	-4418.4730100	-4418.3344540
int1_04	0	-	-4418.8483081	-4418.4709270	-4418.3302430
int1_05	0	-	-4418.8439303	-4418.4671220	-4418.3260830
int1_01	0	-	-4418.8496016	-4418.4647880	-4418.3311760
int1_02	0	-	-4418.8384783	-4418.4598910	-4418.3204650
γ-*Z*-TS2					
ts2_24	1	-342.42	-4418.8390091	-4418.4583890	-4418.3220450
ts2_28	1	-364.14	-4418.8380480	-4418.4570260	-4418.3214120
ts2_26	1	-359.92	-4418.8379665	-4418.4567340	-4418.3212100
γ-*E*-TS2					
ts2_08	1	-262.72	-4418.8375908	-4418.4555140	-4418.3201200
ts2_10	1	-260.98	-4418.8375693	-4418.4554510	-4418.3201000
ts2_01	1	-317.07	-4418.8361198	-4418.4543120	-4418.3191890
ts2_02	1	-317.28	-4418.8361244	-4418.4539220	-4418.3191610

ts2_04	1	-317.24	-4418.8361244	-4418.4539210	-4418.3191620
ts2_03	1	-317.19	-4418.8361243	-4418.4539200	-4418.3191590
γ-*Z*-INT2					
int2_03	0	-	-4418.9022535	-4418.5201120	-4418.3819650
int2_11	0	-	-4418.9005820	-4418.5198170	-4418.3804930
int2_04	0	-	-4418.9020057	-4418.5192280	-4418.3815150
int2_05	0	-	-4418.9001008	-4418.5174880	-4418.3797920
int2_13	0	-	-4418.8959649	-4418.5125770	-4418.3755040
int2_12	0	-	-4418.8920564	-4418.5117300	-4418.3718310
γ-*E*-INT2					
int2_06	0	-	-4418.9047499	-4418.5233730	-4418.3845270
int2_07	0	-	-4418.9052188	-4418.5229960	-4418.3847390
int2_10	0	-	-4418.9022111	-4418.5209560	-4418.3815390
int2_01	0	-	-4418.9022153	-4418.5204200	-4418.3815810
int2_08	0	-	-4418.9002481	-4418.5184810	-4418.3797000
int2_09	0	-	-4418.8954799	-4418.5104380	-4418.3745290
α–TS2					
ts2_09	1	-282.77	-4418.8185250	-4418.4425190	-4418.3024160
α–INT2					
int2_b_03	0	-	-4418.8955610	-4418.5084070	-4418.3750400
int2_b_06	0	-	-4418.8912198	-4418.5078540	-4418.3708200
int2_b_07	0	-	-4418.8872251	-4418.5046400	-4418.3672130
int2_b_04	0	-	-4418.8870006	-4418.5021260	-4418.3663560

int2_b_08	0	-	-4418.8864879	-4418.5015480	-4418.3658530
int2_b_02	0	-	-4418.8851380	-4418.5006520	-4418.3646410
int2_b_05	0	-	-4418.8850599	-4418.5005120	-4418.3643370

Table S3. Electronic energies (in Hartrees) calculated at the PCM(solvent)/M06/Def2-SVP/SDD(Sc)// PCM (acetonitrile)/M06/Def2-SVP/SDD(Sc) level of structures involved in the rate-determining step in different solvents.

Filename	$E_{SCF,298,sol}$ PCM (dichloromethane)/M06/Def2-SVP /SDD(Sc)	$E_{SCF,298,sol}$ PCM (toluene)/M06/Def2-SVP /SDD(Sc)	$E_{SCF,298,sol}$ PCM(diethyl ether)/M06/Def2-SVP /SDD(Sc)
INT1	-4418.8456631	-4418.8496244	-4418.8519244
γ-*E*-TS2	-4418.8306739	-4418.8123840	-4418.8223027
γ-*Z*-TS2	-4418.8328790	-4418.8163161	-4418.8253637
γ-*E*-INT2	-4418.8991624	-4418.8844787	-4418.8924283
γ-*Z*-INT2	-4418.8967560	-4418.8823047	-4418.8901184

CARTESIAN COORDINATES

The best conformer is shown

2a thioether_03
SCF = -899.882698366
Num. Imaginary Freq = 0

C	3.601354	-1.823262	-0.016856
C	2.226240	-1.772022	-0.031754
C	1.545486	-0.527333	-0.008507
C	2.315151	0.673604	0.031531
C	3.729289	0.589820	0.045487
C	4.362382	-0.632156	0.021919
H	-0.430727	-1.391631	-0.042101
H	4.111918	-2.790539	-0.035065
H	1.635481	-2.693694	-0.061826
C	0.127480	-0.451280	-0.020604
C	1.626829	1.916066	0.056945
H	4.308744	1.518675	0.075756
H	5.454667	-0.685954	0.033219
C	0.257669	1.968365	0.041315
C	-0.514036	0.770765	0.000521
H	2.210989	2.841798	0.087095
H	-0.257137	2.934967	0.057757
S	-2.266533	1.002800	-0.001227
C	-2.903373	-0.701929	-0.185543
H	-2.655505	-1.291891	0.713561
H	-2.397876	-1.156839	-1.055844
C	-4.377163	-0.637272	-0.399329
H	-4.709706	-0.144581	-1.323268
C	-5.277702	-1.124889	0.453673
H	-4.973149	-1.614490	1.386229
H	-6.350813	-1.061479	0.251324

4g aleno_methyl
SCF = -589.8709014
Num. Imaginary Freq = 0

C	-2.150436	0.795810	0.102049
O	-2.131623	1.988953	0.170468
O	-3.283147	0.074835	0.159734
C	0.257889	0.310834	-0.161359
O	0.558038	1.452372	-0.426219
N	-1.075558	-0.093988	-0.013070
C	-3.028692	-1.301443	-0.107166
H	-3.653211	-1.915078	0.554184
H	-3.300673	-1.515306	-1.153665
C	-1.538198	-1.468175	0.141967
H	-1.072397	-2.141407	-0.590967
H	-1.323716	-1.846883	1.156091
C	1.254031	-0.771912	0.033170
H	0.937504	-1.757523	0.393890
C	2.532456	-0.550091	-0.200819
C	3.795798	-0.328684	-0.437466
H	4.156174	-0.545507	-1.454377
C	4.787808	0.191430	0.553421
H	4.326915	0.374760	1.534117
H	5.615384	-0.524050	0.683182
H	5.232840	1.133014	0.194393

$Sc(OTf)_3$ scotf3
SCF = -2928.99657282
Num. Imaginary Freq = 0

O	1.677966	-1.039511	0.659045
O	-2.081378	-0.102384	-0.912611
O	-0.076380	1.233085	1.241868
S	2.833572	-1.919799	0.137389
S	0.557388	2.117907	0.182156
S	-2.927423	-0.517965	0.266691
O	3.401079	-2.724914	1.201247
O	2.504267	-2.528167	-1.143231
O	0.570377	1.197335	-1.016142
O	1.765287	2.823968	0.520774
O	-3.943718	0.387755	0.735971
O	-1.884648	-0.991727	1.260225
C	4.081814	-0.605830	-0.229195
C	-0.738158	3.394508	-0.193787
C	-3.782127	-2.072873	-0.276007
F	3.613176	0.210070	-1.152396
F	4.351059	0.075450	0.864567
F	5.178188	-1.186826	-0.670781
F	-0.822019	4.204405	0.833458
F	-4.699120	-1.752756	-1.156377
F	-0.363330	4.050205	-1.265525
F	-4.332185	-2.629012	0.776511
F	-1.889348	2.802186	-0.401194
F	-2.903916	-2.889209	-0.812511
Sc	-0.163863	-0.532440	0.061676

γ-*E*-FP product_E_5
SCF = -1489.81035279
Num. Imaginary Freq = 0

C	-5.359675	-1.995812	-1.501020
C	-4.070901	-1.933525	-0.697949
H	-5.211760	-1.684578	-2.548013
H	-5.835960	-2.984196	-1.488291
H	-3.178099	-2.016858	-1.333142
H	-4.026037	-2.718832	0.076552
N	-4.184770	-0.609913	-0.097525
C	-5.515359	-0.177421	-0.129833
O	-6.006770	0.775466	0.398820
O	-6.220835	-1.057620	-0.861153
C	-0.644175	-0.195081	0.818404
C	-1.907797	-0.667021	0.679173
H	-2.044663	-1.749507	0.774972
C	-3.133402	0.124891	0.472932
O	-3.269948	1.293024	0.770881
S	0.518583	-1.409313	1.410330
C	1.995264	-1.035032	0.485164
C	3.192276	-0.891049	1.151311
C	1.947250	-0.958653	-0.932802
C	4.395187	-0.665045	0.433362
H	3.226559	-0.941661	2.244940
C	3.093461	-0.711004	-1.645043
H	0.991266	-1.098953	-1.447938
C	4.345080	-0.562059	-0.990123
C	5.644018	-0.520673	1.090249
H	3.059951	-0.641196	-2.737115
C	5.544965	-0.319811	-1.704592

C	6.791745	-0.286446	0.369344
H	5.675566	-0.599312	2.181756
C	6.742184	-0.185138	-1.040497
H	5.499458	-0.242798	-2.795790
H	7.749601	-0.177331	0.885721
H	7.662125	0.001355	-1.601637
C	-0.130450	1.215278	0.663976
H	0.966971	1.130613	0.557918
C	-0.381314	2.011927	1.943558
H	-1.461470	2.127139	2.118124
H	0.068804	1.509745	2.814856
H	0.071290	3.012904	1.855779
C	-0.619805	1.947024	-0.595421
H	-0.666580	1.222054	-1.431127
H	-1.641855	2.330082	-0.445064
C	0.299645	3.064381	-0.968112
H	1.336794	2.774627	-1.199688
C	-0.041365	4.352111	-1.024406
H	-1.063738	4.678136	-0.796317
H	0.677259	5.128948	-1.303550

γ-*Z*-FP product_Z_3
SCF = -1489.81581581
Num. Imaginary Freq = 0

C	6.232302	0.762816	0.174093
C	4.803115	0.874913	-0.332451
H	6.971209	1.218689	-0.497048
H	6.350486	1.196959	1.180366
H	4.757856	1.028616	-1.424743
H	4.252024	1.690034	0.158320
N	4.274693	-0.431607	0.036553
C	5.318215	-1.326858	0.279084
O	5.269788	-2.507971	0.461786
O	6.474530	-0.638828	0.248135
C	0.654255	0.146815	-0.431289
C	2.010744	0.203039	-0.518391
H	2.437301	1.034630	-1.085203
C	2.912861	-0.782192	0.064765
O	2.538989	-1.831681	0.555134
S	-0.131599	-1.199406	0.401162
C	-1.845602	-0.690034	0.493388
C	-2.779520	-1.309011	-0.307630
C	-2.252879	0.258521	1.469009
C	-4.157925	-0.995310	-0.187350
H	-2.465490	-2.049758	-1.051359
C	-3.579263	0.588730	1.594582
H	-1.497325	0.726395	2.108181
C	-4.565811	-0.023944	0.776584
C	-5.140419	-1.614099	-1.002181
H	-3.897168	1.326503	2.338446
C	-5.943025	0.293093	0.890163
C	-6.468940	-1.285084	-0.868844
H	-4.819379	-2.357586	-1.738882
C	-6.873536	-0.322970	0.085808
H	-6.250817	1.037942	1.631195
H	-7.219132	-1.767379	-1.501708
H	-7.933193	-0.070237	0.182251
C	-0.189421	1.173981	-1.157484
H	-1.201602	1.167386	-0.720790
C	-0.313795	0.767383	-2.623645
H	-0.998835	1.447301	-3.154734

H	0.667673	0.806913	-3.125612
H	-0.703266	-0.258484	-2.723780
C	0.322236	2.612337	-1.015039
H	1.308603	2.712687	-1.507371
H	-0.365287	3.263659	-1.583823
C	0.395655	3.076500	0.403690
H	1.149410	2.587561	1.038728
C	-0.397577	4.005334	0.938761
H	-1.161557	4.515514	0.338961
H	-0.315262	4.298481	1.989954

α-FP product_b_02
SCF = -1489.81673729
Num. Imaginary Freq = 0

C	-1.887364	-2.357765	0.796523
C	-0.446113	-1.880695	0.926588
H	-2.090729	-3.279641	1.356817
H	-2.607791	-1.583950	1.112794
H	0.224020	-2.657849	1.331050
H	-0.382165	-0.992004	1.572039
N	-0.109068	-1.571086	-0.459511
C	-1.091621	-2.070903	-1.330745
O	-1.111101	-2.051327	-2.525172
O	-2.073246	-2.609179	-0.591856
C	2.510370	0.921865	-0.101501
C	2.030603	-0.487628	0.183601
H	1.536276	-0.472475	1.167296
C	1.063884	-0.954693	-0.902725
O	1.339407	-0.843129	-2.072491
S	1.620278	2.230747	0.743543
C	-0.055945	1.815410	0.284511
C	-0.996561	1.593920	1.268243
C	-0.424047	1.735426	-1.085220
C	-2.331030	1.249114	0.931694
H	-0.713239	1.656581	2.325230
C	-1.702419	1.380760	-1.435741
H	0.329533	1.934563	-1.853312
C	-2.686248	1.116438	-0.445668
C	-3.311601	0.989425	1.924398
H	-1.981461	1.291934	-2.490827
C	-4.005478	0.718285	-0.779643
C	-4.584338	0.607420	1.568393
H	-3.033255	1.094900	2.978065
C	-4.933548	0.467216	0.204502
H	-4.269292	0.613001	-1.837057
H	-5.332255	0.408167	2.340912
H	-5.947662	0.159136	-0.064643
C	3.144376	-1.550702	0.258689
H	3.676304	-1.577333	-0.709887
H	2.673779	-2.545128	0.370001
C	4.090247	-1.318371	1.390592
H	4.685850	-0.395899	1.346270
C	4.229106	-2.137973	2.432693
H	4.928225	-1.921517	3.246106
H	3.648187	-3.065421	2.510073
C	3.556312	1.211863	-0.890878
H	4.109179	0.356494	-1.302573
C	4.074360	2.551392	-1.269962
H	4.251938	2.603053	-2.356592
H	3.385884	3.359897	-0.983292
H	5.049549	2.749411	-0.792500

INT0 rc_04
SCF = -4418.84910115
Num. Imaginary Freq = 0

C	-0.110147	-1.410722	-2.303746
O	0.902681	-0.806124	-1.977575
O	-0.198936	-2.071334	-3.423724
C	-1.400463	-1.052638	-0.292420
O	-0.564125	-0.241102	0.143948
O	1.702339	-1.562728	0.942388
O	1.912784	1.856682	-1.582823
O	3.216878	0.805381	1.057585
S	1.150189	-2.979329	0.985966
S	4.260557	0.049221	0.271036
S	1.259371	2.922664	-0.748075
O	0.591126	-3.320704	2.283110
O	0.376439	-3.308441	-0.213178
O	3.512691	-0.452114	-0.930953
O	5.096252	-0.884544	0.991634
O	1.970413	4.159318	-0.527756
O	0.743266	2.173756	0.450289
C	2.721998	-3.936229	0.834287
C	5.405605	1.360775	-0.368193
C	-0.267295	3.354075	-1.703534
F	3.327938	-3.615423	-0.292037
F	3.510414	-3.661802	1.851990
F	2.438763	-5.223829	0.829833
F	4.721814	2.348260	-0.898757
F	-0.983752	4.214229	-1.009183
F	6.126183	1.808424	0.636458
F	-0.977005	2.261655	-1.915675
F	6.188394	0.819849	-1.276197
F	0.082675	3.886681	-2.850792
N	-1.282209	-1.523640	-1.581623
C	-1.534693	-2.593617	-3.594633
H	-2.063017	-1.931132	-4.296182
H	-1.456875	-3.598739	-4.022433
C	-2.119193	-2.559169	-2.194292
H	-1.979505	-3.508646	-1.650895
H	-3.181543	-2.278543	-2.185914
Sc	1.491512	0.171188	-0.163930
C	-2.487074	-1.556881	0.516165
H	-3.227482	-2.239406	0.083585
C	-2.547773	-1.202724	1.795678
C	-2.549811	-0.852227	3.047648
H	-3.114441	0.068237	3.290076
C	-1.846991	-1.569522	4.154728
H	-2.579580	-1.935515	4.891035
H	-1.253270	-2.413902	3.779957
H	-1.179005	-0.872718	4.684366
S	-3.747990	2.525236	2.398670
C	-4.229185	1.539731	1.001603
C	-5.175446	0.549113	1.177440
C	-3.673322	1.761631	-0.285906
C	-5.583579	-0.269411	0.095511
H	-5.602538	0.362236	2.169559
C	-4.042518	0.971609	-1.346688
H	-2.953473	2.569485	-0.435578
C	-5.001492	-0.063487	-1.191725
C	-6.515225	-1.326312	0.265201
H	-3.606179	1.141149	-2.337634
C	-5.389886	-0.902463	-2.267490

C	-6.855555	-2.138504	-0.791419
H	-6.953153	-1.486630	1.255720
C	-6.292046	-1.923083	-2.071227
H	-4.953180	-0.724183	-3.257058
H	-7.570243	-2.953443	-0.646572
H	-6.580245	-2.568937	-2.905222
C	-1.941591	2.724662	2.088285
H	-1.581882	1.782087	1.635146
H	-1.763672	3.543136	1.371707
C	-1.252745	2.995933	3.379707
H	-1.320944	2.205786	4.141208
C	-0.580512	4.117086	3.644502
H	-0.075152	4.270666	4.602332
H	-0.504601	4.922373	2.903922

TS1 ts1_23
SCF = -4418.83581303
Num. Imaginary Freq = 1

C	-0.067369	0.660803	-2.330596
O	-1.222260	0.517113	-1.943982
O	0.205498	1.105576	-3.531030
C	1.085345	0.093063	-0.271527
O	0.016905	-0.369612	0.223546
O	-1.662987	1.762497	0.845939
O	-2.729997	-1.787041	-1.269235
O	-3.902525	0.000849	1.122734
S	-0.628757	2.873864	0.768097
S	-4.663307	0.893563	0.177684
S	-2.571131	-2.839327	-0.203856
O	0.122178	3.026536	2.006386
O	0.108161	2.868694	-0.495587
O	-3.759760	1.025150	-1.011287
O	-5.263060	2.093358	0.719103
O	-3.660363	-3.764302	0.007742
O	-2.039412	-2.083741	0.977476
C	-1.741527	4.344290	0.674678
C	-6.074734	-0.157145	-0.395199
C	-1.143471	-3.853403	-0.808158
F	-2.527927	4.241428	-0.379356
F	-2.477171	4.421273	1.764814
F	-1.002426	5.430575	0.565044
F	-5.623872	-1.288002	-0.891765
F	-0.872193	-4.785596	0.077299
F	-6.857215	-0.404821	0.633104
F	-0.089061	-3.078489	-0.978444
F	-6.743011	0.499908	-1.318412
F	-1.473894	-4.406069	-1.954297
N	1.082841	0.417819	-1.628642
C	1.628779	1.068980	-3.759002
H	1.845475	0.184408	-4.376016
H	1.913221	1.975603	-4.304080
C	2.218079	0.974580	-2.362589
H	2.479912	1.962261	-1.945434
H	3.093554	0.312114	-2.310721
Sc	-2.006915	-0.073606	-0.057114
C	2.255478	0.354396	0.460624
H	3.122366	0.790130	-0.046076
C	2.306367	0.110163	1.810874
C	1.898627	0.384690	3.028904
H	1.300326	1.316394	3.013559
C	2.063491	-0.286699	4.340523

H	1.077839	-0.597063	4.724108
H	2.706397	-1.175207	4.286913
H	2.480333	0.414884	5.079852
S	3.910245	-1.739693	1.994905
C	4.967999	-1.129727	0.707358
C	5.876391	-0.159399	1.083563
C	4.866651	-1.533652	-0.647331
C	6.714319	0.455656	0.124554
H	5.950489	0.156544	2.130774
C	5.681018	-0.952138	-1.591787
H	4.151896	-2.299990	-0.955358
C	6.615539	0.054042	-1.243335
C	7.649693	1.463119	0.480996
H	5.608772	-1.264035	-2.638943
C	7.455112	0.672677	-2.205207
C	8.447532	2.044142	-0.474682
H	7.721031	1.767034	1.530161
C	8.350114	1.645827	-1.830077
H	7.374806	0.358937	-3.250876
H	9.164083	2.819854	-0.190659
H	8.992484	2.117560	-2.578777
C	2.856670	-2.974074	1.157655
H	2.267284	-2.453085	0.380310
H	3.523160	-3.707756	0.675848
C	1.979617	-3.598537	2.189878
H	2.441529	-4.356195	2.835448
C	0.706356	-3.243081	2.361788
H	0.081291	-3.705430	3.131648
H	0.241695	-2.474379	1.731158

INT1 int1_03

SCF = -4418.85231854
Num. Imaginary Freq = 0

C	-1.482729	3.082287	-0.362578
O	-2.090831	2.069261	-0.011884
O	-1.914167	4.276017	-0.014685
C	0.451046	2.055808	-1.444168
O	-0.049929	0.899224	-1.173925
O	-0.284871	0.313670	1.619890
O	-3.043440	-0.224276	-1.609632
O	-1.885696	-1.949585	0.902066
S	0.556052	1.376743	2.300179
S	-2.956493	-1.455685	1.834742
S	-2.368186	-1.285350	-2.443430
O	1.623581	0.804164	3.104599
O	0.883175	2.495260	1.410978
O	-3.177705	-0.027698	1.439060
O	-2.819103	-1.764226	3.242377
O	-3.171966	-2.412005	-2.864950
O	-1.075987	-1.559241	-1.748467
C	-0.658717	2.080442	3.503634
C	-4.483685	-2.342725	1.285212
C	-1.901765	-0.399385	-4.007658
F	-1.608423	2.726654	2.854126
F	-1.197792	1.116251	4.221875
F	-0.027625	2.920943	4.300613
F	-4.335997	-3.629413	1.520223
F	-0.982919	-1.106348	-4.634373
F	-5.510945	-1.879894	1.965825
F	-1.423603	0.798878	-3.739732
F	-4.680700	-2.147653	-0.000915

F	-2.969302	-0.283818	-4.767104
N	-0.351422	3.168064	-1.104620
C	-1.109862	5.288375	-0.645106
H	-1.691345	5.708660	-1.479230
H	-0.908316	6.077018	0.088913
C	0.131507	4.542424	-1.109928
H	0.981617	4.634436	-0.410906
H	0.455981	4.852270	-2.113201
Sc	-1.463632	0.037600	-0.088098
C	1.675745	2.252911	-2.013392
H	2.056352	3.265196	-2.173839
C	2.497221	1.112204	-2.385966
C	2.235821	0.193025	-3.326064
H	1.304363	0.372560	-3.879806
C	2.999830	-1.028801	-3.675900
H	4.053206	-0.991113	-3.356288
H	2.541462	-1.916222	-3.201688
H	2.976700	-1.204325	-4.761465
S	4.061023	0.823547	-1.424225
C	3.702096	-0.645207	-0.466648
C	4.681705	-1.608184	-0.404969
C	2.459842	-0.789774	0.191659
C	4.447624	-2.793878	0.336794
H	5.638079	-1.477334	-0.922985
C	2.217889	-1.931273	0.912398
H	1.704427	-0.005414	0.117294
C	3.194158	-2.959876	1.003321
C	5.424007	-3.817600	0.429541
H	1.260177	-2.051797	1.430870
C	2.963371	-4.148434	1.738939
C	5.169226	-4.959180	1.152242
H	6.380666	-3.681102	-0.084056
C	3.929417	-5.125207	1.811365
H	2.002433	-4.272441	2.247746
H	5.926678	-5.744645	1.219986
H	3.740540	-6.038270	2.382496
C	3.991374	2.135915	-0.127146
H	4.253772	3.059553	-0.667390
H	2.942132	2.193862	0.211929
C	4.948072	1.814275	0.965975
H	4.621135	1.053992	1.687012
C	6.132623	2.409991	1.103779
H	6.800004	2.162811	1.933756
H	6.474223	3.174460	0.396708

γ-*Z*-TS2 ts2_24
SCF = -4418.83900914
Num. Imaginary Freq = 1

C	-2.276724	-1.445609	2.475861
O	-2.655253	-0.467347	1.830940
O	-3.103806	-2.095199	3.263215
C	0.012343	-1.616207	1.653283
O	-0.199241	-0.581490	0.916116
O	-2.105381	-1.005767	-1.111883
O	-1.594751	2.271081	1.603366
O	-2.242088	1.793258	-1.589002
S	-2.072029	-2.523199	-1.069593
S	-3.728460	1.767735	-1.369571
S	-0.320872	2.872302	1.063634
O	-0.897827	-3.074480	-1.734586
O	-2.441311	-3.067719	0.236243

O	-3.903357	1.077424	-0.049573
O	-4.570211	1.352842	-2.471138
O	-0.298057	4.300977	0.840420
O	0.070945	1.974392	-0.065903
C	-3.500210	-2.899946	-2.177368
C	-4.161399	3.534827	-1.040102
C	0.938204	2.555412	2.391007
F	-4.599637	-2.360093	-1.687290
F	-3.274570	-2.415362	-3.382005
F	-3.649453	-4.207982	-2.250716
F	-3.938367	4.236172	-2.131230
F	2.138182	2.734424	1.879661
F	-5.433574	3.610172	-0.712648
F	0.832188	1.325875	2.848681
F	-3.421380	3.998981	-0.055887
F	0.739570	3.407515	3.373509
N	-1.035058	-1.995733	2.511103
C	-2.397713	-3.119507	3.984667
H	-2.282655	-2.779223	5.024337
H	-3.003341	-4.033051	3.968537
C	-1.068520	-3.247936	3.254497
H	-1.042756	-4.095191	2.547326
H	-0.217309	-3.328646	3.944796
Sc	-1.705575	0.545388	0.221343
C	1.178574	-2.336327	1.632766
H	1.263693	-3.235631	2.245466
C	2.343240	-1.978427	0.858597
C	3.287816	-2.909773	0.465475
H	4.219110	-2.548554	0.018512
C	3.276741	-4.322487	0.942261
H	2.276949	-4.779920	0.865164
H	3.983832	-4.938615	0.369169
H	3.579647	-4.379896	2.003183
S	2.449494	-0.333237	0.250065
C	4.197829	-0.079900	-0.049411
C	4.618333	0.453306	-1.246384
C	5.108577	-0.251481	1.027551
C	5.978747	0.805908	-1.437391
H	3.921906	0.622665	-2.072683
C	6.429541	0.076702	0.858264
H	4.754337	-0.647362	1.983479
C	6.904622	0.607604	-0.369864
C	6.442297	1.345090	-2.664356
H	7.137459	-0.061428	1.681442
C	8.264564	0.953297	-0.567411
C	7.768305	1.671076	-2.826072
H	5.725951	1.495269	-3.478242
C	8.686824	1.472967	-1.769140
H	8.970756	0.799055	0.254492
H	8.117982	2.085952	-3.775347
H	9.738493	1.736369	-1.911694
C	2.345314	-3.186141	-1.670180
H	1.386957	-3.447068	-1.207500
H	3.028457	-4.009414	-1.900053
C	2.513801	-1.945841	-2.244899
H	3.420054	-1.738887	-2.825655
C	1.671889	-0.887432	-1.883882
H	1.755515	0.095746	-2.359555
H	0.685426	-1.118963	-1.464693

γ-*E*-TS2 ts2_08
SCF = -4418.83759076
Num. Imaginary Freq = 1

C	-0.131646	-0.601491	2.517653
O	-1.250974	-0.775166	2.033112
O	0.233021	-1.236206	3.609561
C	0.844748	0.830394	0.801775
O	-0.236203	0.701031	0.117969
O	-0.952250	-1.879063	-0.752007
O	-3.226985	1.216868	1.166046
O	-3.606117	-0.812676	-1.347618
S	0.529061	-2.204637	-0.813094
S	-4.224283	-1.891051	-0.500955
S	-3.297144	2.281827	0.099117
O	1.219242	-1.556035	-1.923730
O	1.177174	-2.178740	0.500029
O	-3.472388	-1.827118	0.794293
O	-4.433615	-3.188514	-1.106278
O	-4.595805	2.853117	-0.183611
O	-2.491965	1.746780	-1.036929
C	0.449133	-3.992328	-1.268066
C	-5.913310	-1.249898	-0.103596
C	-2.292761	3.678561	0.792446
F	-0.221529	-4.662997	-0.352889
F	-0.139201	-4.136193	-2.437883
F	1.681487	-4.464150	-1.337785
F	-6.600967	-1.148088	-1.221038
F	-2.945202	4.220581	1.796023
F	-6.506294	-2.097237	0.710197
F	-2.107057	4.572850	-0.158279
F	-5.825555	-0.070290	0.471988
F	-1.119227	3.244456	1.213516
N	0.858987	0.211501	2.069293
C	1.531194	-0.785840	4.032950
H	1.392542	-0.143432	4.915027
H	2.126331	-1.662392	4.314530
C	2.078724	-0.029498	2.831372
H	2.777971	-0.628000	2.220146
H	2.567468	0.911598	3.119723
Sc	-1.973459	-0.252966	0.102226
C	1.962870	1.489773	0.367139
H	2.853439	1.492152	0.998273
C	2.048062	2.087821	-0.942395
C	1.024477	2.735496	-1.597968
H	0.057359	2.709038	-1.081765
C	0.995710	3.196686	-3.011514
H	1.988974	3.282850	-3.475397
H	0.405844	2.484190	-3.614717
H	0.487685	4.169632	-3.099907
S	3.630338	2.252828	-1.692254
C	4.640812	1.048031	-0.846308
C	4.202582	-0.256815	-0.758663
C	5.910627	1.434911	-0.354676
C	5.015739	-1.230954	-0.133266
H	3.222413	-0.558366	-1.145712
C	6.717697	0.494162	0.240083
H	6.249985	2.470045	-0.447453
C	6.296868	-0.853438	0.374090
C	4.580962	-2.575885	0.001755
H	7.700943	0.781360	0.625194
C	7.103929	-1.840650	0.994951

C	5.386339	-3.507115	0.612031
H	3.590903	-2.844655	-0.379431
C	6.658663	-3.136510	1.110253
H	8.086234	-1.550381	1.380955
H	5.045971	-4.541156	0.714860
H	7.288915	-3.889643	1.591362
C	4.032713	4.364263	-0.557543
H	4.061574	3.866363	0.419392
H	5.001299	4.589494	-1.013225
C	2.885383	5.059222	-0.949829
H	2.932572	5.689841	-1.845147
C	1.666725	4.804133	-0.369103
H	0.757867	5.311603	-0.706461
H	1.595295	4.245365	0.570179

γ-*Z*-INT2 int2_03
SCF = -4418.90225355
Num. Imaginary Freq = 0

C	2.022738	2.043738	2.055308
O	2.573155	1.295499	1.256240
O	2.620695	3.099260	2.539382
C	-0.168411	1.033817	2.034167
O	0.261265	0.078578	1.344987
O	0.780968	0.896753	-1.287187
O	3.252449	-1.514387	1.201277
O	2.343298	-1.428818	-1.831188
S	0.007554	2.204492	-1.221105
S	3.477987	-0.533317	-2.253710
S	2.402662	-2.759373	1.264746
O	-1.401818	2.043111	-1.553142
O	0.356752	2.997139	-0.040785
O	3.644014	0.408512	-1.094515
O	3.439717	0.028612	-3.585058
O	3.026031	-4.021185	0.941436
O	1.146139	-2.376729	0.537690
C	0.757887	3.106805	-2.645624
C	4.972401	-1.625208	-2.200614
C	1.906162	-2.856442	3.046722
F	2.058633	3.224085	-2.462984
F	0.528748	2.450404	-3.763870
F	0.213443	4.305497	-2.716818
F	4.882657	-2.506824	-3.172164
F	0.987896	-3.786301	3.182928
F	6.042653	-0.879450	-2.368094
F	1.424697	-1.693463	3.434597
F	5.035310	-2.243378	-1.042682
F	2.964799	-3.159212	3.764321
N	0.743377	1.941325	2.549522
C	1.780848	3.751462	3.513386
H	2.171643	3.501886	4.510422
H	1.849100	4.833185	3.354104
C	0.397788	3.175456	3.254985
H	-0.218742	3.810995	2.595581
H	-0.149169	2.968949	4.184271
Sc	1.839984	-0.299970	0.031238
C	-1.548826	1.257167	2.255440
H	-1.838646	2.076482	2.914257
C	-2.554164	0.622115	1.554805
C	-3.962661	1.142487	1.681010
H	-4.638342	0.392721	1.241455
C	-4.400224	1.338577	3.126703

H	-3.795787	2.081323	3.669573
H	-5.443996	1.691106	3.146405
H	-4.351032	0.391804	3.686098
S	-2.195256	-0.710328	0.485154
C	-3.729743	-1.005997	-0.383828
C	-4.544871	-2.045409	0.007302
C	-4.021905	-0.243499	-1.544562
C	-5.715072	-2.352720	-0.730901
H	-4.301989	-2.639302	0.894912
C	-5.155313	-0.522897	-2.268642
H	-3.334329	0.552547	-1.848889
C	-6.029466	-1.574170	-1.886415
C	-6.581382	-3.410342	-0.351921
H	-5.395189	0.060282	-3.163443
C	-7.201994	-1.882981	-2.621653
C	-7.711086	-3.684759	-1.085564
H	-6.331909	-4.001681	0.534817
C	-8.023690	-2.914029	-2.230277
H	-7.438701	-1.284631	-3.507233
H	-8.373478	-4.501870	-0.786834
H	-8.925177	-3.143224	-2.805334
C	-4.133185	2.418608	0.814992
H	-5.224047	2.550538	0.683828
H	-3.710623	2.236217	-0.188553
C	-3.557350	3.677492	1.376803
H	-3.997089	4.041720	2.316514
C	-2.587068	4.389240	0.799762
H	-2.118264	4.059582	-0.134889
H	-2.224027	5.323816	1.240406

γ-*E*-INT2 int2_06
SCF = -4418.90474987
Num. Imaginary Freq = 0

C	-0.090622	-0.305687	-2.443661
O	1.006215	-0.568856	-1.968864
O	-0.473581	-0.771357	-3.602993
C	-0.997856	0.949054	-0.581205
O	0.119999	0.953153	-0.019569
O	0.954352	-1.552105	0.867937
O	3.112692	1.277407	-1.469830
O	3.673036	-0.557062	1.173492
S	-0.385085	-2.274189	0.886702
S	4.171770	-1.701816	0.329060
S	3.265569	2.439927	-0.521417
O	-0.893612	-2.453414	2.238277
O	-1.305101	-1.790750	-0.143464
O	3.291702	-1.659145	-0.886928
O	4.384561	-2.976765	0.976142
O	4.580107	3.018760	-0.366270
O	2.530279	1.999635	0.708657
C	0.136259	-3.950165	0.309421
C	5.838466	-1.151958	-0.261151
C	2.205367	3.773673	-1.250399
F	0.615498	-3.866632	-0.917347
F	1.063310	-4.433983	1.110195
F	-0.912763	-4.747891	0.316020
F	6.642783	-1.066877	0.775514
F	2.060658	4.727436	-0.357146
F	6.294949	-2.043903	-1.112676
F	1.023655	3.287238	-1.572889

F	5.744455	0.019429	-0.850064
F	2.795931	4.247386	-2.324269
N	-1.080665	0.466477	-1.879939
C	-1.753426	-0.217530	-3.969007
H	-1.574299	0.569559	-4.715690
H	-2.357873	-1.015221	-4.414184
C	-2.309555	0.322056	-2.661585
H	-2.985677	-0.392556	-2.160453
H	-2.822055	1.284754	-2.787241
Sc	1.944008	-0.027657	-0.116242
C	-2.208570	1.361054	0.038668
H	-3.133270	1.151974	-0.501545
C	-2.307424	1.876306	1.307929
C	-1.155209	2.317379	2.168941
H	-0.303918	2.520712	1.498697
C	-1.455262	3.577224	2.971988
H	-2.225008	3.406307	3.743643
H	-0.547358	3.920702	3.489574
H	-1.793265	4.399232	2.322114
S	-3.859699	1.973389	2.100606
C	-4.855902	0.840367	1.149521
C	-5.988865	1.300777	0.518959
C	-4.503049	-0.536601	1.112758
C	-6.827130	0.401728	-0.190688
H	-6.252290	2.363116	0.552095
C	-5.291484	-1.416019	0.417006
H	-3.591446	-0.882020	1.612912
C	-6.469690	-0.979439	-0.248471
C	-8.002461	0.840408	-0.851097
H	-5.022850	-2.476334	0.371527
C	-7.302921	-1.873219	-0.965535
C	-8.791304	-0.051643	-1.539480
H	-8.268670	1.901011	-0.801667
C	-8.438317	-1.419481	-1.596830
H	-7.025675	-2.931396	-1.006083
H	-9.696494	0.294928	-2.045585
H	-9.074376	-2.118518	-2.146923
C	-0.770385	1.124274	3.073802
H	-0.766329	0.187319	2.488761
H	-1.572618	1.009845	3.830155
C	0.550208	1.283712	3.751808
H	0.715820	2.222568	4.299067
C	1.508968	0.355839	3.753625
H	1.380956	-0.595367	3.221081
H	2.455758	0.509376	4.280525

α-TS2 ts2_09
SCF = -4418.81852504
Num. Imaginary Freq = 1

C	0.168580	-1.038988	-2.040095
O	1.332362	-0.722587	-1.801886
O	-0.131451	-1.793648	-3.072460
C	-0.948936	0.177745	-0.233778
O	0.176653	0.633379	0.148798
O	1.523281	-1.592590	0.946166
O	2.637143	1.843541	-1.304166
O	4.048909	0.112820	1.189008
S	1.706585	-3.042008	1.356772
S	4.856235	-0.703202	0.216296
S	2.549228	2.930584	-0.261775
O	3.099045	-3.400946	1.569956

O	0.704809	-3.447410	2.332706
O	3.895268	-0.971625	-0.906780
O	5.652771	-1.795734	0.725421
O	3.618357	3.903958	-0.218878
O	2.202924	2.212234	1.003081
C	1.210126	-3.901618	-0.204568
C	6.095199	0.484655	-0.480136
C	1.031714	3.908343	-0.715119
F	-0.016384	-3.517808	-0.556525
F	2.040948	-3.603380	-1.182503
F	1.209311	-5.201732	-0.005878
F	6.916559	0.844823	0.483107
F	0.659470	4.598596	0.344392
F	6.766248	-0.124121	-1.434831
F	0.048157	3.122894	-1.095063
F	5.495886	1.547598	-0.969720
F	1.340225	4.729509	-1.695117
N	-0.944853	-0.706508	-1.334841
C	-1.539320	-2.080314	-3.106066
H	-1.926040	-1.777380	-4.087268
H	-1.662921	-3.165884	-2.992134
C	-2.136851	-1.282729	-1.945989
H	-2.673686	-1.922791	-1.226959
H	-2.821941	-0.486191	-2.279283
Sc	2.129390	0.126560	-0.004520
C	-2.158857	0.461324	0.374723
H	-3.053647	0.015307	-0.060142
C	-2.362755	1.479644	1.399517
C	-1.453777	2.328078	1.933389
H	-0.433841	2.242425	1.542606
C	-1.682621	3.342223	2.995827
H	-2.746696	3.593304	3.127960
H	-1.303708	2.993750	3.973749
H	-1.132061	4.269037	2.768516
S	-3.998319	1.451955	2.168817
C	-5.091442	1.049239	0.820975
C	-6.039947	0.066061	0.997026
C	-5.033369	1.798722	-0.384272
C	-6.976657	-0.217712	-0.029333
H	-6.088691	-0.510262	1.927053
C	-5.921476	1.526057	-1.394119
H	-4.281771	2.585315	-0.499635
C	-6.913932	0.520647	-1.249802
C	-7.968152	-1.220605	0.120764
H	-5.880961	2.095348	-2.328108
C	-7.846356	0.230428	-2.276796
C	-8.859616	-1.478729	-0.893966
H	-8.010578	-1.782981	1.058890
C	-8.798475	-0.747061	-2.102806
H	-7.794445	0.800642	-3.209752
H	-9.621774	-2.252751	-0.768800
H	-9.514132	-0.962199	-2.901089
C	-3.431298	-0.629361	3.407953
H	-2.708801	-0.000260	3.940290
H	-4.417654	-0.723937	3.870074
C	-2.981081	-1.542660	2.460273
H	-3.679119	-2.272664	2.036469
C	-1.710230	-1.429631	1.943501
H	-0.979100	-0.747582	2.392744
H	-1.318469	-2.140804	1.210748

α-INT2 int2_b_03
SCF = -4418.89556101
Num. Imaginary Freq = 0

C	-0.781241	1.720866	1.303069
O	0.290206	1.162241	1.125588
O	-0.939241	2.672272	2.175243
C	-2.040626	0.575451	-0.405310
O	-1.039966	-0.034787	-0.787477
O	1.212327	1.712070	-1.577698
O	1.136192	-2.153799	-0.298882
O	3.239344	-0.338285	-1.322332
S	0.606908	3.104590	-1.740181
S	3.920150	0.089549	-0.058596
S	1.159514	-2.496236	-1.777213
O	0.733788	3.597508	-3.097559
O	-0.682341	3.223158	-1.058089
O	2.769600	0.364103	0.880603
O	4.966806	1.082356	-0.138066
O	2.255902	-3.312985	-2.246225
O	0.888868	-1.189078	-2.452224
C	1.778229	4.103701	-0.714384
C	4.729336	-1.431444	0.625636
C	-0.359797	-3.526680	-2.007497
F	1.735505	3.689929	0.538896
F	3.004065	3.975967	-1.177177
F	1.412029	5.367248	-0.771517
F	5.679720	-1.803087	-0.203160
F	-0.509831	-3.777362	-3.287968
F	5.245814	-1.132453	1.798019
F	-1.410700	-2.883623	-1.548553
F	3.851205	-2.398924	0.761192
F	-0.204202	-4.649634	-1.341119
N	-1.968705	1.453654	0.644882
C	-2.317233	3.093116	2.239506
H	-2.726243	2.732723	3.194229
H	-2.338061	4.188646	2.222083
C	-2.975399	2.448440	1.026265
H	-3.118763	3.158776	0.196533
H	-3.933609	1.972252	1.272572
Sc	1.108010	0.005610	-0.496751
C	-3.384441	0.406276	-1.071383
C	-4.377059	-0.289233	-0.144815
C	-6.700786	-0.369923	0.891835
H	-7.011516	0.331076	1.684649
H	-7.590623	-0.527008	0.259905
H	-6.420934	-1.328251	1.350987
S	-3.908490	-1.915835	0.467099
C	-2.803166	-1.442202	1.796897
C	-1.517944	-1.939399	1.823335
C	-3.251992	-0.568471	2.823216
C	-0.609414	-1.543639	2.840499
H	-1.163365	-2.611228	1.033888
C	-2.384219	-0.153764	3.803158
H	-4.289242	-0.218211	2.818613
C	-1.037957	-0.608335	3.830090
C	0.729317	-2.012881	2.869323
H	-2.724751	0.527043	4.591300
C	-0.106807	-0.153326	4.796526
C	1.610884	-1.551228	3.819217
H	1.051501	-2.727361	2.105127
C	1.191670	-0.608997	4.786842

H	-0.439968	0.569902	5.547922
H	2.644945	-1.907919	3.823966
H	1.904513	-0.246627	5.532711
H	-3.755275	1.436155	-1.243974
C	-3.240228	-0.302165	-2.417681
H	-3.093584	-1.380285	-2.238315
H	-2.302362	0.022630	-2.906226
C	-4.367563	-0.110039	-3.381889
H	-4.358752	-0.821162	-4.218570
C	-5.325161	0.816877	-3.360487
H	-5.410212	1.574295	-2.573460
H	-6.077844	0.864055	-4.152786
C	-5.599727	0.217070	0.092170
H	-5.818822	1.192876	-0.366735