

Supplementary Material

Computational study on the iodobenzene-catalyzed oxidative cyclization of a δ -alkynyl β -ketoester

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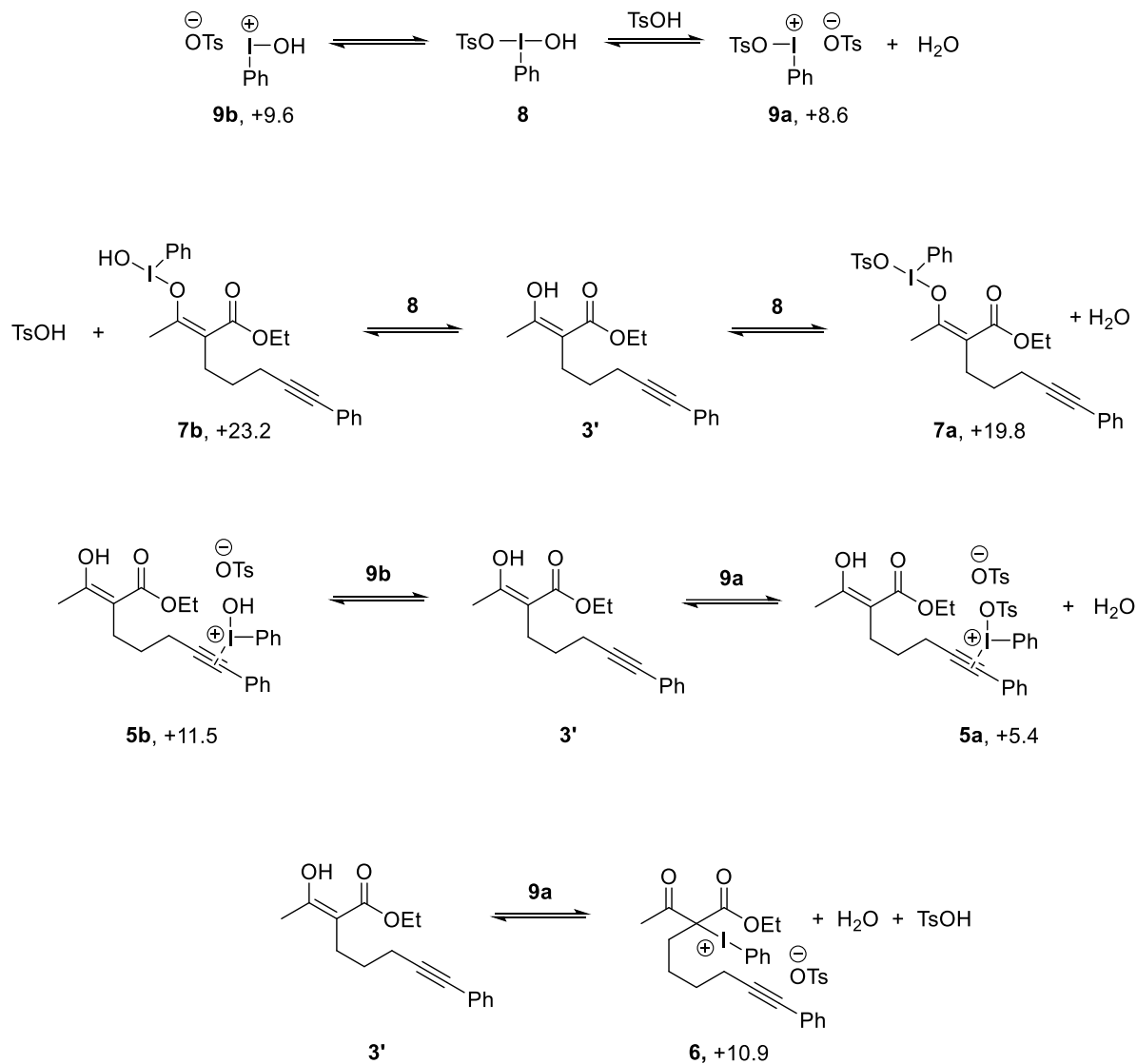
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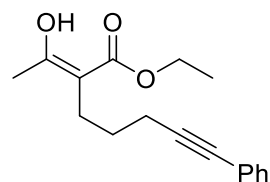
Formation of Possible Intermediates and their Energies



Supplementary Figure 1: Formation of different intermediates. Free energies are reported in kcal/mol

Cartesian Coordinates and Energies of Calculated Structures

3'

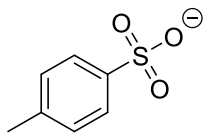


C	-3.00408	-3.26596	-0.27003
H	-3.93959	-3.80464	-0.45365
H	-2.41251	-3.25618	-1.18293
H	-2.46065	-3.82643	0.49796
C	-3.32296	-1.89649	0.25549
C	-2.9262	-0.70039	-0.30202
C	-3.37012	0.51609	0.37264
C	-3.40251	2.89177	0.38911
H	-3.02241	2.91884	1.41475
H	-4.49527	2.90421	0.443
C	-2.85909	4.03022	-0.45199
H	-3.24678	3.98247	-1.47352
H	-3.15869	4.98762	-0.01481
H	-1.76678	3.99929	-0.49557
C	-2.08999	-0.57197	-1.56116
H	-2.13811	-1.49877	-2.14102
H	-2.53415	0.20164	-2.19592
C	-0.61064	-0.19744	-1.32948
H	-0.55541	0.73874	-0.76582
H	-0.13486	-0.00857	-2.29882
C	0.19013	-1.28603	-0.58469
H	0.15672	-2.22225	-1.16044
H	-0.29647	-1.50076	0.37547
C	1.58426	-0.91415	-0.3504
C	2.73788	-0.58595	-0.16784
C	4.09878	-0.20763	0.05336
C	4.95099	0.07316	-1.03222
C	4.61298	-0.10911	1.36091
C	6.27605	0.44058	-0.8131
H	4.56038	-0.0011	-2.04195
C	5.93933	0.25855	1.57174
H	3.96123	-0.3243	2.20145
C	6.77557	0.53463	0.48774
H	6.92134	0.65405	-1.66036
H	6.32198	0.32989	2.5858
H	7.80954	0.82107	0.65568

O -4.06701 -1.97102 1.36005
O -4.05418 0.55028 1.40925
O -2.98023 1.65508 -0.23279
H -4.24042 -1.02874 1.65015
Zero-point correction= 0.333400 (Hartree/Particle)
Thermal correction to Energy= 0.354069
Thermal correction to Enthalpy= 0.355013
Thermal correction to Gibbs Free Energy= 0.279760
SCF Done: E(RB3LYP) = -885.555870 Hartree

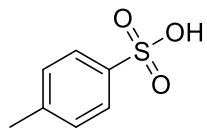
Water

O -1.08285 -1.2936 0.
H -0.12285 -1.2936 0.
H -1.4033 -0.38867 0.
Zero-point correction= 0.021287 (Hartree/Particle)
Thermal correction to Energy= 0.024122
Thermal correction to Enthalpy= 0.025067
Thermal correction to Gibbs Free Energy= 0.003638
SCF Done: E(RB3LYP) = -76.434048 Hartree

Tosylate ion

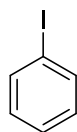
O -0.22019 0.04793 -0.77169
S -0.91651 1.02449 0.25088
O -0.76166 2.41076 -0.20751
O -0.47498 0.67952 1.62107
C -2.65268 0.58692 0.10306
C -3.42546 1.18695 -0.89338
C -3.2111 -0.34457 0.97828
C -4.76948 0.83663 -1.01494
H -2.97818 1.92312 -1.55255
C -4.55966 -0.6809 0.84504
H -2.60139 -0.78287 1.76121
C -5.35888 -0.09901 -0.14966
H -5.37214 1.30219 -1.79087
H -4.99763 -1.40307 1.52941
C -6.82485 -0.44358 -0.26991
H -7.0482 -1.40936 0.19275
H -7.44669 0.31173 0.22687
H -7.14026 -0.4865 -1.31728
Zero-point correction= 0.129791 (Hartree/Particle)

Thermal correction to Energy= 0.140040
 Thermal correction to Enthalpy= 0.140985
 Thermal correction to Gibbs Free Energy= 0.091310
 SCF Done: E(RB3LYP) = -894.880428 Hartree

***p*-Toluenesulfonic acid**

C	-0.20949	-4.51301	0.63571
C	1.18566	-4.41856	0.7282
C	1.8636	-3.38672	0.06515
C	1.14639	-2.44933	-0.69038
C	-0.24877	-2.54379	-0.78287
C	-0.9267	-3.57562	-0.11983
H	-0.72711	-5.30084	1.14196
H	1.73327	-5.13428	1.30506
H	1.66401	-1.6615	-1.19663
H	-0.79637	-1.82807	-1.35974
C	-2.45984	-3.67942	-0.22146
H	-2.87592	-2.70174	-0.34765
H	-2.72116	-4.28933	-1.06088
H	-2.84765	-4.1193	0.67353
S	3.63566	-3.26675	0.18263
O	4.10092	-2.10966	-0.5948
O	4.07586	-3.07602	1.78224
H	5.03158	-3.01132	1.8456
O	4.24607	-4.49263	-0.35061

Zero-point correction= 0.141819 (Hartree/Particle)
 Thermal correction to Energy= 0.152664
 Thermal correction to Enthalpy= 0.153608
 Thermal correction to Gibbs Free Energy= 0.103983
 SCF Done: E(RB3LYP) = -895.396787 Hartree

Iodobenzene

C	0.00001	2.65469	1.2079
C	0.00002	0.56859	0.
C	0.00001	2.65469	-1.2079
H	0.00002	3.1913	2.15234

H	0.00002	3.1913	-2.15234
I	-0.00001	-1.56105	0.
C	0.00001	1.25605	-1.2156
H	0.00002	0.71609	-2.15614
C	0.00002	3.35638	0.
H	0.00003	4.44215	0.
C	0.00001	1.25605	1.2156
H	0.00002	0.71609	2.15614

Zero-point correction= 0.089984 (Hartree/Particle)

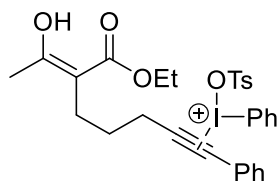
Thermal correction to Energy= 0.095875

Thermal correction to Enthalpy= 0.096819

Thermal correction to Gibbs Free Energy= 0.058229

SCF Done: E(RB3LYP) = -243.079684 Hartree

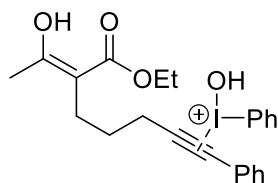
5a



C	3.00411	-3.915	0.01838
H	3.3978	-4.85099	-0.38968
H	2.75316	-4.0653	1.06595
H	2.08678	-3.69741	-0.54077
C	4.01096	-2.83009	-0.22427
C	4.51425	-1.94826	0.70849
C	5.55873	-1.02715	0.25962
C	7.1822	0.61282	0.87066
H	6.83778	1.29682	0.09015
H	7.98233	-0.00151	0.4505
C	7.61973	1.34037	2.12592
H	7.95319	0.6363	2.89407
H	8.45533	2.00581	1.8875
H	6.80816	1.94707	2.53822
C	4.10137	-1.93568	2.16626
H	3.57772	-2.86243	2.41365
H	5.00331	-1.92601	2.78742
C	3.23833	-0.74472	2.6304
H	3.76904	0.19623	2.462
H	3.09804	-0.83863	3.71366
C	1.81585	-0.64734	2.01771
H	1.21206	0.00521	2.65912
H	1.33609	-1.63416	2.03438
C	1.77892	-0.11412	0.64255

O	4.3871	-2.81462	-1.50912
O	5.96738	-0.94169	-0.91251
O	6.07836	-0.26551	1.23527
H	5.08501	-2.10091	-1.60292
C	2.10574	0.29144	-0.4766
I	-0.89922	-0.00438	-0.08158
C	-1.0126	1.99955	0.60793
C	-1.41591	2.22193	1.92399
C	-0.71522	3.02471	-0.29169
C	-1.50148	3.54718	2.35772
H	-1.70047	1.40397	2.57616
C	-0.80631	4.33979	0.17092
H	-0.42766	2.81927	-1.31587
C	-1.19298	4.59807	1.48948
H	-1.82068	3.75015	3.37455
H	-0.5838	5.15798	-0.506
H	-1.26487	5.6231	1.83784
O	-3.00308	-0.14046	-0.33406
S	-3.78394	-0.96288	0.87773
O	-3.28304	-2.3374	0.86021
O	-3.65808	-0.16481	2.10205
C	-5.42599	-0.86273	0.21729
C	-6.23549	0.2258	0.55942
C	-5.87505	-1.8733	-0.63792
C	-7.52276	0.28848	0.03446
H	-5.86751	0.99294	1.23095
C	-7.16571	-1.78738	-1.14983
H	-5.2313	-2.71084	-0.88097
C	-8.00896	-0.71172	-0.82544
H	-8.16346	1.12445	0.29881
H	-7.52772	-2.5709	-1.80864
C	-9.41512	-0.65028	-1.36291
H	-9.48856	-1.12196	-2.34649
H	-10.10461	-1.17969	-0.69327
H	-9.7681	0.38071	-1.44732
C	2.48692	0.75311	-1.76405
C	2.57043	-0.15169	-2.84826
C	2.73787	2.12675	-1.98154
C	2.93346	0.3082	-4.10977
H	2.37078	-1.2037	-2.68284
C	3.1031	2.57238	-3.24696
H	2.65752	2.82135	-1.15135
C	3.20428	1.66629	-4.3095
H	3.01295	-0.39139	-4.93572

H 3.31461 3.62382 -3.40899
 H 3.49346 2.01991 -5.29396
 Zero-point correction= 0.555646 (Hartree/Particle)
 Thermal correction to Energy= 0.596372
 Thermal correction to Enthalpy= 0.597316
 Thermal correction to Gibbs Free Energy= 0.469546
 SCF Done: E(RB3LYP) = -2023.113423 Hartree

5b

C	-3.63603	-2.93403	0.54498
H	-4.68721	-3.1936	0.37174
H	-3.05656	-3.32957	-0.29151
H	-3.31916	-3.42207	1.46809
C	-3.48901	-1.44694	0.7018
C	-3.48591	-0.52779	-0.33941
C	-3.40089	0.88874	0.02185
C	-3.54707	3.15468	-0.71835
H	-2.64359	3.4596	-0.18274
H	-4.40106	3.30096	-0.05175
C	-3.71321	3.88841	-2.03345
H	-4.60962	3.55167	-2.56195
H	-3.81487	4.96083	-1.83984
H	-2.84695	3.74046	-2.68547
C	-3.7566	-0.92195	-1.77619
H	-4.06034	-1.97176	-1.816
H	-4.60484	-0.34436	-2.16009
C	-2.55616	-0.708	-2.71539
H	-2.38115	0.36066	-2.86328
H	-2.75761	-1.14938	-3.69695
C	-1.2836	-1.3613	-2.14214
H	-0.4397	-1.16116	-2.81621
H	-1.40703	-2.45217	-2.10999
C	-0.91863	-0.89307	-0.80016
O	-3.3743	-1.08215	1.9701
O	-3.30294	1.30641	1.18815
O	-3.44776	1.73058	-1.02049
H	-3.33478	-0.07765	1.99185
C	-0.33135	-0.58756	0.24733

I	2.05409	-1.24105	-0.7702
C	2.66898	0.76351	-0.39793
C	2.67125	1.65776	-1.46878
C	3.14101	1.09197	0.87297
C	3.17115	2.94277	-1.24479
H	2.31427	1.37122	-2.45147
C	3.63841	2.38371	1.06988
H	3.12535	0.37939	1.68959
C	3.65351	3.30256	0.01751
H	3.19063	3.65533	-2.06323
H	4.01461	2.66338	2.04873
H	4.04648	4.30121	0.17944
C	-0.14012	-0.20566	1.6232
C	0.04152	-1.19555	2.60744
C	-0.15812	1.15094	1.98937
C	0.17332	-0.82822	3.94403
H	0.04781	-2.24368	2.32472
C	-0.02931	1.50742	3.33013
H	-0.30337	1.91125	1.23044
C	0.13431	0.52231	4.3082
H	0.29364	-1.5945	4.70326
H	-0.0681	2.55472	3.61264
H	0.22582	0.80442	5.3524
O	3.89395	-1.73058	-1.54306
H	4.49184	-2.02293	-0.83309

Zero-point correction= 0.437479 (Hartree/Particle)

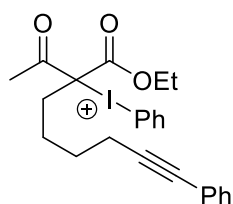
Thermal correction to Energy= 0.468335

Thermal correction to Enthalpy= 0.469279

Thermal correction to Gibbs Free Energy= 0.367793

SCF Done: E(RB3LYP) = -1204.137816 Hartree

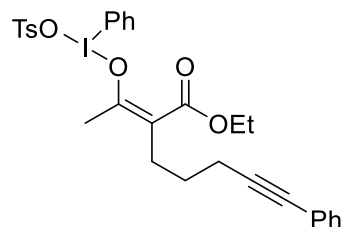
6



C	-3.295755	-2.267949	0.022274
O	-4.147728	-2.199390	0.879221
C	-3.425991	-3.158753	-1.191378
H	-4.481168	-3.232508	-1.459911
H	-2.840307	-2.833336	-2.055367
H	-3.081809	-4.165216	-0.924319

C	-1.974694	-1.486740	0.278400
C	-0.729868	-2.349005	0.224929
H	-0.837840	-3.000381	1.106441
H	-0.769590	-3.000458	-0.653613
C	-2.110824	-0.639019	1.555751
O	-1.543391	-0.997832	2.561280
O	-2.930704	0.393638	1.428916
C	-3.286886	1.096185	2.672744
C	-4.588807	1.828984	2.432909
H	-2.459813	1.769700	2.913064
H	-3.368321	0.349532	3.463963
H	-4.879921	2.348226	3.350597
H	-4.495108	2.576170	1.639736
H	-5.386490	1.130919	2.167554
C	0.627903	-1.638824	0.303281
C	1.797162	-2.638365	0.439072
H	0.647127	-0.948854	1.150275
H	0.782587	-1.052031	-0.608847
H	1.696226	-3.190304	1.382891
H	1.739315	-3.386419	-0.363696
I	-1.914596	0.017669	-1.608268
C	-1.015288	1.827647	-0.890642
C	-1.866188	2.836928	-0.444359
C	0.369687	1.958920	-0.964159
C	-1.282964	4.041804	-0.046834
H	-2.939349	2.698821	-0.406393
C	0.923368	3.174201	-0.554696
H	1.007912	1.160442	-1.322640
C	0.102669	4.207831	-0.099397
H	-1.919727	4.849402	0.299497
H	1.999666	3.304451	-0.598475
H	0.544658	5.148529	0.211961
C	3.090560	-1.962535	0.390210
C	4.150473	-1.374226	0.343240
C	5.406821	-0.692569	0.295316
C	6.123795	-0.599550	-0.913164
C	5.944333	-0.106711	1.457679
C	7.346840	0.064241	-0.953644
H	5.716057	-1.056249	-1.809212
C	7.168232	0.554781	1.407724
H	5.397481	-0.182600	2.391882
C	7.871816	0.643010	0.204207
H	7.894208	0.126703	-1.889171
H	7.576569	0.998995	2.310293

H 8.827428 1.156956 0.169591
 Zero-point correction= 0.411596 (Hartree/Particle)
 Thermal correction to Energy= 0.440589
 Thermal correction to Enthalpy= 0.441533
 Thermal correction to Gibbs Free Energy= 0.344317
 SCF Done: E(RB3LYP) = -1127.676348 Hartree

7a

C	0.978708	-1.191481	-2.950452
C	1.020968	-1.977947	-1.661115
H	0.376902	-0.283918	-2.822822
H	1.960794	-0.884039	-3.304879
H	0.490662	-1.786633	-3.731168
C	2.173055	-2.409268	-1.066022
O	-0.181066	-2.357383	-1.182925
C	2.233275	-3.160654	0.222512
O	3.249652	-3.733957	0.588030
O	1.109603	-3.136380	0.969892
C	1.143583	-3.907527	2.194489
C	1.786784	-3.139065	3.338964
H	1.674067	-4.843894	2.006704
H	0.092407	-4.122214	2.401470
H	1.723316	-3.729266	4.259635
H	2.840679	-2.947268	3.126434
H	1.275626	-2.186805	3.506176
C	3.537801	-2.242322	-1.708183
C	4.328667	-1.044488	-1.150843
H	3.452678	-2.153101	-2.794858
H	4.106696	-3.155097	-1.509644
C	5.749322	-0.957167	-1.749492
H	3.793786	-0.109056	-1.357124
H	4.405080	-1.135684	-0.062514
H	6.291142	-1.885543	-1.524211
H	5.681165	-0.903325	-2.845153
C	-0.943748	-0.260421	0.971242
C	-1.705090	-0.329137	2.132970
C	0.343756	0.264050	0.926356
C	-1.132145	0.165189	3.307269

H	-2.718474	-0.717758	2.126587
C	0.894681	0.744348	2.116707
H	0.915041	0.298346	0.007340
C	0.159148	0.696525	3.301366
H	-1.706589	0.131658	4.227802
H	1.897350	1.159863	2.107881
H	0.591473	1.078628	4.220965
C	6.513765	0.186156	-1.254553
C	7.127996	1.142270	-0.829724
C	7.861798	2.263715	-0.331901
C	8.681735	2.136184	0.806198
C	7.778873	3.516587	-0.969945
C	9.395260	3.230513	1.288006
H	8.750261	1.172978	1.301273
C	8.495459	4.606149	-0.481883
H	7.149733	3.620624	-1.848047
C	9.305500	4.468391	0.647450
H	10.024205	3.116828	2.166222
H	8.422232	5.566036	-0.984928
H	9.863726	5.319778	1.025394
I	-1.798912	-1.010441	-0.843870
O	-3.465110	0.437837	-0.375996
S	-4.865004	-0.232597	-0.062388
O	-4.862604	-0.771403	1.309801
O	-5.230582	-1.138058	-1.162215
C	-5.937332	1.197385	-0.104614
C	-6.168341	1.919019	1.066068
C	-6.529199	1.573625	-1.310978
C	-6.997363	3.037662	1.019393
H	-5.718677	1.592645	1.997050
C	-7.355316	2.694050	-1.338450
H	-6.356756	0.981200	-2.202652
C	-7.597455	3.446432	-0.179629
H	-7.187133	3.598900	1.930408
H	-7.826143	2.986166	-2.273406
C	-8.470424	4.676976	-0.228711
H	-9.291474	4.557153	-0.941750
H	-8.900092	4.903087	0.751062
H	-7.892763	5.554908	-0.543606

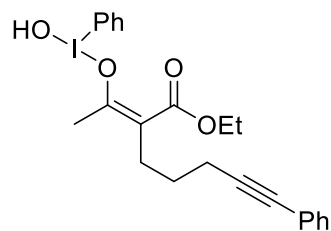
Zero-point correction= 0.545053 (Hartree/Particle)

Thermal correction to Energy= 0.585191

Thermal correction to Enthalpy= 0.586135

Thermal correction to Gibbs Free Energy= 0.460072

SCF Done: E(RB3LYP) = -2022.65151585 Hartree

7b

C	1.130657	0.258589	-2.536156
C	1.402304	1.135685	-1.332454
H	1.148804	-0.797458	-2.242056
H	0.166813	0.448974	-3.002615
H	1.915564	0.397876	-3.289057
C	0.481341	2.039121	-0.856987
O	2.611041	1.014601	-0.783295
O	0.648809	2.860231	0.360182
O	-0.161905	3.711606	0.703599
O	1.757181	2.599630	1.113163
C	1.931967	3.428445	2.282605
C	1.159536	2.896129	3.481361
H	1.620563	4.448031	2.045395
H	3.009555	3.411661	2.466838
H	1.362008	3.516127	4.361506
H	0.085821	2.921492	3.283162
H	1.457616	1.869075	3.716328
C	-0.841163	2.306547	-1.558508
C	-2.006055	1.458849	-1.016984
H	-0.751058	2.157841	-2.639337
H	-1.086134	3.362045	-1.410450
C	-3.348176	1.815284	-1.692687
H	-1.799380	0.392009	-1.164327
H	-2.094840	1.618361	0.062475
H	-3.565366	2.878189	-1.521034
H	-3.250774	1.698077	-2.781456
C	2.742227	-1.608762	0.715917
C	2.822680	-2.982719	0.893539
C	1.963374	-0.768455	1.497210
C	2.062226	-3.546135	1.922466
H	3.468920	-3.581473	0.261531
C	1.213688	-1.360699	2.519657
H	1.939641	0.302182	1.324707
C	1.259500	-2.739195	2.730383
H	2.100296	-4.619285	2.083892
H	0.593641	-0.730281	3.149880

H	0.670019	-3.185515	3.525373
C	-4.470837	1.007041	-1.219960
C	-5.388023	0.323208	-0.815759
C	-6.476958	-0.474106	-0.344755
C	-7.319545	-0.004439	0.681741
C	-6.730181	-1.743896	-0.899348
C	-8.381312	-0.782664	1.135479
H	-7.129702	0.973116	1.112924
C	-7.793863	-2.516243	-0.440112
H	-6.084918	-2.111222	-1.690801
C	-8.623329	-2.040038	0.577658
H	-9.022735	-0.406311	1.927226
H	-7.976786	-3.493186	-0.878426
H	-9.452635	-2.644310	0.933417
I	3.919291	-0.742910	-0.895471
O	5.115709	-2.436803	-0.853609
I	5.743193	-2.334724	-0.120909

Zero-point correction= 0.426689 (Hartree/Particle)

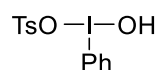
Thermal correction to Energy= 0.456625

Thermal correction to Enthalpy= 0.457569

Thermal correction to Gibbs Free Energy= 0.357873

SCF Done: E(RB3LYP) = -1203.68855760 Hartree

8



I	-1.38281	-1.43738	0.14472
C	-2.7185	0.21927	0.07223
C	-2.74492	1.00254	-1.07858
C	-3.53706	0.46031	1.17442
C	-3.64835	2.06868	-1.12157
H	-2.06031	0.81971	-1.89856
C	-4.43543	1.52836	1.10654
H	-3.47726	-0.14956	2.06934
C	-4.49138	2.32755	-0.03853
H	-3.67961	2.69975	-2.00416
H	-5.08017	1.73764	1.95459
H	-5.1866	3.16036	-0.08171
O	-2.88745	-2.74008	-0.37874
H	-3.38753	-3.00981	0.40721
O	0.22017	0.04759	0.77169
S	0.91648	1.02441	-0.25065
O	0.76151	2.41058	0.20801

O	0.47503	0.6797	-1.62092
C	2.65266	0.58689	-0.10283
C	3.42533	1.18665	0.89381
C	3.21117	-0.34437	-0.97829
C	4.76938	0.83633	1.01537
H	2.97799	1.9226	1.55319
C	4.55971	-0.68068	-0.84505
H	2.60151	-0.7825	-1.76133
C	5.35887	-0.09901	0.14986
H	5.37196	1.30167	1.79149
H	4.99774	-1.40267	-1.52958
C	6.82489	-0.44346	0.26974
H	7.04695	-1.41242	-0.18688
H	7.44612	0.30817	-0.23337
H	7.14226	-0.47946	1.31676

Zero-point correction= 0.234981 (Hartree/Particle)

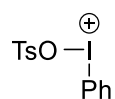
Thermal correction to Energy= 0.254950

Thermal correction to Enthalpy= 0.255894

Thermal correction to Gibbs Free Energy= 0.180731

SCF Done: E(RB3LYP) = -1213.614807 Hartree

9a



I	1.71244	-1.31679	-0.54557
C	2.75457	0.4732	-0.1864
C	2.96785	0.86911	1.14019
C	3.23736	1.18524	-1.29324
C	3.70695	2.03199	1.35428
H	2.56035	0.30934	1.97413
C	3.9783	2.34034	-1.04585
H	3.04926	0.8573	-2.30954
C	4.21082	2.7593	0.26929
H	3.88739	2.36682	2.37048
H	4.37089	2.91053	-1.88137
H	4.78881	3.66007	0.44994
O	-0.20617	-0.67524	-0.52653
S	-1.03899	-0.7951	0.9991
O	-0.29776	0.06786	1.91403
O	-1.18954	-2.21964	1.25981
C	-2.52399	-0.05187	0.41132
C	-2.66795	1.34096	0.49059
C	-3.52729	-0.87732	-0.11644
C	-3.85451	1.90624	0.04059

H	-1.87894	1.95443	0.91085
C	-4.70247	-0.28288	-0.56036
H	-3.39136	-1.95218	-0.15923
C	-4.88853	1.11077	-0.49046
H	-3.98699	2.98204	0.10524
H	-5.49287	-0.90905	-0.96292
C	-6.17929	1.73655	-0.94541
H	-6.66286	1.1402	-1.72329
H	-6.88037	1.80947	-0.10416
H	-6.02209	2.74874	-1.32743

Zero-point correction= 0.221305 (Hartree/Particle)

Thermal correction to Energy= 0.239282

Thermal correction to Enthalpy= 0.240226

Thermal correction to Gibbs Free Energy= 0.170574

SCF Done: E(RB3LYP) = -1137.531731 Hartree

9b



I	1.34288	0.01984	-0.30325
C	-0.74599	0.00805	-0.08307
C	-1.40137	-1.23158	-0.06251
C	-1.41547	1.23726	0.0092
C	-2.7904	-1.22538	0.05557
H	-0.85833	-2.1675	-0.13384
C	-2.80447	1.20974	0.12293
H	-0.88441	2.18262	-0.01392
C	-3.48554	-0.01347	0.14738
H	-3.32683	-2.16835	0.07417
H	-3.35178	2.1441	0.19178
H	-4.56726	-0.02207	0.23571
O	1.94975	-0.20056	1.57454
H	2.0777	0.67624	1.98518

Zero-point correction= 0.103482 (Hartree/Particle)

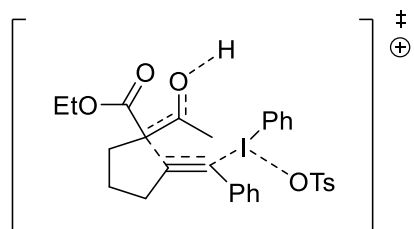
Thermal correction to Energy= 0.111516

Thermal correction to Enthalpy= 0.112460

Thermal correction to Gibbs Free Energy= 0.068866

SCF Done: E(RB3LYP) = -318.555934 Hartree

TS[5-10a]



C	-2.57661	-0.91834	-3.66935
H	-2.67031	-1.70373	-4.43044
H	-3.55362	-0.45282	-3.54625
H	-1.86249	-0.18299	-4.04429
C	-2.04322	-1.52582	-2.40659
C	-2.83312	-2.08354	-1.38608
C	-2.11798	-2.80683	-0.31058
C	-2.26078	-4.26765	1.57257
H	-1.67976	-3.58862	2.20188
H	-1.56694	-4.955	1.08318
C	-3.34917	-4.98633	2.34092
H	-3.92224	-5.65148	1.68874
H	-2.88954	-5.59384	3.12657
H	-4.03673	-4.28029	2.81585
C	-4.31027	-2.33595	-1.5713
H	-4.60643	-2.11876	-2.60044
H	-4.52055	-3.39643	-1.40191
C	-5.16955	-1.49559	-0.60739
H	-5.05432	-1.85746	0.41794
H	-6.22804	-1.57115	-0.87344
C	-4.72121	-0.03527	-0.69934
H	-5.31273	0.58698	-0.00606
H	-4.89333	0.36269	-1.70723
C	-3.3456	0.22825	-0.27558
O	-0.73043	-1.52959	-2.36707
O	-0.88542	-2.80984	-0.19935
O	-2.91276	-3.4682	0.52702
H	-0.42514	-2.04384	-1.5522
C	-2.47653	0.92296	0.34651
I	-0.13075	0.3833	0.5706
C	0.36926	1.95425	-0.78205
C	0.77529	1.6007	-2.06761
C	0.3309	3.26791	-0.31884
C	1.14634	2.63427	-2.9327
H	0.83729	0.56286	-2.37319
C	0.70371	4.28133	-1.20734
H	0.03111	3.5051	0.69499
C	1.10641	3.96588	-2.50749

H	1.47656	2.38945	-3.9375
H	0.68658	5.31353	-0.87212
H	1.4004	4.75878	-3.18805
O	2.05451	0.1205	0.88853
S	2.67013	-1.2248	0.24736
O	2.40184	-2.35434	1.14204
O	2.20647	-1.30944	-1.15247
C	4.40711	-0.8208	0.29158
C	4.99086	-0.15252	-0.78808
C	5.15436	-1.17836	1.41633
C	6.34885	0.15191	-0.73493
H	4.39442	0.10554	-1.65603
C	6.51135	-0.86153	1.44988
H	4.68207	-1.70441	2.23857
C	7.13091	-0.19641	0.37982
H	6.81186	0.66404	-1.57401
H	7.09933	-1.14017	2.31983
C	8.60928	0.10322	0.4062
H	8.94145	0.38937	1.40836
H	9.1847	-0.78564	0.11629
H	8.87204	0.90486	-0.28844
C	-2.79196	2.16728	1.10481
C	-2.59538	2.23221	2.49414
C	-3.31155	3.28098	0.42341
C	-2.92661	3.39547	3.19043
H	-2.19594	1.37708	3.03055
C	-3.63164	4.44361	1.12765
H	-3.4467	3.24015	-0.65321
C	-3.44281	4.50345	2.51075
H	-2.77914	3.43493	4.26521
H	-4.02876	5.30088	0.59276
H	-3.69501	5.40707	3.05651

Zero-point correction= 0.554605 (Hartree/Particle)

Thermal correction to Energy= 0.594172

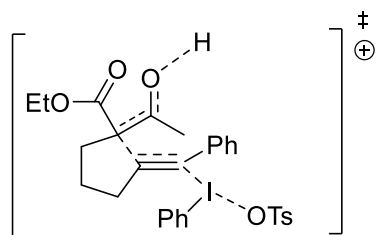
Thermal correction to Enthalpy= 0.595116

Thermal correction to Gibbs Free Energy= 0.473163

SCF Done: E(RB3LYP) = -2023.083617 Hartree

Imaginary Frequency = -125.17 cm⁻¹

TS[5-10b]



C	-3.81561	-2.17584	-3.17589
H	-4.64262	-2.14875	-3.89713
H	-2.97874	-1.62814	-3.61077
H	-3.53681	-3.21965	-3.02427
C	-4.277	-1.59384	-1.8776
C	-4.34017	-0.20529	-1.59082
C	-5.04345	0.1679	-0.33867
C	-6.04834	1.89689	0.9695
H	-5.45195	1.6318	1.84623
H	-6.98395	1.33398	1.00505
C	-6.27083	3.38879	0.84469
H	-6.85571	3.62944	-0.04742
H	-6.82558	3.74098	1.71977
H	-5.32222	3.93161	0.80156
C	-4.23715	0.82756	-2.69793
H	-4.12404	0.32958	-3.66391
H	-5.16361	1.40714	-2.74826
C	-3.03962	1.76362	-2.46215
H	-3.25403	2.44843	-1.6369
H	-2.82772	2.36514	-3.3505
C	-1.82854	0.89062	-2.11032
H	-0.98682	1.52061	-1.79771
H	-1.49948	0.32059	-2.98903
C	-2.13209	-0.03409	-0.99595
O	-4.64114	-2.49204	-1.00183
O	-5.36951	-0.66117	0.52798
O	-5.30915	1.46011	-0.22303
H	-5.02551	-2.00114	-0.19935
C	-1.71229	-0.65169	0.04121
I	0.72822	-0.40444	0.11117
C	0.88719	-1.72358	1.79534
C	0.9624	-1.14837	3.06112
C	0.94136	-3.09721	1.56753
C	1.08158	-2.01375	4.15499
H	0.98201	-0.07115	3.19736
C	1.05594	-3.93693	2.67913
H	0.91002	-3.51436	0.56752

C	1.12211	-3.39727	3.96718
H	1.15123	-1.59247	5.15298
H	1.11044	-5.01075	2.52972
H	1.22055	-4.05663	4.82372
O	2.96472	-0.31743	0.11601
S	3.5378	1.12183	0.55722
O	2.96666	2.14086	-0.33629
O	3.33576	1.28086	2.00935
C	5.26896	0.89162	0.20881
C	6.11548	0.41371	1.21224
C	5.74746	1.18436	-1.0717
C	7.4666	0.2354	0.92135
H	5.72422	0.20308	2.20126
C	7.10118	0.99856	-1.34011
H	5.07397	1.56452	-1.83184
C	7.98159	0.52323	-0.3532
H	8.13311	-0.12892	1.69805
H	7.48233	1.23056	-2.3307
C	9.45162	0.359	-0.64879
H	9.98425	1.30509	-0.4909
H	9.91099	-0.38893	0.00328
H	9.61947	0.06012	-1.68754
C	-2.18077	-1.60847	1.15328
C	-2.19892	-2.98507	0.92719
C	-2.58683	-1.09888	2.38656
C	-2.62369	-3.85177	1.93399
H	-1.87946	-3.38645	-0.04548
C	-3.01082	-1.96577	3.3941
H	-2.57241	-0.01395	2.56498
C	-3.02944	-3.34202	3.16798
H	-2.63862	-4.93678	1.75564
H	-3.33053	-1.56373	4.36653
H	-3.36426	-4.02558	3.96167

Zero-point correction= 0.555109 (Hartree/Particle)

Thermal correction to Energy= 0.594635

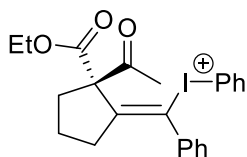
Thermal correction to Enthalpy= 0.595579

Thermal correction to Gibbs Free Energy= 0.472820

SCF Done: E(RB3LYP) = -2023.101181 Hartree

Imaginary Frequency = -212.56 cm⁻¹

10a



C	1.07268	-1.20389	2.84715
H	1.18387	-1.64917	3.84157
H	1.66585	-0.28899	2.79267
H	0.00933	-0.9785	2.71116
C	1.45893	-2.2429	1.81445
C	2.74977	-2.07128	0.95948
C	2.59117	-2.97575	-0.28978
C	1.1902	-3.45587	-2.16464
H	1.01499	-4.43479	-1.71247
H	2.02742	-3.54051	-2.86361
C	-0.06164	-2.89488	-2.80769
H	0.12879	-1.92539	-3.28031
H	-0.39306	-3.58576	-3.59053
H	-0.87336	-2.78628	-2.0815
C	3.92168	-2.61588	1.83412
H	3.79311	-2.25779	2.8633
H	3.91928	-3.70626	1.84439
C	5.18088	-1.99749	1.21915
H	5.45865	-2.54998	0.31637
H	6.03567	-2.01653	1.90172
C	4.74039	-0.56823	0.87055
H	5.3018	-0.12016	0.04618
H	4.87368	0.09309	1.73672
C	3.24156	-0.66982	0.55125
O	0.84751	-3.28769	1.71796
O	3.26927	-3.95226	-0.51933
O	1.59659	-2.54944	-1.08672
C	2.59657	0.35017	-0.03462
I	0.45878	0.17881	-0.53619
C	-0.07002	2.12134	0.1914
C	-0.81294	2.19356	1.36721
C	0.28564	3.24585	-0.54921
C	-1.18277	3.46033	1.82952
H	-1.15291	1.29303	1.86846
C	-0.09523	4.50225	-0.06705
H	0.84083	3.16242	-1.47595
C	-0.82134	4.60945	1.1211
H	-1.77115	3.53897	2.73867
H	0.17249	5.39093	-0.63048

H	-1.11974	5.58764	1.48632
O	-2.12526	0.12844	-0.85381
S	-2.77909	-0.86674	0.10423
O	-2.63579	-2.25976	-0.37621
O	-2.33764	-0.62116	1.50983
C	-4.53232	-0.45124	0.03507
C	-5.19493	-0.00903	1.17736
C	-5.22194	-0.59314	-1.17327
C	-6.55828	0.29668	1.10693
H	-4.64538	0.0847	2.10763
C	-6.57816	-0.28224	-1.2298
H	-4.69902	-0.94501	-2.05645
C	-7.27024	0.16686	-0.09149
H	-7.07361	0.63835	2.0014
H	-7.11126	-0.39243	-2.17145
C	-8.74597	0.48447	-0.16603
H	-8.96118	1.19321	-0.97392
H	-9.33606	-0.41893	-0.3627
H	-9.10799	0.92067	0.76949
C	3.23882	1.62397	-0.43678
C	3.54575	1.87305	-1.78647
C	3.5622	2.59842	0.52143
C	4.17546	3.06	-2.16371
H	3.29747	1.12808	-2.53758
C	4.19282	3.78543	0.14254
H	3.31344	2.42484	1.56409
C	4.50115	4.01996	-1.19979
H	4.41475	3.2335	-3.20882
H	4.43639	4.52857	0.89613
H	4.9904	4.94366	-1.49414

Zero-point correction= 0.545275 (Hartree/Particle)

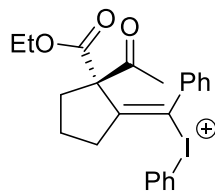
Thermal correction to Energy= 0.584349

Thermal correction to Enthalpy= 0.585294

Thermal correction to Gibbs Free Energy= 0.466164

SCF Done: E(RB3LYP) = -2022.769357 Hartree

10b



C	1.07268	-1.20389	2.84715
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H	1.18387	-1.64917	3.84157
H	1.66585	-0.28899	2.79267
H	0.00933	-0.9785	2.71116
C	1.45893	-2.2429	1.81445
C	2.74977	-2.07128	0.95948
C	2.59117	-2.97575	-0.28978
C	1.1902	-3.45587	-2.16464
H	1.01499	-4.43479	-1.71247
H	2.02742	-3.54051	-2.86361
C	-0.06164	-2.89488	-2.80769
H	0.12879	-1.92539	-3.28031
H	-0.39306	-3.58576	-3.59053
H	-0.87336	-2.78628	-2.0815
C	3.92168	-2.61588	1.83412
H	3.79311	-2.25779	2.8633
H	3.91928	-3.70626	1.84439
C	5.18088	-1.99749	1.21915
H	5.45865	-2.54998	0.31637
H	6.03567	-2.01653	1.90172
C	4.74039	-0.56823	0.87055
H	5.3018	-0.12016	0.04618
H	4.87368	0.09309	1.73672
C	3.24156	-0.66982	0.55125
O	0.84751	-3.28769	1.71796
O	3.26927	-3.95226	-0.51933
O	1.59659	-2.54944	-1.08672
C	2.59657	0.35017	-0.03462
I	0.45878	0.17881	-0.53619
C	-0.07002	2.12134	0.1914
C	-0.81294	2.19356	1.36721
C	0.28564	3.24585	-0.54921
C	-1.18277	3.46033	1.82952
H	-1.15291	1.29303	1.86846
C	-0.09523	4.50225	-0.06705
H	0.84083	3.16242	-1.47595
C	-0.82134	4.60945	1.1211
H	-1.77115	3.53897	2.73867
H	0.17249	5.39093	-0.63048
H	-1.11974	5.58764	1.48632
O	-2.12526	0.12844	-0.85381
S	-2.77909	-0.86674	0.10423
O	-2.63579	-2.25976	-0.37621
O	-2.33764	-0.62116	1.50983
C	-4.53232	-0.45124	0.03507

C	-5.19493	-0.00903	1.17736
C	-5.22194	-0.59314	-1.17327
C	-6.55828	0.29668	1.10693
H	-4.64538	0.0847	2.10763
C	-6.57816	-0.28224	-1.2298
H	-4.69902	-0.94501	-2.05645
C	-7.27024	0.16686	-0.09149
H	-7.07361	0.63835	2.0014
H	-7.11126	-0.39243	-2.17145
C	-8.74597	0.48447	-0.16603
H	-8.96118	1.19321	-0.97392
H	-9.33606	-0.41893	-0.3627
H	-9.10799	0.92067	0.76949
C	3.23882	1.62397	-0.43678
C	3.54575	1.87305	-1.78647
C	3.5622	2.59842	0.52143
C	4.17546	3.06	-2.16371
H	3.29747	1.12808	-2.53758
C	4.19282	3.78543	0.14254
H	3.31344	2.42484	1.56409
C	4.50115	4.01996	-1.19979
H	4.41475	3.2335	-3.20882
H	4.43639	4.52857	0.89613
H	4.9904	4.94366	-1.49414

Zero-point correction= 0.545275 (Hartree/Particle)

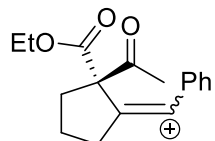
Thermal correction to Energy= 0.584349

Thermal correction to Enthalpy= 0.585294

Thermal correction to Gibbs Free Energy= 0.466164

SCF Done: E(RB3LYP) = -2022.769357 Hartree

11



C	-1.52457	-2.28974	-1.85497
H	-1.24697	-3.32084	-2.08051
H	-1.98617	-1.82063	-2.73056
H	-0.60716	-1.72777	-1.62159
C	-2.43657	-2.27893	-0.66198
C	-3.384	-1.05372	-0.43143
C	-3.52812	-0.86277	1.092
C	-2.24395	-0.45649	3.06996
H	-2.52824	-1.44251	3.44786

H	-2.96644	0.27595	3.44389
C	-0.80994	-0.10173	3.406
H	-0.55015	0.89801	3.04634
H	-0.68284	-0.12398	4.49405
H	-0.11418	-0.80861	2.94648
C	-4.75095	-1.37924	-1.11458
H	-4.59659	-2.12837	-1.8992
H	-5.43732	-1.79763	-0.37712
C	-5.23891	-0.06348	-1.73634
H	-5.72404	0.55995	-0.97694
H	-5.95343	-0.21744	-2.55089
C	-3.94599	0.6118	-2.22438
H	-4.03249	1.68573	-2.40499
H	-3.58399	0.14049	-3.14709
C	-2.96623	0.27942	-1.0891
O	-2.53687	-3.20942	0.11174
O	-4.55673	-1.02063	1.71385
O	-2.35424	-0.50242	1.61437
C	-2.0484	1.11345	-0.71852
C	-1.20213	2.12274	-0.38824
C	-1.64262	3.15754	0.51786
C	0.10137	2.21391	-0.99099
C	-0.85575	4.26081	0.71996
H	-2.60418	3.04805	1.00792
C	0.84724	3.38598	-0.81406
H	0.42381	1.42345	-1.65865
C	0.38328	4.37972	0.03244
H	-1.17648	5.05041	1.39148
H	1.81192	3.48126	-1.29912
H	0.98364	5.27219	0.18637

Zero-point correction= 0.321778 (Hartree/Particle)

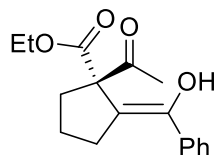
Thermal correction to Energy= 0.341903

Thermal correction to Enthalpy= 0.342847

Thermal correction to Gibbs Free Energy= 0.270451

SCF Done: E(RB3LYP) = -884.681062 Hartree

12a



C	-1.66852	-1.76927	2.17009
H	-2.26589	-1.81505	3.08233

H	-1.76421	-2.70367	1.61082
H	-0.61819	-1.65722	2.46491
C	-2.08455	-0.5521	1.3721
C	-1.96141	-0.58483	-0.18129
C	-1.88528	0.8769	-0.68741
C	-0.65398	2.91077	-0.53016
H	-1.57392	3.3758	-0.16937
H	-0.59566	3.05633	-1.61244
C	0.57151	3.42395	0.19583
H	1.48672	2.94753	-0.16982
H	0.66244	4.50145	0.02753
H	0.4909	3.2539	1.27309
C	-3.19213	-1.33109	-0.78366
H	-3.55834	-2.07464	-0.06719
H	-3.99266	-0.61553	-0.97638
C	-2.67059	-2.02361	-2.04673
H	-2.58901	-1.30595	-2.86941
H	-3.31245	-2.84435	-2.37927
C	-1.27696	-2.53529	-1.63977
H	-0.60373	-2.74398	-2.47384
H	-1.35244	-3.44214	-1.02734
C	-0.76015	-1.39611	-0.73433
O	-2.56223	0.43126	1.89341
O	-2.74507	1.39953	-1.35511
O	-0.75788	1.4694	-0.2731
C	0.49142	-1.1508	-0.55917
C	1.72173	-1.59498	-0.97049
C	2.30476	-1.07663	-2.17277
C	2.42234	-2.58876	-0.21201
C	3.53668	-1.54338	-2.59158
H	1.76563	-0.32304	-2.7365
C	3.65418	-3.04016	-0.64779
H	1.97155	-2.97781	0.69472
C	4.20657	-2.51874	-1.83126
H	3.9874	-1.16175	-3.50141
H	4.19359	-3.79305	-0.08332
H	5.1746	-2.87936	-2.16728
O	1.2203	-0.25475	0.47052
H	1.38666	-0.67343	1.18517

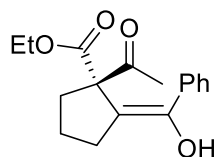
Zero-point correction= 0.338212 (Hartree/Particle)

Thermal correction to Energy= 0.359319

Thermal correction to Enthalpy= 0.360263

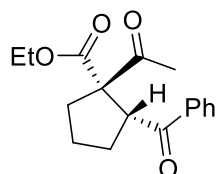
Thermal correction to Gibbs Free Energy= 0.286806

SCF Done: E(RB3LYP) = -960.806585 Hartree

12b

C	-4.64743	-0.7475	-2.04744
H	-5.3734	-0.3015	-2.73768
H	-3.72094	-0.9423	-2.58967
H	-5.07098	-1.68473	-1.68042
C	-4.46781	0.19624	-0.87125
C	-3.23909	1.13116	-0.86113
C	-3.38066	2.06376	0.37146
C	-2.95758	2.36542	2.68647
H	-4.02552	2.46368	2.90229
H	-2.56051	3.36488	2.48731
C	-2.20614	1.66593	3.80304
H	-1.14559	1.55731	3.55662
H	-2.28691	2.25639	4.72174
H	-2.61975	0.67234	4.00035
C	-3.24468	2.04016	-2.13234
H	-3.44579	1.42181	-3.01334
H	-4.00938	2.81565	-2.06228
C	-1.80904	2.58499	-2.19128
H	-1.70581	3.42304	-1.49364
H	-1.54798	2.95771	-3.18637
C	-0.93252	1.39214	-1.7554
H	-0.06667	1.69963	-1.15724
H	-0.52491	0.85786	-2.62242
C	-1.86274	0.46952	-0.97106
O	-5.31062	0.2624	0.00594
O	-3.94352	3.13795	0.34027
O	-2.80898	1.56534	1.48263
C	-1.46101	-0.76445	-0.60694
C	-2.20552	-1.86581	0.05642
C	-2.1301	-3.16324	-0.49353
C	-2.94398	-1.67922	1.23576
C	-2.7851	-4.23497	0.11225
H	-1.57674	-3.32476	-1.41486
C	-3.60054	-2.75532	1.83765
H	-2.99656	-0.69153	1.67481
C	-3.52397	-4.0343	1.28275
H	-2.72454	-5.22405	-0.3328

H -4.17141 -2.5903 2.74673
 H -4.03474 -4.86782 1.75597
 O -0.16636 -1.1065 -0.98691
 H 0.10743 -1.89585 -0.50058
 Zero-point correction= 0.338718 (Hartree/Particle)
 Thermal correction to Energy= 0.359558
 Thermal correction to Enthalpy= 0.360503
 Thermal correction to Gibbs Free Energy= 0.288537
 SCF Done: E(RB3LYP) = -960.804340 Hartree

13

C -4.47696 -0.79509 -2.3313
 H -5.17817 -0.31798 -3.02645
 H -3.48841 -0.81307 -2.7936
 H -4.82555 -1.81319 -2.14801
 C -4.50307 -0.03029 -1.02057
 C -3.4416 1.06852 -0.79294
 C -3.81754 1.79862 0.52421
 C -3.55901 1.89252 2.88232
 H -4.63082 1.75003 3.04928
 H -3.36854 2.96726 2.81389
 C -2.71524 1.23013 3.95514
 H -1.64765 1.36689 3.75714
 H -2.94494 1.67728 4.92795
 H -2.92079 0.15721 4.01755
 C -3.48717 2.13485 -1.93307
 H -3.51405 1.62357 -2.90073
 H -4.36758 2.77428 -1.84545
 C -2.15404 2.88293 -1.77464
 H -2.23759 3.61523 -0.96385
 H -1.87671 3.43301 -2.67898
 C -1.13998 1.77613 -1.41626
 H -0.37695 2.11278 -0.70495
 H -0.59432 1.43325 -2.30436
 C -1.97614 0.62988 -0.85205
 O -5.37593 -0.23594 -0.19634
 O -4.57476 2.7453 0.57111
 O -3.21214 1.28349 1.60982
 C -1.41989 -0.57132 -0.603

C	-2.0476	-1.8407	-0.15087
C	-1.83164	-3.01714	-0.89663
C	-2.80743	-1.9211	1.02647
C	-2.37079	-4.23437	-0.48013
H	-1.2612	-2.97452	-1.82015
C	-3.34723	-3.14141	1.43956
H	-2.97162	-1.02269	1.60778
C	-3.13056	-4.30081	0.6924
H	-2.2026	-5.12854	-1.0736
H	-3.93792	-3.18337	2.35001
H	-3.55022	-5.24817	1.01808
O	-0.03878	-0.68472	-0.87024
H	-2.3936	-0.26048	-1.8338

Zero-point correction= 0.339269 (Hartree/Particle)

Thermal correction to Energy= 0.359896

Thermal correction to Enthalpy= 0.360840

Thermal correction to Gibbs Free Energy= 0.287174

SCF Done: E(RB3LYP) = -960.819859 Hartree