

## Supplemental Information

### Exploring $\alpha$ Electron-Deficiency Induced [1,2]-Fluorine Migration

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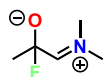
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## 1. Geometric Structures

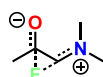
This part records all of the optimized geometric structures in Cartesian coordinate. The imaginary frequency of each transition state is attached to corresponding geometric structure.

### 1-IM1



1	C	-1.155012	-0.027265	-0.160966
2	O	-1.203282	0.514636	-1.313352
3	C	0.194174	-0.753514	0.005922
4	H	0.220526	-1.849498	-0.010620
5	N	1.332866	-0.163298	0.019250
6	C	1.456752	1.300289	-0.003146
7	H	0.597223	1.703066	-0.543787
8	H	1.475915	1.674951	1.027438
9	H	2.396145	1.549152	-0.508259
10	C	2.593727	-0.904715	0.045621
11	H	2.391620	-1.976814	0.125335
12	H	3.151775	-0.691181	-0.874735
13	H	3.179886	-0.567528	0.909497
14	C	-2.309506	-0.942541	0.242573
15	H	-2.377591	-1.782514	-0.462658
16	H	-2.195799	-1.329937	1.264949
17	H	-3.233897	-0.353747	0.177102
18	F	-1.110047	0.957392	0.943087

### 1-TS (Frequency: 248.8620 i cm<sup>-1</sup>)



1	C	-1.186804	0.222256	-0.169410
2	O	-1.243307	1.440907	-0.033283
3	C	0.122306	-0.532687	-0.287466
4	H	0.046921	-1.598831	-0.508103
5	N	1.320771	-0.068282	-0.175119
6	C	1.653972	1.334858	0.082256
7	H	0.733355	1.916565	0.147196
8	H	2.218166	1.386043	1.022867
9	H	2.293074	1.694428	-0.734667
10	C	2.476772	-0.963710	-0.214464
11	H	2.156172	-1.976945	-0.475134
12	H	3.188854	-0.593709	-0.962477
13	H	2.961497	-0.968693	0.770713
14	F	-0.992089	-0.652413	1.376824
15	C	-2.382626	-0.544726	-0.692921
16	H	-2.551227	-0.267960	-1.743997
17	H	-2.261664	-1.630720	-0.615478

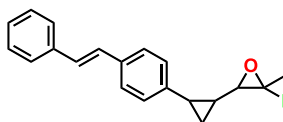
18	H	-3.257016	-0.233691	-0.108216
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### 1-IM2



1	C	1.301496	0.336713	0.269970
2	O	1.378399	1.493876	0.595903
3	C	-0.025320	-0.422581	0.447395
4	H	-0.064880	-0.776485	1.491771
5	N	-1.158568	0.355023	0.173149
6	C	-1.230189	0.884014	-1.179474
7	H	-0.293403	1.394339	-1.439144
8	H	-1.425752	0.096722	-1.930609
9	H	-2.042064	1.621580	-1.236573
10	C	-2.408870	-0.240492	0.612485
11	H	-2.317993	-0.567345	1.657302
12	H	-3.210612	0.508311	0.553583
13	H	-2.704022	-1.111383	-0.002260
14	C	2.455969	-0.456466	-0.270978
15	H	2.591388	-1.377588	0.313311
16	H	2.226734	-0.767386	-1.300448
17	H	3.364768	0.154042	-0.248333
18	F	0.044456	-1.579789	-0.346029

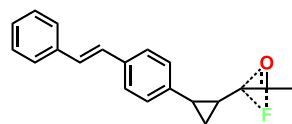
### 2-IM1



1	C	2.868523	0.704445	-0.545242
2	C	3.733330	-0.350849	0.107409
3	H	3.291923	1.712333	-0.543412
4	H	3.197725	-1.144312	0.636741
5	C	4.988888	0.096175	0.783861
6	C	6.323394	-0.430437	0.490104
7	H	4.865196	0.539002	1.779359
8	O	5.944640	0.791290	-0.031513
9	C	1.387233	0.661875	-0.417306
10	C	0.672183	-0.547530	-0.425042
11	C	0.661784	1.850324	-0.280479
12	C	-0.710579	-0.566191	-0.300957
13	H	1.202961	-1.496948	-0.529468
14	C	-0.725346	1.832589	-0.156630
15	H	1.192515	2.804518	-0.271329
16	C	-1.442936	0.627236	-0.164662

17	H	-1.225170	-1.528078	-0.310172
18	H	-1.268394	2.774510	-0.051751
19	C	-2.906140	0.668159	-0.032854
20	C	-3.737811	-0.388408	-0.042252
21	H	-3.322112	1.673798	0.080430
22	H	-3.322299	-1.393901	-0.158269
23	C	-5.202553	-0.345641	0.088815
24	C	-5.917859	-1.553816	0.055203
25	C	-5.927391	0.849485	0.246376
26	C	-7.306667	-1.573346	0.173818
27	H	-5.370303	-2.491113	-0.066253
28	C	-7.313385	0.830627	0.364824
29	H	-5.405782	1.807131	0.277132
30	C	-8.011047	-0.380173	0.329229
31	H	-7.839616	-2.525006	0.144445
32	H	-7.856305	1.769367	0.486127
33	H	-9.097954	-0.390371	0.422345
34	C	3.615424	-0.303777	-1.379442
35	H	4.477307	0.068951	-1.935798
36	H	3.033214	-1.083811	-1.873553
37	C	6.681933	-1.549553	-0.434558
38	H	6.797308	-2.477705	0.138991
39	H	5.904482	-1.685620	-1.192768
40	H	7.635423	-1.316749	-0.928104
41	F	7.240767	-0.303718	1.487349

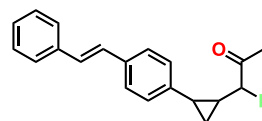
**2-TS (Frequency: 153.8032 i cm<sup>-1</sup>)**



1	C	2.997511	-0.336889	-0.716492
2	C	3.751644	-1.094718	0.549389
3	H	3.530088	0.552465	-1.061225
4	H	3.039609	-1.515440	1.260115
5	C	4.627553	-0.118609	1.015823
6	C	5.732312	0.660333	0.341576
7	H	4.464005	0.255461	2.029288
8	O	5.677365	1.889808	0.508155
9	C	6.376103	0.103235	-0.918598
10	H	5.771977	0.347200	-1.805396
11	H	7.341082	0.615488	-1.021165
12	H	6.552311	-0.977160	-0.862882
13	F	6.664612	-0.138101	1.463063
14	C	1.537801	-0.165395	-0.570989
15	C	0.672680	-1.243997	-0.323948
16	C	0.994957	1.118661	-0.695612
17	C	-0.693417	-1.041205	-0.205964
18	H	1.063618	-2.258051	-0.220528
19	C	-0.376281	1.318518	-0.581275

20	H	1.653382	1.968554	-0.884803
21	C	-1.248806	0.246806	-0.333537
22	H	-1.335539	-1.900945	-0.013903
23	H	-0.784050	2.325710	-0.684184
24	C	-2.687469	0.518518	-0.220114
25	C	-3.649377	-0.395044	0.001084
26	H	-2.961658	1.571063	-0.333434
27	H	-3.372130	-1.447877	0.108497
28	C	-5.091197	-0.131245	0.116792
29	C	-5.958622	-1.217110	0.317649
30	C	-5.646033	1.158618	0.036355
31	C	-7.334620	-1.026993	0.432406
32	H	-5.541988	-2.224557	0.383265
33	C	-7.019136	1.348665	0.151180
34	H	-5.001072	2.025153	-0.115639
35	C	-7.870353	0.257557	0.349248
36	H	-7.989634	-1.885551	0.587746
37	H	-7.431009	2.356936	0.086658
38	H	-8.946657	0.411392	0.438879
39	C	3.692743	-1.618751	-0.865717
40	H	4.616572	-1.623774	-1.440248
41	H	3.082706	-2.517362	-0.959382

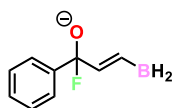
**2-IM2**



1	C	-2.994183	0.423630	0.407098
2	C	-3.778922	-0.741073	-0.137486
3	H	-3.468501	1.399650	0.289578
4	H	-3.182195	-1.557974	-0.553699
5	C	-5.057948	-0.544946	-0.916951
6	C	-6.029407	0.425155	-0.247974
7	H	-4.836699	-0.167544	-1.927883
8	O	-5.752733	1.599488	-0.184825
9	C	-7.290909	-0.164496	0.312591
10	H	-7.868593	0.616536	0.817876
11	H	-7.878673	-0.614090	-0.500375
12	H	-7.042283	-0.978983	1.008475
13	F	-5.676154	-1.774457	-1.052657
14	C	-1.508506	0.442948	0.301076
15	C	-0.732464	-0.720153	0.433943
16	C	-0.843661	1.650740	0.065216
17	C	0.651618	-0.676085	0.334020
18	H	-1.214611	-1.682991	0.619583
19	C	0.544929	1.696205	-0.035174
20	H	-1.423503	2.569793	-0.040983
21	C	1.323551	0.536938	0.096854
22	H	1.215176	-1.603732	0.442944

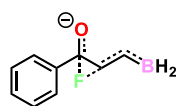
23	H	1.040079	2.652140	-0.219750
24	C	2.785205	0.642735	-0.016353
25	C	3.667606	-0.365905	0.093085
26	H	3.152737	1.655433	-0.207474
27	H	3.299489	-1.378203	0.284992
28	C	5.130688	-0.260903	-0.019379
29	C	5.902377	-1.425797	0.121723
30	C	5.799904	0.952257	-0.262024
31	C	7.292412	-1.386191	0.024750
32	H	5.398482	-2.376338	0.310574
33	C	7.187142	0.992377	-0.358982
34	H	5.233311	1.877453	-0.376613
35	C	7.941327	-0.175898	-0.216283
36	H	7.869918	-2.304990	0.138098
37	H	7.686446	1.944100	-0.547658
38	H	9.028960	-0.139881	-0.292978
39	C	-3.697836	-0.529449	1.340498
40	H	-4.577865	-0.149825	1.865245
41	H	-3.081967	-1.218877	1.921069

### 3a-IM1



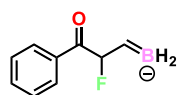
1	C	2.539297	1.023886	0.835988
2	C	1.243445	0.548024	1.040350
3	C	0.621581	-0.254608	0.077185
4	C	1.319643	-0.579782	-1.086540
5	C	2.616196	-0.106805	-1.296532
6	C	3.228622	0.699192	-0.335478
7	H	3.018246	1.645105	1.595545
8	H	0.707203	0.782011	1.961856
9	H	0.817655	-1.226098	-1.808372
10	H	3.153435	-0.368912	-2.210040
11	H	4.241999	1.071637	-0.496000
12	C	-0.821833	-0.788650	0.237247
13	O	-1.134897	-1.786729	-0.479763
14	C	-1.781409	0.413567	0.200220
15	C	-2.836880	0.476093	-0.637477
16	H	-1.569051	1.246689	0.883344
17	H	-2.958501	-0.404630	-1.280101
18	F	-0.876330	-1.088030	1.717582
19	B	-3.781324	1.680927	-0.642457
20	H	-3.552684	2.616951	0.087317
21	H	-4.757506	1.733201	-1.351175

### 3a-TS (Frequency: 216.2276 i cm<sup>-1</sup>)



1	C	2.405531	-1.574207	0.164436
2	C	1.063754	-1.193690	0.216603
3	C	0.709499	0.158536	0.158193
4	C	1.720700	1.121259	0.063760
5	C	3.059244	0.743542	-0.000634
6	C	3.405606	-0.608804	0.049600
7	H	2.669975	-2.631635	0.215973
8	H	0.298604	-1.964143	0.314721
9	H	1.430796	2.172513	0.042415
10	H	3.837380	1.504007	-0.086108
11	H	4.453814	-0.908798	0.004117
12	C	-0.712849	0.647473	0.253320
13	O	-0.933215	1.796119	0.594276
14	C	-1.831175	-0.322920	0.038969
15	C	-3.127678	-0.027611	0.379453
16	H	-1.573474	-1.344766	-0.235692
17	H	-3.303434	0.998874	0.719535
18	F	-1.136777	0.288860	-1.744575
19	B	-4.200716	-1.078660	0.298634
20	H	-3.922937	-2.190574	-0.098867
21	H	-5.346226	-0.872330	0.635504

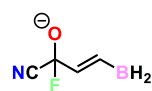
### 3a-IM2



1	C	-2.479213	-1.436736	-0.241516
2	C	-1.132686	-1.085820	-0.150762
3	C	-0.764653	0.259835	-0.016932
4	C	-1.762255	1.242671	0.026980
5	C	-3.106044	0.891738	-0.060586
6	C	-3.465959	-0.451254	-0.196474
7	H	-2.759381	-2.486010	-0.344588
8	H	-0.368298	-1.861914	-0.163589
9	H	-1.457793	2.285245	0.127301
10	H	-3.876102	1.663809	-0.025314
11	H	-4.518691	-0.729970	-0.266918
12	C	0.671115	0.711035	0.049556
13	O	0.932484	1.890075	0.128319
14	C	1.773826	-0.358217	-0.006320
15	C	3.158803	0.134940	0.061373
16	H	1.619294	-0.966570	-0.914444
17	H	3.314376	0.872276	0.861569
18	F	1.433318	-1.219389	1.087344
19	B	4.202968	-0.284571	-0.862947

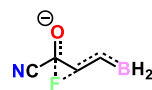
20	H	3.962709	-1.085539	-1.761851
21	H	5.351701	0.136282	-0.801992

### 3b-IM1



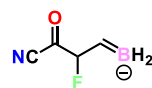
1	C	0.548706	-0.426952	-0.098147
2	O	0.580619	-1.096683	-1.158089
3	C	-0.793617	0.141033	0.378201
4	C	-1.911437	0.047881	-0.363302
5	H	-0.799567	0.630802	1.359774
6	H	-1.788237	-0.456776	-1.328288
7	F	1.000007	-1.161074	1.097415
8	C	1.565588	0.755439	-0.075053
9	N	2.331677	1.616038	-0.168143
10	B	-3.253828	0.597830	0.149401
11	H	-3.291113	1.154200	1.219597
12	H	-4.274143	0.489075	-0.483301

### 3b-TS (Frequency: 313.6585 i cm<sup>-1</sup>)



1	C	-0.579514	0.548676	-0.077219
2	O	-0.640319	1.706390	0.249671
3	C	0.668136	-0.245575	-0.249241
4	C	1.913036	0.330481	-0.096599
5	H	0.566645	-1.192902	-0.783288
6	H	1.920110	1.340709	0.326367
7	F	-0.152617	-0.910661	1.312249
8	C	-1.848338	-0.180510	-0.385212
9	N	-2.850278	-0.682602	-0.657100
10	B	3.147006	-0.414381	-0.504577
11	H	3.048724	-1.533779	-0.962954
12	H	4.257624	0.062492	-0.415513

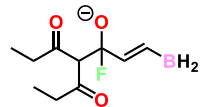
### 3b-IM2



1	C	0.574649	0.677133	0.248581
2	O	0.765241	1.854771	0.409534
3	C	-0.649096	-0.107779	0.643253
4	C	-1.392833	-0.384268	-0.603379
5	H	-1.225807	0.501124	1.354794
6	H	-0.834617	-1.024046	-1.302044
7	F	-0.192612	-1.262785	1.299966
8	C	1.594752	-0.136832	-0.493176

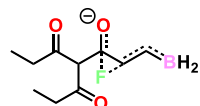
9	N	2.417761	-0.744298	-1.026548
10	B	-2.696912	0.207402	-0.909532
11	H	-3.264752	0.923130	-0.097349
12	H	-3.267843	0.010234	-1.969549

### 3c-IM1



1	C	-0.710501	-0.918905	-0.295738
2	O	-0.562034	-0.612455	-1.513219
3	C	-2.142685	-0.967374	0.246863
4	C	-3.209940	-0.595618	-0.485630
5	H	-2.271672	-1.326371	1.275326
6	H	-2.976652	-0.255198	-1.501217
7	F	-0.275123	-2.334855	0.009485
8	C	0.189774	-0.132675	0.746640
9	H	-0.119207	-0.383897	1.770211
10	C	-0.092278	1.346565	0.568454
11	O	-0.960195	1.880342	1.226602
12	C	1.664195	-0.507576	0.655283
13	O	2.325944	-0.527919	1.672130
14	C	0.669208	2.090033	-0.499993
15	H	1.747387	1.998554	-0.281135
16	H	0.495581	1.504419	-1.418941
17	C	0.246988	3.541636	-0.640709
18	H	0.402254	4.088309	0.299611
19	H	0.821098	4.041490	-1.431719
20	H	-0.820482	3.611752	-0.890241
21	C	2.276982	-0.871806	-0.676994
22	H	1.763656	-1.797532	-0.980437
23	H	1.958914	-0.139475	-1.429965
24	C	3.785414	-1.035244	-0.608324
25	H	4.064381	-1.801024	0.127638
26	H	4.189754	-1.329303	-1.585991
27	H	4.270105	-0.096119	-0.304264
28	B	-4.630232	-0.664239	0.089975
29	H	-5.602129	-0.351352	-0.553025
30	H	-4.788398	-1.043336	1.225692

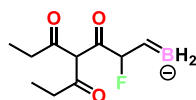
### 3c-TS (Frequency: 248.1467 i cm<sup>-1</sup>)



1	C	-0.950110	0.410996	-0.315747
2	O	-0.720740	0.571989	-1.494643
3	C	-2.345764	0.414333	0.233534
4	C	-3.438256	0.655165	-0.568419
5	H	-2.440619	0.504949	1.316935

6	H	-3.241305	0.665283	-1.645983
7	F	-1.813150	-1.455586	0.419013
8	C	0.179521	0.197774	0.691970
9	H	-0.212465	0.291240	1.710298
10	C	1.255388	1.280312	0.552097
11	O	1.302127	2.183464	1.353571
12	C	0.790115	-1.210464	0.605922
13	O	1.251528	-1.695340	1.612096
14	C	2.220449	1.180070	-0.603384
15	H	2.760238	0.222094	-0.498948
16	H	1.610327	1.076018	-1.515189
17	C	3.183497	2.351902	-0.678225
18	H	3.779260	2.426584	0.241310
19	H	3.867809	2.238351	-1.528643
20	H	2.636241	3.296978	-0.796316
21	C	0.829053	-1.925418	-0.722540
22	H	-0.224811	-2.192391	-0.899279
23	H	1.090647	-1.210969	-1.515951
24	C	1.739477	-3.141400	-0.708630
25	H	1.437633	-3.843218	0.079799
26	H	1.702701	-3.664793	-1.672941
27	H	2.782918	-2.853701	-0.513408
28	B	-4.793912	0.882557	0.034749
29	H	-5.776119	1.120230	-0.634357
30	H	-4.928063	0.850310	1.240143

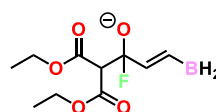
### 3c-IM2



1	C	0.693457	-0.948045	-0.008029
2	O	0.426435	-1.714491	-0.900679
3	C	2.135670	-0.689103	0.430127
4	C	3.128419	-0.585885	-0.657566
5	H	2.398311	-1.510196	1.121538
6	H	2.808472	0.066413	-1.483838
7	F	2.062542	0.479834	1.249861
8	C	-0.398984	-0.227726	0.785911
9	H	-0.196452	-0.370400	1.856239
10	C	-1.766977	-0.854747	0.499197
11	O	-2.238956	-1.644522	1.279272
12	C	-0.421744	1.291412	0.550713
13	O	-0.933135	2.007873	1.375240
14	C	-2.461798	-0.463272	-0.782166
15	H	-2.602086	0.632109	-0.768072
16	H	-1.749956	-0.668086	-1.598608
17	C	-3.780842	-1.187150	-0.989614
18	H	-4.475682	-0.974446	-0.166284
19	H	-4.250194	-0.875589	-1.931240

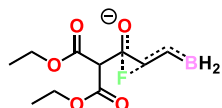
20	H	-3.624566	-2.273759	-1.021122
21	C	0.161478	1.813987	-0.739191
22	H	1.247465	1.629180	-0.670815
23	H	-0.194303	1.175206	-1.564644
24	C	-0.140143	3.282415	-0.980578
25	H	0.233848	3.894150	-0.149322
26	H	0.331933	3.627872	-1.908801
27	H	-1.223385	3.450920	-1.058366
28	B	4.386831	-1.319955	-0.658031
29	H	5.199591	-1.236197	-1.568681
30	H	4.674007	-2.068110	0.269939

### 3d-IM1



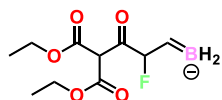
1	C	-1.414509	-0.819479	-0.286703
2	O	-1.258981	-0.661016	-1.522407
3	C	-2.786285	-0.475709	0.305641
4	C	-3.796438	0.010140	-0.440867
5	H	-2.927122	-0.662690	1.377740
6	H	-3.552718	0.161023	-1.498870
7	F	-1.312646	-2.266202	0.154246
8	C	-0.279860	-0.202046	0.654515
9	H	-0.640869	-0.160033	1.690552
10	C	-0.048462	1.218490	0.214884
11	O	-0.891186	2.076678	0.306281
12	C	0.943908	-1.081953	0.683642
13	O	1.417451	-1.523052	1.704448
14	C	1.474959	2.773522	-0.703295
15	H	2.311150	2.660226	-1.403397
16	H	0.608237	3.177240	-1.242908
17	C	2.634581	-2.129988	-0.574414
18	H	2.550124	-2.960317	0.139328
19	H	2.658603	-2.537048	-1.592474
20	B	-5.167820	0.309479	0.175314
21	H	-6.093492	0.721783	-0.480129
22	H	-5.336059	0.128292	1.357714
23	C	1.851464	3.654829	0.470326
24	H	2.144219	4.650779	0.111176
25	H	1.000243	3.767858	1.154460
26	H	2.697590	3.221135	1.020838
27	C	3.861521	-1.286026	-0.290126
28	H	3.920728	-0.445069	-0.994671
29	H	3.824684	-0.889949	0.733465
30	H	4.770231	-1.894297	-0.395790
31	O	1.444709	-1.341065	-0.519874
32	O	1.172018	1.440806	-0.273879

### 3d-TS (Frequency: 243.2318 i cm<sup>-1</sup>)



1	C	1.459890	-0.494051	-0.400669
2	O	1.354535	-0.535335	-1.602740
3	C	2.781884	-0.545986	0.300953
4	C	3.964143	-0.697694	-0.386026
5	H	2.756029	-0.734437	1.375860
6	H	3.893410	-0.607836	-1.475457
7	F	2.166709	1.293362	0.591943
8	C	0.209830	-0.393572	0.484909
9	H	0.441660	-0.733191	1.503595
10	C	-0.876892	-1.315236	-0.043814
11	O	-0.672386	-2.437231	-0.424383
12	C	-0.272063	1.040159	0.621772
13	O	-0.566295	1.553411	1.669123
14	C	-3.200865	-1.549700	-0.414139
15	H	-3.979231	-0.822595	-0.672670
16	H	-2.915833	-2.106858	-1.316160
17	C	-0.918173	2.960437	-0.568785
18	H	-0.433306	3.518938	0.243106
19	H	-0.596910	3.379907	-1.529727
20	B	5.245922	-0.967108	0.348119
21	H	6.304078	-1.129251	-0.220033
22	H	5.238637	-1.048206	1.558646
23	C	-3.652669	-2.480536	0.691695
24	H	-4.547512	-3.030546	0.370642
25	H	-2.865412	-3.207741	0.930043
26	H	-3.900650	-1.910781	1.597438
27	C	-2.427491	2.985917	-0.432828
28	H	-2.894347	2.396359	-1.234027
29	H	-2.731702	2.570816	0.536958
30	H	-2.794141	4.019202	-0.501742
31	O	-0.422301	1.619907	-0.564907
32	O	-2.082344	-0.752869	0.003788

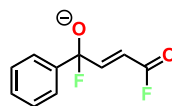
### 3d-IM2



1	C	1.084007	-1.196522	-0.080958
2	O	0.830931	-1.887192	-1.033547
3	C	2.513803	-0.832728	0.312248
4	C	3.335424	-0.240616	-0.764707
5	H	2.975809	-1.766166	0.679656
6	H	2.846439	0.611305	-1.257565
7	F	2.380904	0.007184	1.455299
8	C	-0.031095	-0.678714	0.841335

9	H	0.144759	-1.047112	1.859716
10	C	-1.363339	-1.219840	0.359578
11	O	-1.844266	-2.253023	0.738792
12	C	-0.043720	0.840038	0.891330
13	O	-0.475810	1.480753	1.811143
14	C	-3.176076	-0.817634	-1.102927
15	H	-3.242594	-0.284728	-2.058177
16	H	-3.149523	-1.898200	-1.294819
17	C	0.420778	2.785589	-0.364042
18	H	0.709466	3.233992	0.595633
19	H	1.191663	3.008932	-1.110527
20	B	4.631624	-0.776752	-1.155020
21	H	5.298813	-0.298163	-2.062758
22	H	5.104671	-1.750664	-0.578673
23	C	-4.314243	-0.445692	-0.175764
24	H	-5.273865	-0.699885	-0.645546
25	H	-4.235545	-0.994450	0.772025
26	H	-4.303551	0.632852	0.032931
27	C	-0.947139	3.257535	-0.811530
28	H	-1.231024	2.770088	-1.754134
29	H	-1.702719	3.025183	-0.048967
30	H	-0.934368	4.344325	-0.969390
31	O	0.443716	1.357920	-0.229702
32	O	-1.911459	-0.420544	-0.550359

### 4a-IM1

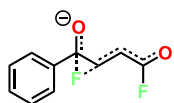


1	C	-3.026704	-1.282239	0.810717
2	C	-1.873793	-0.532101	1.044004
3	C	-1.361265	0.308926	0.049770
4	C	-2.022600	0.392739	-1.175831
5	C	-3.176640	-0.355332	-1.414471
6	C	-3.680252	-1.197008	-0.421243
7	H	-3.422127	-1.932576	1.593514
8	H	-1.369263	-0.581870	2.010978
9	H	-1.609861	1.069343	-1.925784
10	H	-3.687600	-0.281094	-2.376623
11	H	-4.582256	-1.783760	-0.604424
12	C	-0.075236	1.144464	0.246855
13	O	0.096328	2.114033	-0.551395
14	C	1.106428	0.166390	0.389588
15	C	2.186688	0.299749	-0.386158
16	H	1.041514	-0.641548	1.125024
17	H	2.221526	1.115895	-1.110299
18	F	-0.197205	1.576499	1.682213
19	C	3.352127	-0.581485	-0.321420
20	O	4.352242	-0.521047	-0.962283



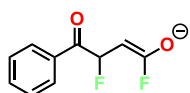
21 F 3.224648 -1.564599 0.591807

**4a-TS (Frequency: 166.3151 i cm<sup>-1</sup>)**



1	C	3.012609	1.566875	0.066534
2	C	1.748130	1.048377	0.337914
3	C	1.462013	-0.289961	0.041523
4	C	2.456196	-1.102365	-0.512346
5	C	3.720337	-0.581163	-0.787740
6	C	3.998401	0.756037	-0.502056
7	H	3.236346	2.607213	0.308912
8	H	0.977486	1.634024	0.837256
9	H	2.222016	-2.146684	-0.725260
10	H	4.489817	-1.218677	-1.226265
11	H	4.986781	1.166406	-0.716180
12	C	0.103337	-0.899486	0.266841
13	O	-0.011396	-2.097115	0.449818
14	C	-1.093082	-0.034230	0.035910
15	C	-2.322552	-0.587447	-0.111472
16	H	-0.931136	1.013271	-0.211950
17	H	-2.470030	-1.655587	0.046396
18	F	-0.418697	0.315253	1.926616
19	C	-3.499033	0.186848	-0.422330
20	O	-4.626622	-0.180862	-0.567108
21	F	-3.239666	1.511742	-0.576754

**4a-IM2**



1	C	-3.058090	-1.560413	-0.113363
2	C	-1.753956	-1.081593	0.004730
3	C	-1.507188	0.297533	-0.022481
4	C	-2.581876	1.185229	-0.164675
5	C	-3.883531	0.706800	-0.278833
6	C	-4.122509	-0.669411	-0.254992
7	H	-3.244321	-2.634996	-0.091218
8	H	-0.930046	-1.781537	0.138878
9	H	-2.371153	2.255093	-0.187495
10	H	-4.714588	1.404933	-0.388966
11	H	-5.141879	-1.048009	-0.346342
12	C	-0.122004	0.878776	0.058977
13	O	0.042186	2.074968	-0.016215
14	C	1.055175	-0.090424	0.230891
15	C	2.362820	0.544400	0.277197
16	H	1.010761	-0.856267	-0.557877
17	H	2.466501	1.522511	0.744873

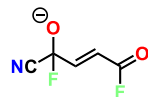
18 F 0.703342 -0.800568 1.435597

19 C 3.514828 -0.049107 -0.215733

20 O 4.679305 0.307866 -0.248472

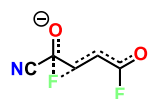
21 F 3.266746 -1.298892 -0.805005

**4b-IM1**



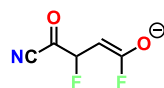
1	C	1.400689	-0.447783	0.079498
2	O	1.507249	-1.501638	-0.591478
3	C	-0.003268	0.129845	0.304668
4	C	-1.048756	-0.432576	-0.303164
5	H	-0.114046	0.995532	0.963876
6	H	-0.892207	-1.292929	-0.956208
7	F	1.898193	-0.548911	1.456502
8	C	2.286333	0.721039	-0.440288
9	N	2.963791	1.528492	-0.913952
10	C	-2.430876	0.033492	-0.139390
11	O	-3.411161	-0.417068	-0.635574
12	F	-2.535273	1.095966	0.676661

**4b-TS (Frequency: 291.9022 i cm<sup>-1</sup>)**



1	C	-1.401383	0.575757	-0.163063
2	O	-1.573520	1.762557	-0.065085
3	C	-0.088555	-0.119492	-0.106263
4	C	1.060991	0.619539	-0.017688
5	H	-0.051207	-1.148056	-0.464150
6	H	1.021124	1.688486	0.186511
7	F	-0.923409	-0.591199	1.490009
8	C	-2.580307	-0.313329	-0.384945
9	N	-3.517017	-0.949754	-0.601269
10	C	2.362940	0.031483	-0.124005
11	O	3.441081	0.548428	-0.061196
12	F	2.321919	-1.313665	-0.348615

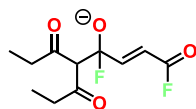
**4b-IM2**



1	C	1.357648	0.535840	-0.456295
2	O	1.593431	1.290906	-1.362428
3	C	0.173783	0.579398	0.473131
4	C	-0.692596	-0.541918	0.119174
5	H	-0.329814	1.545206	0.343430
6	H	-0.276844	-1.549606	0.077591

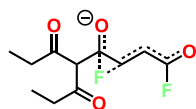
7	F	0.698221	0.523361	1.783581
8	C	2.268167	-0.630503	-0.212901
9	N	2.997691	-1.503644	-0.024009
10	C	-2.057068	-0.411558	-0.148640
11	O	-2.900545	-1.227633	-0.451894
12	F	-2.500428	0.902879	-0.048603

#### 4c-IMI



1	C	-0.275211	-0.755413	-0.304994
2	O	-0.093283	-0.552834	-1.538572
3	C	-1.708802	-0.609680	0.219834
4	C	-2.683389	-0.188442	-0.589995
5	H	-1.913096	-0.862899	1.263898
6	H	-2.453297	0.056260	-1.628443
7	F	-0.000875	-2.176569	0.101841
8	C	0.695960	0.011159	0.687109
9	H	0.353349	-0.121516	1.721785
10	C	0.554042	1.492845	0.383866
11	O	-0.229859	2.155153	1.030745
12	C	2.104727	-0.569170	0.651358
13	O	2.708043	-0.699383	1.695769
14	C	1.345572	2.099927	-0.749951
15	H	1.331218	1.383303	-1.583002
16	H	0.812732	3.009655	-1.059364
17	C	2.773220	2.459244	-0.323071
18	H	3.344077	1.583188	0.017116
19	H	3.320295	2.906050	-1.163822
20	H	2.758033	3.187696	0.499825
21	C	2.717045	-1.019640	-0.655961
22	H	2.064353	-1.828617	-1.017041
23	H	2.598362	-0.225759	-1.405808
24	C	4.163127	-1.459924	-0.505538
25	H	4.250283	-2.275857	0.224122
26	H	4.564656	-1.807752	-1.466507
27	H	4.794053	-0.632714	-0.148540
28	C	-4.078613	-0.034357	-0.170451
29	O	-5.000752	0.327660	-0.827063
30	F	-4.281823	-0.353998	1.120995

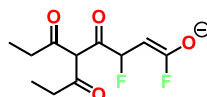
#### 4c-TS (Frequency: 234.6067 i cm<sup>-1</sup>)



1	C	-0.389177	0.357035	-0.412911
2	O	-0.198208	0.438616	-1.605420
3	C	-1.759646	0.157225	0.157847

4	C	-2.842888	0.139439	-0.673990
5	H	-1.896576	0.345193	1.221355
6	H	-2.711823	0.092288	-1.754373
7	F	-0.945444	-1.545160	0.541536
8	C	0.752530	0.431083	0.595948
9	H	0.349352	0.545417	1.607334
10	C	1.668021	1.640411	0.372495
11	O	1.734781	2.496780	1.222496
12	C	1.581653	-0.868629	0.636093
13	O	2.109932	-1.175247	1.677554
14	C	2.519456	1.708079	-0.875156
15	H	2.028537	1.171605	-1.696194
16	H	2.602345	2.769340	-1.148704
17	C	3.918458	1.144536	-0.592931
18	H	3.887972	0.081454	-0.312708
19	H	4.551633	1.238063	-1.484686
20	H	4.392834	1.697826	0.229134
21	C	1.737752	-1.686252	-0.621906
22	H	0.726922	-2.080763	-0.807710
23	H	1.958420	-1.014770	-1.465443
24	C	2.766375	-2.794451	-0.476899
25	H	2.504328	-3.459359	0.356521
26	H	2.822332	-3.392930	-1.395392
27	H	3.767066	-2.386878	-0.271192
28	C	-4.192877	0.119547	-0.187818
29	O	-5.222065	0.094855	-0.798601
30	F	-4.269757	0.152420	1.172820

#### 4c-IM2



1	C	0.251953	-0.936949	-0.092824
2	O	0.214735	-1.658612	-1.058050
3	C	1.572330	-0.402095	0.460193
4	C	2.498429	0.080586	-0.557787
5	H	2.020158	-1.217044	1.052035
6	H	2.118717	0.563988	-1.458289
7	F	1.198272	0.579006	1.439746
8	C	-1.006950	-0.570059	0.689113
9	H	-0.841840	-0.825055	1.744916
10	C	-2.210614	-1.389556	0.214881
11	O	-2.700020	-2.211178	0.950995
12	C	-1.328957	0.936531	0.673439
13	O	-1.982017	1.407476	1.570667
14	C	-2.789853	-1.109718	-1.153811
15	H	-2.003715	-0.761329	-1.836130
16	H	-3.172269	-2.065616	-1.537693
17	C	-3.938175	-0.096649	-1.062307

18	H	-3.598370	0.886182	-0.704782
19	H	-4.394543	0.045795	-2.050240
20	H	-4.712446	-0.458561	-0.372059
21	C	-0.846047	1.749817	-0.502208
22	H	0.256431	1.729189	-0.454729
23	H	-1.111726	1.211060	-1.427527
24	C	-1.372453	3.174201	-0.499442
25	H	-1.084414	3.688364	0.426690
26	H	-0.970674	3.736648	-1.351472
27	H	-2.469759	3.188903	-0.561165
28	C	3.877042	-0.031989	-0.436153
29	O	4.797140	0.314273	-1.152380
30	F	4.255674	-0.685995	0.742701

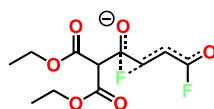
#### 4d-IM1



1	C	-0.801583	-0.820527	-0.407005
2	O	-0.573603	-0.437197	-1.581008
3	C	-2.220575	-0.604332	0.136399
4	C	-3.142243	0.005229	-0.613089
5	H	-2.462789	-0.974481	1.136911
6	H	-2.871447	0.366351	-1.606647
7	F	-0.692806	-2.311037	-0.225062
8	C	0.241165	-0.354590	0.707014
9	H	-0.176605	-0.536188	1.705878
10	C	0.410389	1.134705	0.565341
11	O	-0.483697	1.916518	0.774411
12	C	1.509777	-1.168114	0.639133
13	O	1.954368	-1.778004	1.582810
14	C	1.846979	2.917792	0.034141
15	H	1.612559	3.422863	0.982484
16	H	1.144609	3.294797	-0.723193
17	C	3.305991	-1.888706	-0.701874
18	H	3.225532	-2.842244	-0.163197
19	H	3.391388	-2.092652	-1.775964
20	C	-4.523047	0.228041	-0.181204
21	O	-5.400723	0.755478	-0.785192
22	F	-4.773530	-0.239770	1.056577
23	C	4.481985	-1.073712	-0.201299
24	H	5.418849	-1.621821	-0.370778
25	H	4.538812	-0.113882	-0.732586
26	H	4.382722	-0.878981	0.874965
27	C	3.285509	3.121329	-0.376697
28	H	3.492521	2.609724	-1.326423
29	H	3.488294	4.192392	-0.506335
30	H	3.966501	2.727805	0.390226
31	O	2.081155	-1.165831	-0.560072

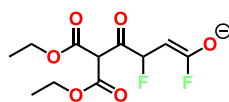
32	O	1.632499	1.511648	0.197283
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#### 4d-TS (Frequency: 225.5265 i cm<sup>-1</sup>)



1	C	0.913809	-0.429107	-0.441028
2	O	0.756487	-0.591558	-1.625720
3	C	2.262148	-0.223669	0.171948
4	C	3.379137	-0.288983	-0.608872
5	H	2.349552	-0.323509	1.252575
6	H	3.295237	-0.323107	-1.694514
7	F	1.443175	1.521660	0.390101
8	C	-0.284381	-0.419921	0.514520
9	H	0.045300	-0.648052	1.537282
10	C	-1.275806	-1.504218	0.122676
11	O	-0.958717	-2.607689	-0.231948
12	C	-0.936609	0.951037	0.582687
13	O	-1.234107	1.503252	1.608335
14	C	-3.554774	-2.078086	-0.016522
15	H	-3.385379	-2.957109	0.621502
16	H	-3.447880	-2.399849	-1.062311
17	C	-1.840357	2.700727	-0.698228
18	H	-1.356787	3.361780	0.033593
19	H	-1.621021	3.068298	-1.707810
20	C	4.708494	-0.255860	-0.067096
21	O	5.761958	-0.296329	-0.633415
22	F	4.727640	-0.184927	1.293627
23	C	-3.333443	2.606408	-0.458005
24	H	-3.794745	3.597137	-0.569918
25	H	-3.796147	1.923494	-1.183765
26	H	-3.535872	2.239018	0.556672
27	C	-4.893763	-1.433405	0.246972
28	H	-5.039613	-0.560597	-0.403210
29	H	-5.697387	-2.154034	0.047632
30	H	-4.967351	-1.109387	1.293794
31	O	-1.220674	1.413557	-0.630294
32	O	-2.536443	-1.108008	0.266869

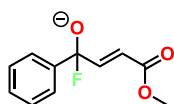
#### 4d-IM2



1	C	0.548144	-1.150733	0.076128
2	O	0.349486	-1.839665	-0.889697
3	C	1.939889	-0.650450	0.450056
4	C	2.616823	0.082908	-0.614931
5	H	2.524342	-1.535917	0.744726
6	H	2.050583	0.778068	-1.233901

7	F	1.760919	0.090400	1.663055
8	C	-0.593296	-0.769585	1.029302
9	H	-0.377196	-1.169472	2.027914
10	C	-1.879195	-1.397485	0.525951
11	O	-2.266616	-2.487594	0.846913
12	C	-0.719839	0.740393	1.148432
13	O	-1.191762	1.306949	2.096398
14	C	-3.709829	-1.111724	-0.924994
15	H	-4.406254	-1.382053	-0.118716
16	H	-3.463022	-2.030288	-1.476483
17	C	-0.357780	2.770470	-0.004972
18	H	-0.086242	3.177215	0.978033
19	H	0.401798	3.067064	-0.737552
20	C	3.981416	-0.013067	-0.846539
21	O	4.720361	0.525838	-1.649785
22	F	4.609316	-0.923957	0.014696
23	C	-1.745478	3.207077	-0.425678
24	H	-1.780049	4.300667	-0.520912
25	H	-2.009751	2.762886	-1.394928
26	H	-2.488718	2.898872	0.321988
27	C	-4.270104	-0.039387	-1.826929
28	H	-3.548594	0.220465	-2.613129
29	H	-5.190774	-0.399967	-2.303530
30	H	-4.506564	0.865984	-1.251835
31	O	-0.271596	1.340036	0.051814
32	O	-2.504395	-0.603318	-0.335192

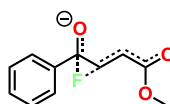
#### 5a-IMI1



1	C	3.154609	1.656837	0.615736
2	C	2.109119	0.796440	0.951965
3	C	1.753497	-0.256155	0.101095
4	C	2.465049	-0.438247	-1.085078
5	C	3.511709	0.419893	-1.427300
6	C	3.857642	1.471901	-0.577525
7	H	3.427873	2.472489	1.288235
8	H	1.567844	0.926178	1.891284
9	H	2.177377	-1.278490	-1.719154
10	H	4.062264	0.267743	-2.358037
11	H	4.675472	2.144894	-0.841607
12	C	0.586014	-1.221937	0.413303
13	O	0.579371	-2.319781	-0.222333
14	C	-0.720477	-0.408946	0.389357
15	C	-1.743634	-0.786152	-0.380437
16	H	-0.793211	0.492678	1.005789
17	H	-1.640082	-1.688631	-0.987045
18	F	0.729764	-1.408233	1.902146

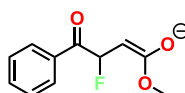
19	C	-3.034980	-0.076332	-0.472890
20	O	-3.959195	-0.434853	-1.165599
21	O	-3.100866	1.022048	0.292209
22	C	-4.323183	1.742624	0.245892
23	H	-5.158267	1.110795	0.577051
24	H	-4.204789	2.596034	0.920172
25	H	-4.529032	2.091532	-0.774924

#### 5a-TS (Frequency: 219.4071 i cm<sup>-1</sup>)



1	C	3.196899	1.716730	0.237587
2	C	2.003281	1.030003	0.452555
3	C	1.862258	-0.285208	-0.007625
4	C	2.928408	-0.907208	-0.666154
5	C	4.118705	-0.215911	-0.886945
6	C	4.252291	1.099018	-0.437826
7	H	3.310063	2.737610	0.606444
8	H	1.181887	1.456986	1.027300
9	H	2.806688	-1.937291	-1.005310
10	H	4.943869	-0.702220	-1.409769
11	H	5.183478	1.642010	-0.608768
12	C	0.587104	-1.065970	0.161477
13	O	0.617480	-2.279638	0.207612
14	C	-0.703676	-0.309180	0.150076
15	C	-1.880414	-0.976844	-0.029037
16	H	-0.661013	0.755224	-0.075470
17	H	-1.910934	-2.063944	0.044393
18	F	-0.155246	0.031290	1.964968
19	C	-3.150854	-0.315889	-0.243569
20	O	-4.222349	-0.872370	-0.397787
21	O	-3.063902	1.037122	-0.280673
22	C	-4.273821	1.729226	-0.521640
23	H	-5.012501	1.518045	0.264192
24	H	-4.027512	2.796186	-0.524528
25	H	-4.707730	1.442277	-1.489796

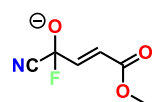
#### 5a-IM2



1	C	3.242014	1.720355	0.114587
2	C	2.003854	1.088064	0.221452
3	C	1.887410	-0.280498	-0.056342
4	C	3.026014	-1.002802	-0.437102
5	C	4.261522	-0.371177	-0.543835
6	C	4.370209	0.994105	-0.268575
7	H	3.326803	2.785353	0.335234

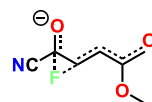
8	H	1.130660	1.652508	0.546015
9	H	2.917341	-2.066869	-0.650672
10	H	5.142551	-0.940740	-0.843307
11	H	5.337323	1.492737	-0.351892
12	C	0.575260	-1.017380	0.009845
13	O	0.540424	-2.208896	-0.200955
14	C	-0.684597	-0.210489	0.342580
15	C	-1.923752	-0.953672	0.284782
16	H	-0.722917	0.692143	-0.284956
17	H	-1.926629	-2.012554	0.540450
18	F	-0.348242	0.317020	1.664551
19	C	-3.156503	-0.368681	-0.034368
20	O	-4.267414	-0.906065	-0.101117
21	O	-3.069791	0.991572	-0.322528
22	C	-4.262200	1.601709	-0.747259
23	H	-5.058896	1.509802	0.005928
24	H	-4.035431	2.662705	-0.911101
25	H	-4.637766	1.161639	-1.684438

#### 5b-IM1



1	C	1.873121	-0.341712	0.209267
2	O	2.162414	-1.510313	-0.144105
3	C	0.399443	0.077074	0.227880
4	C	-0.537623	-0.750505	-0.233123
5	H	0.144797	1.062939	0.627368
6	H	-0.243212	-1.725070	-0.628164
7	F	2.294615	-0.000048	1.576812
8	C	2.642871	0.757134	-0.583127
9	N	3.246174	1.492725	-1.239515
10	C	-1.987885	-0.450482	-0.241120
11	O	-2.830679	-1.211677	-0.652036
12	O	-2.283987	0.755108	0.254588
13	C	-3.662020	1.101085	0.278745
14	H	-4.226724	0.391381	0.897754
15	H	-3.719929	2.106091	0.706579
16	H	-4.079112	1.095513	-0.736950

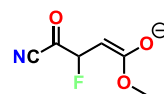
#### 5b-TS (Frequency: 286.1846 i cm<sup>-1</sup>)



1	C	1.873121	-0.341712	0.209267
2	O	2.162414	-1.510313	-0.144105
3	C	0.399443	0.077074	0.227880
4	C	-0.537623	-0.750505	-0.233123
5	H	0.144797	1.062939	0.627368

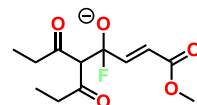
6	H	-0.243212	-1.725070	-0.628164
7	F	2.294615	-0.000048	1.576812
8	C	2.642871	0.757134	-0.583127
9	N	3.246174	1.492725	-1.239515
10	C	-1.987885	-0.450482	-0.241120
11	O	-2.830679	-1.211677	-0.652036
12	O	-2.283987	0.755108	0.254588
13	C	-3.662020	1.101085	0.278745
14	H	-4.226724	0.391381	0.897754
15	H	-3.719929	2.106091	0.706579
16	H	-4.079112	1.095513	-0.736950

#### 5b-IM2



1	C	-1.691554	0.616177	0.450697
2	O	-1.830910	1.418447	1.341598
3	C	-0.563732	0.542513	-0.535943
4	C	0.187791	-0.652530	-0.180111
5	H	0.041899	1.451808	-0.438888
6	H	-0.326526	-1.613227	-0.125474
7	F	-1.141325	0.529734	-1.831843
8	C	-2.688812	-0.494338	0.304490
9	N	-3.498025	-1.308008	0.183341
10	C	1.580503	-0.665405	0.064681
11	O	2.275315	-1.633761	0.364691
12	O	2.173763	0.574016	-0.052032
13	C	3.560823	0.614703	0.191476
14	H	4.113688	-0.021359	-0.515369
15	H	3.871851	1.658518	0.067176
16	H	3.801731	0.276360	1.209964

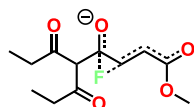
#### 5c-IM1



1	C	0.092596	-0.746295	-0.402120
2	O	0.364977	-0.534658	-1.617904
3	C	-1.369729	-0.595025	0.027772
4	C	-2.290980	-0.155275	-0.830587
5	H	-1.642379	-0.859058	1.053542
6	H	-1.992494	0.099442	-1.849604
7	F	0.338718	-2.176466	0.008282
8	C	1.003823	-0.001279	0.664799
9	H	0.593438	-0.150728	1.672052
10	C	0.896724	1.486315	0.384286
11	O	0.098324	2.152482	1.009650
12	C	2.407822	-0.590955	0.709517

13	O	2.942062	-0.746708	1.787938
14	C	1.748039	2.100715	-0.701720
15	H	1.777222	1.391852	-1.540743
16	H	1.235700	3.015627	-1.030249
17	C	3.150878	2.451047	-0.192826
18	H	3.697740	1.569346	0.171773
19	H	3.746688	2.902318	-0.997352
20	H	3.091882	3.172610	0.634223
21	C	3.099868	-1.022189	-0.564027
22	H	2.470311	-1.826749	-0.973184
23	H	3.023187	-0.219802	-1.309947
24	C	4.534779	-1.463773	-0.332724
25	H	4.578752	-2.286740	0.392833
26	H	4.993063	-1.802168	-1.271454
27	H	5.143533	-0.640293	0.068913
28	C	-3.724542	0.013805	-0.510459
29	O	-4.551389	0.406016	-1.299911
30	O	-4.033807	-0.309573	0.750909
31	C	-5.398776	-0.164587	1.115768
32	H	-5.471444	-0.464743	2.165204
33	H	-5.722233	0.877945	0.995517
34	H	-6.035775	-0.806165	0.492412

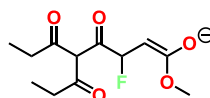
**5c-TS (Frequency: 270.2855 i cm<sup>-1</sup>)**



1	C	0.002830	0.416243	-0.518220
2	O	0.269191	0.556367	-1.689782
3	C	-1.388049	0.121924	-0.033291
4	C	-2.419486	0.088033	-0.943240
5	H	-1.613972	0.402251	0.996021
6	H	-2.208761	0.009398	-2.009407
7	F	-0.701763	-1.480067	0.468754
8	C	1.079928	0.464856	0.563900
9	H	0.612630	0.605949	1.544175
10	C	2.050314	1.638356	0.389391
11	O	2.076886	2.511493	1.224389
12	C	1.855066	-0.863921	0.672092
13	O	2.310051	-1.176168	1.745599
14	C	2.998850	1.653091	-0.788076
15	H	2.549931	1.128142	-1.639870
16	H	3.147665	2.706359	-1.064428
17	C	4.346778	1.035201	-0.393528
18	H	4.251225	-0.023409	-0.111362
19	H	5.050954	1.095661	-1.233388
20	H	4.778382	1.575484	0.460207
21	C	2.049351	-1.702820	-0.566498
22	H	1.036005	-2.058940	-0.809455

23	H	2.348527	-1.050565	-1.401379
24	C	3.018769	-2.852150	-0.351478
25	H	2.680255	-3.493660	0.472652
26	H	3.100816	-3.464377	-1.258772
27	H	4.022601	-2.484877	-0.092753
28	C	-3.808642	0.074412	-0.563331
29	O	-4.760664	0.041935	-1.324830
30	O	-4.008538	0.123525	0.782225
31	C	-5.356151	0.160810	1.206276
32	H	-5.338536	0.197425	2.300794
33	H	-5.872919	1.047138	0.811553
34	H	-5.901688	-0.732791	0.871834

**5c-IM2**



1	C	0.078765	-0.924132	0.161203
2	O	0.137804	-1.637877	1.132285
3	C	-1.245896	-0.358411	-0.344063
4	C	-2.096072	0.202137	0.691291
5	H	-1.756636	-1.171227	-0.886920
6	H	-1.652489	0.670627	1.570625
7	F	-0.871256	0.563503	-1.399174
8	C	1.319771	-0.605698	-0.671591
9	H	1.115271	-0.896038	-1.711189
10	C	2.518996	-1.433554	-0.203327
11	O	2.964568	-2.298496	-0.917829
12	C	1.670373	0.892700	-0.724407
13	O	2.301910	1.316266	-1.660516
14	C	3.149633	-1.111425	1.133102
15	H	2.394497	-0.716671	1.825120
16	H	3.523375	-2.059213	1.544607
17	C	4.315959	-0.129731	0.962418
18	H	3.985832	0.844506	0.573593
19	H	4.807343	0.043885	1.928366
20	H	5.059389	-0.538286	0.264277
21	C	1.244037	1.760261	0.433970
22	H	0.140284	1.757862	0.425217
23	H	1.532548	1.253126	1.370321
24	C	1.795757	3.172950	0.357228
25	H	1.487427	3.655582	-0.579399
26	H	1.431659	3.776754	1.197916
27	H	2.894624	3.169786	0.383922
28	C	-3.496869	0.177172	0.622212
29	O	-4.311358	0.617901	1.438218
30	O	-3.981340	-0.440964	-0.524593
31	C	-5.379813	-0.561725	-0.606880
32	H	-5.599966	-1.056798	-1.560697

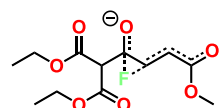
33	H	-5.787537	-1.163652	0.219715
34	H	-5.874827	0.420337	-0.580378

### 5d-IMI



1	C	-0.605550	0.691168	1.597382
2	O	-0.195963	1.589985	2.369957
3	C	0.408821	-0.330556	1.081196
4	C	1.712273	-0.116265	1.264767
5	H	0.045310	-1.177159	0.493749
6	H	2.030007	0.755580	1.840719
7	F	-1.642546	-0.188338	2.226521
8	C	-1.444560	1.234633	0.314580
9	H	-1.870121	2.174963	0.684230
10	C	-2.579359	0.319705	-0.049737
11	O	-3.747076	0.603777	0.061434
12	C	-0.526196	1.526978	-0.843889
13	O	-0.557301	0.982825	-1.920952
14	C	-3.180466	-1.846406	-0.735845
15	H	-3.865101	-1.452613	-1.501430
16	H	-3.767350	-2.001342	0.181994
17	C	1.357255	2.771606	-1.521236
18	H	0.876519	2.822020	-2.507178
19	H	1.729007	3.768182	-1.255261
20	C	2.790474	-0.945202	0.687903
21	O	3.968963	-0.713197	0.828567
22	O	2.344160	-1.973728	-0.042684
23	C	3.338136	-2.784487	-0.652919
24	H	2.804577	-3.565840	-1.202007
25	H	3.951819	-2.187951	-1.341244
26	H	3.992406	-3.232456	0.106672
27	C	-2.496156	-3.114095	-1.189661
28	H	-1.824172	-3.492673	-0.407225
29	H	-3.244049	-3.886906	-1.410288
30	H	-1.906507	-2.928942	-2.097834
31	C	2.475245	1.746936	-1.513624
32	H	3.218393	2.005830	-2.280638
33	H	2.978795	1.719536	-0.537598
34	H	2.080904	0.744878	-1.735110
35	O	-2.167902	-0.875550	-0.473856
36	O	0.361740	2.474119	-0.535431

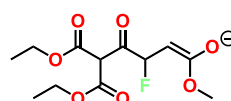
### 5d-TS (Frequency: 261.8994 i cm<sup>-1</sup>)



1	C	0.574071	-0.090566	1.804505
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2	O	0.552416	-0.314883	2.988997
3	C	-0.647076	0.221291	0.994692
4	C	-1.897154	-0.037305	1.507886
5	H	-0.519247	0.190146	-0.086037
6	H	-2.039955	-0.202512	2.575426
7	F	-0.062000	1.937176	1.103516
8	C	1.911918	-0.133653	1.041355
9	H	2.716973	-0.223770	1.781632
10	C	2.142231	1.143580	0.245668
11	O	2.832249	2.055064	0.610158
12	C	1.985933	-1.331916	0.104089
13	O	2.907133	-1.540667	-0.638311
14	C	1.223910	2.363258	-1.540461
15	H	2.140022	2.724777	-2.030669
16	H	0.936643	3.063459	-0.745774
17	C	0.764088	-3.180087	-0.733269
18	H	1.742455	-3.651414	-0.890907
19	H	0.093175	-3.895171	-0.244319
20	C	-3.083172	-0.027671	0.692320
21	O	-4.222685	-0.238062	1.072118
22	O	-2.839694	0.226083	-0.626649
23	C	-3.967036	0.206227	-1.478465
24	H	-3.602008	0.441585	-2.484179
25	H	-4.448021	-0.782275	-1.478032
26	H	-4.712250	0.951852	-1.167721
27	C	0.094928	2.144215	-2.519791
28	H	-0.795568	1.788721	-1.981625
29	H	-0.151451	3.085801	-3.028186
30	H	0.371567	1.399958	-3.279537
31	C	0.176917	-2.650699	-2.025393
32	H	0.011009	-3.476227	-2.730295
33	H	-0.784716	-2.154945	-1.831817
34	H	0.861566	-1.927889	-2.490584
35	O	1.491032	1.104289	-0.913527
36	O	0.912108	-2.107666	0.209985

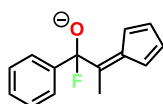
### 5d-IM2



1	C	-0.628076	0.144098	1.804471
2	O	-0.565807	0.386611	2.980678
3	C	0.479802	-0.538361	1.009584
4	C	1.804549	-0.428329	1.556164
5	H	0.439927	-0.241630	-0.043901
6	H	1.948264	-0.381538	2.635028
7	F	-0.090538	-1.913635	0.972263
8	C	-1.907441	0.489663	1.011995
9	H	-2.685542	0.787209	1.726369

10	C	-2.391028	-0.736189	0.250011
11	O	-3.193121	-1.522078	0.674499
12	C	-1.649778	1.640838	0.046258
13	O	-2.439057	2.014671	-0.777043
14	C	-1.787818	-2.129617	-1.558837
15	H	-2.741342	-2.234636	-2.096811
16	H	-1.737946	-2.902996	-0.781271
17	C	0.053636	3.088381	-0.745778
18	H	-0.764676	3.747701	-1.061714
19	H	0.811513	3.679135	-0.219387
20	C	2.953711	-0.412255	0.745891
21	O	4.132780	-0.314645	1.091467
22	O	2.674622	-0.502166	-0.615992
23	C	3.782927	-0.394354	-1.475375
24	H	3.402069	-0.508642	-2.497923
25	H	4.280285	0.583173	-1.378520
26	H	4.531243	-1.174277	-1.271785
27	C	-0.594022	-2.186225	-2.482360
28	H	0.328194	-2.052578	-1.899396
29	H	-0.556804	-3.158836	-2.990280
30	H	-0.649837	-1.396414	-3.244018
31	C	0.646656	2.314308	-1.905444
32	H	1.100153	3.004363	-2.629548
33	H	1.416668	1.618446	-1.540545
34	H	-0.135250	1.736254	-2.418816
35	O	-1.759498	-0.851763	-0.911354
36	O	-0.443768	2.165150	0.235581

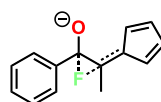
**6a-IMI**



1	C	2.437753	-2.108232	-0.091686
2	C	1.393334	-1.324129	0.394925
3	C	1.434991	0.070754	0.293159
4	C	2.550467	0.669768	-0.298484
5	C	3.604252	-0.112038	-0.781228
6	C	3.550334	-1.502022	-0.682276
7	H	2.389642	-3.195838	-0.007866
8	H	0.522553	-1.783985	0.868687
9	H	2.590401	1.757231	-0.365783
10	H	4.473632	0.368813	-1.234477
11	H	4.372008	-2.112451	-1.061249
12	C	0.238102	0.862094	0.891994
13	O	-0.118814	0.496762	2.052215
14	C	-0.843643	0.927442	-0.226645
15	F	0.744362	2.276846	0.882743
16	C	-2.991949	0.033811	-1.228110
17	C	-2.321209	-0.850161	0.842043

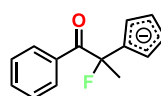
18	C	-3.899834	-0.894826	-0.830643
19	H	-3.030609	0.614650	-2.147444
20	C	-3.480048	-1.447383	0.459645
21	H	-1.739331	-1.002802	1.745275
22	H	-4.795936	-1.191196	-1.376147
23	H	-4.022402	-2.214273	1.013063
24	C	-1.940453	0.121579	-0.199612
25	C	-0.575911	1.870773	-1.358571
26	H	-0.625506	2.902352	-0.981581
27	H	0.452223	1.733490	-1.726184
28	H	-1.272528	1.753728	-2.195768

**6a-TS (Frequency: 222.4965 i cm<sup>-1</sup>)**



1	C	3.678751	-1.047846	-1.002619
2	C	2.317065	-1.190115	-0.733893
3	C	1.659267	-0.280213	0.102231
4	C	2.386285	0.760301	0.692222
5	C	3.751045	0.889463	0.435986
6	C	4.399115	-0.007002	-0.416298
7	H	4.179130	-1.756384	-1.664863
8	H	1.755969	-2.016446	-1.175482
9	H	1.841870	1.432886	1.353932
10	H	4.315112	1.696804	0.906827
11	H	5.465893	0.102543	-0.618801
12	C	0.191350	-0.550555	0.375912
13	O	-0.097468	-1.625953	0.861297
14	C	-0.844507	0.417925	-0.149955
15	F	-0.196203	1.126224	1.631889
16	C	-3.238388	0.895874	-0.790434
17	C	-2.868749	-1.061254	0.413077
18	C	-4.438355	0.262329	-0.610213
19	H	-3.089595	1.833107	-1.323916
20	C	-4.207279	-0.955115	0.143290
21	H	-2.372958	-1.854854	0.961416
22	H	-5.407233	0.608624	-0.970853
23	H	-4.978612	-1.665315	0.443214
24	C	-2.192107	0.094108	-0.165222
25	C	-0.345466	1.582476	-0.956556
26	H	0.570218	1.992026	-0.524879
27	H	-0.126388	1.257601	-1.987155
28	H	-1.095994	2.378756	-1.001988

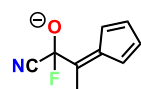
**6a-IM2**





1	C	3.828455	0.066199	0.686565
2	C	2.632046	-0.612638	0.897932
3	C	1.485339	-0.289159	0.159063
4	C	1.553461	0.735376	-0.796478
5	C	2.749616	1.422773	-0.997635
6	C	3.888007	1.088187	-0.263080
7	H	4.715598	-0.198224	1.263904
8	H	2.562643	-1.406659	1.642279
9	H	0.667080	1.000001	-1.369035
10	H	2.793289	2.224486	-1.736269
11	H	4.823175	1.625271	-0.430291
12	C	0.235411	-1.069070	0.473483
13	O	0.200533	-1.782980	1.453638
14	C	-0.993623	-0.987013	-0.443983
15	F	-0.503916	-0.833055	-1.770731
16	C	-3.276675	0.199462	-0.135893
17	C	-1.440782	1.396663	0.531688
18	C	-3.717167	1.440969	0.352712
19	H	-3.913626	-0.597171	-0.522878
20	C	-2.583422	2.179329	0.768504
21	H	-0.414561	1.683260	0.763597
22	H	-4.755322	1.775334	0.401981
23	H	-2.591526	3.180727	1.203024
24	C	-1.860532	0.161352	-0.037768
25	C	-1.713984	-2.326264	-0.450306
26	H	-1.028225	-3.120931	-0.776304
27	H	-2.088474	-2.565612	0.550343
28	H	-2.555974	-2.276141	-1.151682

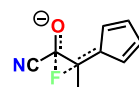
**6b-IM1**



1	C	1.372892	-0.395374	0.413556
2	O	1.141499	-1.543429	0.858100
3	C	0.220778	0.612572	0.165728
4	F	2.292346	0.380337	1.264612
5	C	2.198470	-0.404739	-0.916864
6	N	2.784147	-0.532614	-1.905495
7	C	-2.234129	1.066640	-0.216392
8	C	-1.595139	-1.176270	0.108781
9	C	-3.335951	0.280216	-0.280396
10	H	-2.208848	2.148893	-0.323764
11	C	-2.936029	-1.119287	-0.081551
12	H	-0.970491	-2.044842	0.284724
13	H	-4.357337	0.618507	-0.453936
14	H	-3.620707	-1.967257	-0.092158
15	C	-1.065203	0.200964	0.036867
16	C	0.638298	2.045801	0.040827

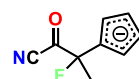
17	H	1.504947	2.128593	-0.633289
18	H	-0.161165	2.693617	-0.333137
19	H	0.977535	2.412066	1.020374

**6b-TS (Frequency: 325.1692 i cm<sup>-1</sup>)**



1	C	1.311125	-0.653421	-0.216183
2	O	1.107963	-1.836122	-0.310352
3	C	0.290041	0.438281	-0.100080
4	F	1.146087	0.301865	1.596540
5	C	2.742017	-0.205793	-0.273439
6	N	3.866883	0.033957	-0.359184
7	C	-2.132180	1.112256	-0.156512
8	C	-1.712986	-1.167650	0.026433
9	C	-3.333292	0.450270	-0.111871
10	H	-1.994538	2.188901	-0.248407
11	C	-3.071238	-0.967761	0.006758
12	H	-1.196290	-2.119013	0.110666
13	H	-4.320977	0.909419	-0.159436
14	H	-3.832458	-1.746009	0.069396
15	C	-1.066121	0.128940	-0.081838
16	C	0.735995	1.844394	-0.388345
17	H	0.501003	2.114384	-1.428364
18	H	0.206059	2.536395	0.276087
19	H	1.810379	1.973322	-0.221231

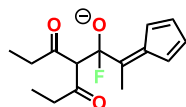
**6b-IM2**



1	C	1.380678	0.090793	-0.618104
2	O	1.705624	0.572199	-1.672744
3	C	0.551752	0.763616	0.460478
4	F	1.045696	0.294499	1.679335
5	C	1.748427	-1.328412	-0.314765
6	N	2.129975	-2.398595	-0.113762
7	C	-1.849704	0.858162	-0.535007
8	C	-1.276950	-1.061118	0.600056
9	C	-2.935562	-0.027925	-0.586498
10	H	-1.803002	1.852284	-0.981542
11	C	-2.584058	-1.209839	0.117391
12	H	-0.712836	-1.779568	1.195713
13	H	-3.891282	0.164318	-1.076912
14	H	-3.225035	-2.079973	0.267757
15	C	-0.819687	0.230876	0.213678
16	C	0.697057	2.266824	0.408671
17	H	0.430712	2.633006	-0.589723

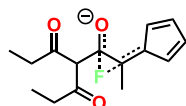
18	H	0.027926	2.721401	1.149619
19	H	1.735726	2.552749	0.623955

**6c-IM1**



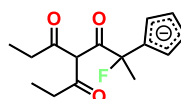
1	C	0.117664	-0.966981	-0.293097
2	O	0.165491	-0.554693	-1.486628
3	C	-1.258246	-1.025856	0.430365
4	F	0.547621	-2.393237	-0.186734
5	C	1.156464	-0.291270	0.720935
6	H	1.138687	-0.819947	1.679791
7	C	0.799379	1.155217	1.027126
8	O	0.834377	1.540487	2.178458
9	C	2.568758	-0.509108	0.198323
10	O	3.272674	-1.351828	0.711918
11	C	0.343264	2.078741	-0.081018
12	H	0.952500	1.911665	-0.977474
13	H	-0.656257	1.713299	-0.373298
14	C	0.302392	3.535963	0.347001
15	H	1.303738	3.891681	0.630116
16	H	-0.070319	4.170567	-0.467740
17	H	-0.352038	3.667090	1.218471
18	C	3.047796	0.311583	-0.972990
19	H	2.243301	0.242083	-1.723316
20	H	3.072661	1.366866	-0.649034
21	C	4.401707	-0.130224	-1.500694
22	H	4.364670	-1.174688	-1.840147
23	H	4.714544	0.496397	-2.346256
24	H	5.169049	-0.065987	-0.717328
25	C	-3.725679	-0.497241	0.516769
26	C	-2.568987	0.147101	-1.426973
27	C	-4.591592	0.116028	-0.327313
28	H	-3.964156	-0.899321	1.499119
29	C	-3.869349	0.516764	-1.540348
30	H	-1.758624	0.279403	-2.134985
31	H	-5.651642	0.291411	-0.144555
32	H	-4.320169	1.028906	-2.390451
33	C	-2.392909	-0.516631	-0.118829
34	C	-1.259184	-1.636080	1.804130
35	H	-0.898217	-0.903127	2.544769
36	H	-2.255211	-1.967252	2.117231
37	H	-0.570299	-2.489679	1.825374

**6c-TS (Frequency: 262.9840 i cm<sup>-1</sup>)**



1	C	-0.088685	-0.518981	0.109141
2	O	-0.035755	-1.261968	-0.850111
3	C	-1.380173	0.059977	0.634181
4	F	-0.789794	-1.377010	1.853098
5	C	1.220329	-0.031608	0.748723
6	H	1.120065	-0.087617	1.835492
7	C	1.579459	1.403426	0.357190
8	O	2.315411	2.050884	1.064161
9	C	2.345624	-1.011367	0.389321
10	O	2.635626	-1.892831	1.160174
11	C	1.007931	1.951312	-0.930035
12	H	1.183750	1.205474	-1.722567
13	H	-0.090827	1.972722	-0.812751
14	C	1.555605	3.319119	-1.294355
15	H	2.644528	3.275832	-1.435115
16	H	1.099502	3.686148	-2.222257
17	H	1.352303	4.042653	-0.493988
18	C	3.041598	-0.840203	-0.939230
19	H	2.249590	-0.881354	-1.704375
20	H	3.453027	0.183810	-0.977294
21	C	4.120740	-1.879773	-1.186622
22	H	3.694319	-2.891580	-1.164787
23	H	4.594806	-1.722653	-2.163793
24	H	4.896480	-1.829458	-0.410698
25	C	-3.844850	0.462977	0.348648
26	C	-2.882124	-1.034149	-1.150787
27	C	-4.817613	0.016424	-0.505804
28	H	-3.982556	1.176900	1.159493
29	C	-4.217283	-0.918156	-1.437382
30	H	-2.156535	-1.658863	-1.660727
31	H	-5.867103	0.311552	-0.494506
32	H	-4.747806	-1.440928	-2.233848
33	C	-2.583421	-0.165567	-0.019354
34	C	-1.330766	1.130576	1.694279
35	H	-0.362858	1.194876	2.197824
36	H	-1.569870	2.115029	1.264306
37	H	-2.083144	0.907828	2.460421

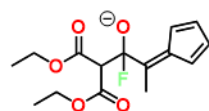
**6c-IM2**



1	C	0.389421	0.851751	-0.475075
2	O	0.725317	0.853304	-1.638605
3	C	-0.625914	1.844177	0.086215
4	F	-0.183578	2.197389	1.366539
5	C	0.916191	-0.218022	0.486361
6	H	0.868765	0.156681	1.517183
7	C	2.375838	-0.468615	0.107863

8	O	2.715171	-1.464749	-0.483415
9	C	0.160050	-1.556062	0.447548
10	O	0.203172	-2.271362	1.420121
11	C	3.348053	0.612335	0.517900
12	H	2.890054	1.589767	0.293138
13	H	3.404674	0.568237	1.619517
14	C	4.719665	0.459870	-0.115545
15	H	4.651028	0.525125	-1.210162
16	H	5.400935	1.244598	0.236860
17	H	5.152896	-0.517507	0.134079
18	C	-0.521265	-1.942514	-0.835202
19	H	-1.341539	-1.216103	-0.988154
20	H	0.201368	-1.766701	-1.648706
21	C	-1.042728	-3.368174	-0.817777
22	H	-1.760223	-3.500595	0.003396
23	H	-1.548505	-3.610340	-1.761748
24	H	-0.225753	-4.088115	-0.666708
25	C	-2.828235	0.847054	-0.861376
26	C	-2.212948	0.166152	1.242847
27	C	-3.733557	-0.142668	-0.435056
28	H	-2.833463	1.354442	-1.827461
29	C	-3.357727	-0.557596	0.865567
30	H	-1.669104	0.082025	2.184521
31	H	-4.589242	-0.511218	-1.003577
32	H	-3.878219	-1.295850	1.478167
33	C	-1.888986	1.048546	0.180519
34	C	-0.705137	3.098932	-0.754240
35	H	0.269248	3.607365	-0.772088
36	H	-0.983005	2.842348	-1.782933
37	H	-1.463315	3.770789	-0.332267

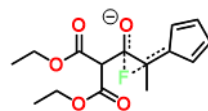
**6d-IM1**



1	C	-0.046496	-1.479111	0.589590
2	O	-0.408931	-0.886220	1.635957
3	C	1.443782	-1.464370	0.167565
4	F	-0.355246	-2.924814	0.637732
5	C	-0.899482	-1.072797	-0.760119
6	H	-0.904199	-1.933576	-1.434656
7	C	-0.206799	0.053009	-1.474502
8	O	0.361175	-0.097307	-2.533395
9	C	-2.304903	-0.879986	-0.268295
10	O	-3.081280	-1.794218	-0.129784
11	C	0.687840	2.215287	-1.311970
12	H	0.451203	2.383542	-2.372202
13	H	1.726884	1.851581	-1.248541
14	C	-3.888519	0.589613	0.642213

15	H	-3.946518	-0.017822	1.557634
16	H	-4.677186	0.235452	-0.037933
17	C	3.669009	-0.258167	0.109673
18	C	1.960732	0.694367	1.416570
19	C	4.130094	0.887111	0.672439
20	H	4.228802	-0.919485	-0.548167
21	C	3.064290	1.480085	1.488813
22	H	0.989203	0.835871	1.877127
23	H	5.127286	1.308396	0.544791
24	H	3.157070	2.409500	2.051150
25	C	2.270193	-0.451190	0.539191
26	C	1.876946	-2.553390	-0.765267
27	H	1.694202	-3.529878	-0.297824
28	H	1.263809	-2.521215	-1.679924
29	H	2.929912	-2.473993	-1.054953
30	C	0.477554	3.458376	-0.481020
31	H	0.726517	3.260343	0.570093
32	H	1.123964	4.267047	-0.847599
33	H	-0.567659	3.792245	-0.542431
34	C	-4.013980	2.065826	0.936196
35	H	-3.950634	2.651655	0.008973
36	H	-4.979444	2.274191	1.415494
37	H	-3.210306	2.391530	1.610481
38	O	-0.169737	1.194671	-0.797079
39	O	-2.614634	0.376820	0.034607

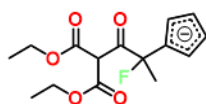
**6d-TS (Frequency: 238.9347 i cm<sup>-1</sup>)**



1	C	0.259813	-0.842039	-0.234676
2	O	0.091832	-1.515120	0.757357
3	C	1.594718	-0.287473	-0.660470
4	F	1.190193	-1.851899	-1.828421
5	C	-0.970767	-0.446521	-1.074173
6	H	-0.804004	-0.784295	-2.101140
7	C	-1.231589	1.048401	-1.057999
8	O	-1.911207	1.627824	-1.863149
9	C	-2.167318	-1.197668	-0.523253
10	O	-2.519848	-2.282237	-0.899379
11	C	-0.746099	3.064124	0.066887
12	H	-1.805920	3.305485	0.233725
13	H	-0.446246	3.514558	-0.890651
14	C	-3.873221	-1.151222	1.098524
15	H	-3.519647	-2.095280	1.537715
16	H	-4.631427	-1.398193	0.341746
17	C	3.993677	0.223781	-0.108680
18	C	2.870786	-1.141547	1.405659
19	C	4.852214	-0.095977	0.909196

20	H	4.222921	0.854680	-0.966260
21	C	4.152860	-0.949585	1.849659
22	H	2.095808	-1.733353	1.881401
23	H	5.886993	0.234005	1.004037
24	H	4.583148	-1.366898	2.760587
25	C	2.708061	-0.408022	0.157090
26	C	1.654642	0.661047	-1.828637
27	H	0.788616	0.572635	-2.490702
28	H	1.731529	1.701581	-1.479191
29	H	2.542529	0.435014	-2.430382
30	C	0.130541	3.515713	1.209712
31	H	1.179531	3.250268	1.018750
32	H	0.060662	4.604900	1.325671
33	H	-0.185282	3.042372	2.148968
34	C	-4.400655	-0.199669	2.144767
35	H	-4.741057	0.735655	1.680357
36	H	-5.248787	-0.656996	2.670441
37	H	-3.619751	0.036320	2.880040
38	O	-0.615125	1.640840	-0.041139
39	O	-2.766569	-0.514486	0.447440

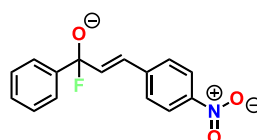
#### 6d-IM2



1	C	0.470052	-0.091382	0.585988
2	O	0.182594	-0.494872	1.682273
3	C	1.653156	0.833742	0.316154
4	F	1.317103	1.517540	-0.891429
5	C	-0.329794	-0.494783	-0.658853
6	H	0.365296	-0.768073	-1.462429
7	C	-1.161924	0.678514	-1.154412
8	O	-1.508850	0.823141	-2.294607
9	C	-1.181761	-1.700374	-0.316140
10	O	-0.775845	-2.831070	-0.347431
11	C	-2.262628	2.653812	-0.510360
12	H	-3.183655	2.308010	-1.000893
13	H	-1.699081	3.253904	-1.239588
14	C	-3.285412	-2.411079	0.466356
15	H	-2.821401	-2.936948	1.312930
16	H	-3.380066	-3.126888	-0.362422
17	C	4.213044	0.422787	0.320069
18	C	2.905945	-1.355251	-0.308189
19	C	5.057625	-0.653525	-0.001534
20	H	4.531297	1.412561	0.651283
21	C	4.251502	-1.752862	-0.383377
22	H	2.040133	-1.989753	-0.512354
23	H	6.148399	-0.642665	0.040842
24	H	4.609511	-2.741057	-0.677461

25	C	2.873504	-0.001544	0.127937
26	C	1.751806	1.899502	1.390908
27	H	0.831283	2.499789	1.406700
28	H	1.888989	1.425654	2.369922
29	H	2.606184	2.555589	1.183122
30	C	-2.549163	3.418257	0.758943
31	H	-1.616815	3.759754	1.228305
32	H	-3.165355	4.297460	0.530678
33	H	-3.093076	2.786636	1.474093
34	C	-4.608837	-1.788213	0.837559
35	H	-5.045570	-1.265494	-0.023955
36	H	-5.308152	-2.568958	1.163243
37	H	-4.480140	-1.069612	1.658032
38	O	-1.475014	1.506771	-0.164790
39	O	-2.405935	-1.353143	0.056620

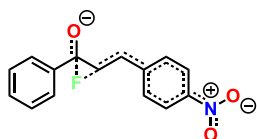
#### 7a-IM1



1	C	5.175487	1.870450	-0.915084
2	C	4.847769	0.772103	-1.712012
3	C	3.971162	-0.202466	-1.231622
4	C	3.410946	-0.092291	0.041781
5	C	3.748659	1.008007	0.838169
6	C	4.625127	1.984567	0.364043
7	H	5.861061	2.634144	-1.286913
8	H	5.280534	0.675007	-2.709944
9	H	3.706716	-1.080574	-1.823249
10	H	3.329565	1.083043	1.843475
11	H	4.886082	2.836338	0.995522
12	C	2.422399	-1.188010	0.507060
13	O	2.493835	-2.299437	-0.103483
14	C	1.024219	-0.552642	0.617206
15	C	-0.020190	-1.097192	-0.015413
16	H	0.193314	-2.005395	-0.588499
17	C	-1.407370	-0.614438	-0.019926
18	C	-2.366952	-1.313836	-0.774217
19	C	-1.823755	0.522971	0.699604
20	C	-3.693607	-0.903615	-0.818648
21	H	-2.058586	-2.196851	-1.336134
22	C	-3.143372	0.947929	0.667502
23	H	-1.102967	1.083318	1.295361
24	C	-4.061297	0.225689	-0.094055
25	H	-4.439520	-1.441103	-1.401471
26	H	-3.472443	1.825468	1.221158
27	H	0.929858	0.358986	1.217470
28	F	2.763171	-1.305021	1.970666

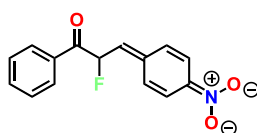
29	N	-5.458183	0.670072	-0.131635
30	O	-6.240540	0.027477	-0.795116
31	O	-5.757072	1.656828	0.502641

**7a-TS (Frequency: 272.1695 i cm<sup>-1</sup>)**



1	C	5.732604	1.412376	-0.728046
2	C	5.730371	0.051263	-1.039276
3	C	4.630970	-0.735705	-0.701337
4	C	3.523383	-0.164675	-0.064474
5	C	3.532878	1.198334	0.257331
6	C	4.637503	1.981407	-0.073929
7	H	6.593163	2.030247	-0.990408
8	H	6.587265	-0.395823	-1.545740
9	H	4.612371	-1.802339	-0.931125
10	H	2.686179	1.591416	0.819858
11	H	4.649812	3.041009	0.186993
12	C	2.350700	-1.054293	0.242168
13	O	2.519541	-2.245929	0.410163
14	C	0.986208	-0.443370	0.241871
15	C	-0.112109	-1.258478	0.196027
16	H	0.038153	-2.336730	0.284230
17	C	-1.460412	-0.763023	0.089864
18	C	-2.530489	-1.635589	-0.231829
19	C	-1.777025	0.601654	0.318267
20	C	-3.828477	-1.175397	-0.362160
21	H	-2.317585	-2.694276	-0.390584
22	C	-3.069450	1.075572	0.183240
23	H	-0.986726	1.276899	0.647512
24	C	-4.088817	0.183683	-0.163128
25	H	-4.646557	-1.846630	-0.618661
26	H	-3.310564	2.122528	0.360796
27	H	0.911002	0.587754	-0.103727
28	F	1.490535	0.233900	1.973673
29	N	-5.448220	0.675020	-0.298832
30	O	-6.320332	-0.117757	-0.592883
31	O	-5.654311	1.857830	-0.114521

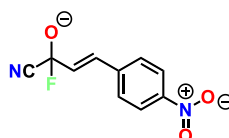
**7a-IM2**



1	C	-6.006078	-1.237712	-0.154780
2	C	-6.013106	0.157787	-0.219538
3	C	-4.810511	0.857009	-0.207535
4	C	-3.590945	0.171880	-0.121925

5	C	-3.590293	-1.228023	-0.053595
6	C	-4.795906	-1.927523	-0.074652
7	H	-6.947562	-1.789210	-0.166850
8	H	-6.958623	0.698200	-0.282040
9	H	-4.792609	1.945894	-0.266825
10	H	-2.651590	-1.774869	0.026832
11	H	-4.789999	-3.017102	-0.024861
12	C	-2.331262	0.987773	-0.152229
13	O	-2.370210	2.173488	-0.387293
14	C	-1.001208	0.268272	0.104490
15	C	0.154194	1.176314	0.199895
16	H	-0.047317	2.239541	0.331600
17	C	1.452261	0.724761	0.129099
18	C	2.579696	1.639932	0.184201
19	C	1.801088	-0.681274	0.003347
20	C	3.872699	1.214692	0.082294
21	H	2.369087	2.705421	0.301293
22	C	3.098137	-1.100083	-0.104528
23	H	1.004535	-1.426871	0.022352
24	C	4.165215	-0.166971	-0.074516
25	H	4.701383	1.921341	0.117622
26	H	3.337528	-2.158812	-0.200696
27	H	-0.868258	-0.488981	-0.690763
28	F	-1.198016	-0.495921	1.284337
29	N	5.491999	-0.604483	-0.179351
30	O	6.405918	0.223520	-0.145807
31	O	5.724004	-1.809618	-0.305825

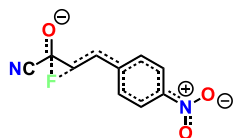
**7b-IM1**



1	C	-3.652282	0.233528	0.246814
2	O	-3.889966	1.462482	0.139491
3	C	-2.194609	-0.234497	0.268799
4	C	-1.214663	0.643560	0.040663
5	H	-2.015759	-1.294928	0.472175
6	H	-1.530322	1.674087	-0.151166
7	C	0.231111	0.375674	0.026701
8	C	1.113002	1.442359	-0.216808
9	C	0.769720	-0.906409	0.244443
10	C	2.489179	1.249334	-0.244861
11	H	0.706547	2.440446	-0.386996
12	C	2.140296	-1.118564	0.219364
13	H	0.107799	-1.751354	0.434946
14	C	2.979774	-0.033255	-0.025790
15	H	3.178627	2.070400	-0.432673
16	H	2.567236	-2.105945	0.385385

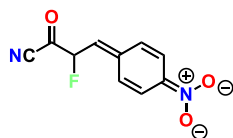
17	N	4.431704	-0.252235	-0.054363
18	O	5.143992	0.701956	-0.268389
19	O	4.838544	-1.375366	0.137554
20	F	-4.195017	-0.379408	1.469687
21	C	-4.386518	-0.633055	-0.821538
22	N	-4.953074	-1.182431	-1.666325

**7b-TS (Frequency: 344.2083 i cm<sup>-1</sup>)**



1	C	3.637861	-0.446758	-0.202435
2	O	4.015210	-1.579192	-0.057881
3	C	2.237636	0.041192	-0.087536
4	C	1.234250	-0.886344	0.097503
5	H	2.021783	0.986804	-0.590257
6	H	1.516508	-1.919480	0.308041
7	C	-0.160181	-0.554253	0.067789
8	C	-1.143014	-1.580057	0.039795
9	C	-0.626823	0.789025	0.070688
10	C	-2.493258	-1.293455	-0.020195
11	H	-0.815835	-2.621235	0.055214
12	C	-1.974807	1.086851	0.001929
13	H	0.091632	1.604132	0.164512
14	C	-2.905184	0.043470	-0.048230
15	H	-3.240570	-2.084891	-0.050162
16	H	-2.326380	2.117515	0.005192
17	N	-4.318811	0.351774	-0.110867
18	O	-5.109995	-0.570757	-0.141865
19	O	-4.655117	1.519814	-0.131719
20	F	2.892948	0.874825	1.367345
21	C	4.648285	0.615460	-0.494359
22	N	5.459803	1.390230	-0.760078

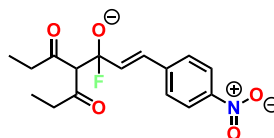
**7b-IM2**



1	C	-3.616136	0.417818	-0.432211
2	O	-3.767732	1.461537	-0.996140
3	C	-2.280243	-0.219201	-0.094854
4	C	-1.250151	0.772811	0.242864
5	H	-1.999660	-0.830934	-0.974099
6	H	-1.579227	1.762512	0.563524
7	C	0.100047	0.489792	0.171631
8	C	1.095910	1.501251	0.464574
9	C	0.624965	-0.812797	-0.188261
10	C	2.437250	1.256076	0.369485

11	H	0.748884	2.493535	0.760804
12	C	1.969866	-1.051316	-0.287766
13	H	-0.068201	-1.638247	-0.359264
14	C	2.904586	-0.024840	-0.017896
15	H	3.167183	2.035406	0.586182
16	H	2.342609	-2.037951	-0.561335
17	N	4.286129	-0.278644	-0.113934
18	O	5.080797	0.627941	0.132139
19	O	4.669846	-1.400170	-0.444076
20	F	-2.558443	-1.159680	0.920765
21	C	-4.817994	-0.376817	-0.028084
22	N	-5.780055	-0.946830	0.251794

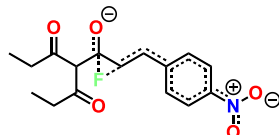
**7c-IM1**



1	C	2.048359	-0.295482	1.607268
2	O	2.191445	-1.506716	1.949096
3	C	0.648577	0.157066	1.183360
4	C	-0.347395	-0.722341	1.041274
5	H	0.496436	1.231945	1.036038
6	H	-0.099624	-1.768615	1.249103
7	C	-1.731882	-0.429012	0.644646
8	C	-2.672369	-1.473889	0.639133
9	C	-2.156570	0.857706	0.260973
10	C	-3.995005	-1.253956	0.273805
11	H	-2.354631	-2.476280	0.930183
12	C	-3.472155	1.096209	-0.107782
13	H	-1.446033	1.684589	0.245788
14	C	-4.373519	0.032944	-0.093920
15	H	-4.728828	-2.057922	0.269599
16	H	-3.809226	2.087192	-0.406417
17	N	-5.767093	0.279367	-0.482778
18	O	-6.533937	-0.656555	-0.466428
19	O	-6.076248	1.405756	-0.799128
20	F	2.310946	0.658183	2.715187
21	C	3.169733	0.191596	0.569442
22	H	4.074609	0.226661	1.188762
23	C	2.975779	1.600317	0.044713
24	O	3.502439	2.537736	0.605493
25	C	3.435147	-0.866940	-0.492089
26	O	4.579937	-1.169520	-0.754394
27	C	2.130757	1.844684	-1.193619
28	H	1.265713	1.167370	-1.219749
29	H	1.754522	2.874711	-1.121720
30	C	2.970112	1.689102	-2.467083
31	H	3.355671	0.666091	-2.586615

32	H	2.366430	1.925666	-3.353078
33	H	3.830159	2.372828	-2.444182
34	C	2.278242	-1.563274	-1.174048
35	H	1.776540	-2.121039	-0.367256
36	H	1.542452	-0.816260	-1.507511
37	C	2.715806	-2.472221	-2.309768
38	H	3.425014	-3.229097	-1.949778
39	H	1.852025	-2.986201	-2.751546
40	H	3.219115	-1.901524	-3.103795

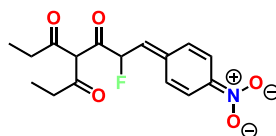
**7c-TS (Frequency: 305.4423 i cm<sup>-1</sup>)**



1	C	1.538487	0.615137	-0.360048
2	O	1.824696	1.072769	-1.442929
3	C	0.137266	0.233466	0.015916
4	C	-0.879942	0.475786	-0.882827
5	H	-0.082589	0.231463	1.085624
6	H	-0.613817	0.791336	-1.893523
7	C	-2.264875	0.297212	-0.563644
8	C	-3.278929	0.786391	-1.431528
9	C	-2.691408	-0.376925	0.614634
10	C	-4.620558	0.657078	-1.129216
11	H	-2.982650	1.288488	-2.354374
12	C	-4.030638	-0.503882	0.930658
13	H	-1.943755	-0.837896	1.260913
14	C	-4.993186	0.019749	0.060262
15	H	-5.391859	1.043657	-1.793676
16	H	-4.351825	-1.020961	1.833675
17	N	-6.396434	-0.117598	0.385398
18	O	-7.216713	0.336250	-0.389311
19	O	-6.698048	-0.679149	1.421102
20	F	0.738048	-1.484740	0.114586
21	C	2.600044	0.321844	0.697538
22	H	2.125664	0.223782	1.679711
23	C	3.631768	1.446557	0.840457
24	O	3.689642	2.064551	1.877118
25	C	3.307388	-1.027543	0.453368
26	O	3.736450	-1.630450	1.406648
27	C	4.598984	1.721108	-0.288959
28	H	4.138249	1.465227	-1.250527
29	H	4.805388	2.800505	-0.275993
30	C	5.907286	0.950089	-0.069613
31	H	5.753603	-0.138746	-0.078996
32	H	6.626881	1.193622	-0.861908
33	H	6.351868	1.220999	0.897837
34	C	3.472401	-1.520374	-0.962630

35	H	2.444737	-1.751646	-1.284160
36	H	3.809642	-0.687017	-1.598261
37	C	4.383206	-2.731754	-1.061712
38	H	4.006608	-3.549656	-0.433617
39	H	4.442897	-3.087442	-2.098359
40	H	5.401579	-2.495265	-0.720401

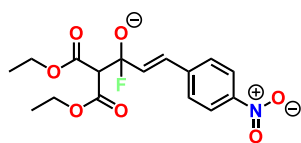
**7c-IM2**



1	C	-1.510527	0.074883	0.642601
2	O	-1.687288	-0.279600	1.783874
3	C	-0.275698	0.832778	0.199248
4	C	0.664532	-0.105566	-0.429496
5	H	0.148738	1.341015	1.075222
6	H	0.241899	-0.898898	-1.052887
7	C	2.041691	-0.068405	-0.267839
8	C	2.877499	-1.076483	-0.885787
9	C	2.749784	0.938140	0.494360
10	C	4.238694	-1.086991	-0.750739
11	H	2.389994	-1.855018	-1.476579
12	C	4.113117	0.923301	0.629105
13	H	2.190697	1.745913	0.968148
14	C	4.886119	-0.087731	0.014421
15	H	4.843889	-1.859430	-1.224114
16	H	4.624219	1.693319	1.206195
17	N	6.289152	-0.096685	0.155767
18	O	6.939651	-0.984294	-0.392262
19	O	6.830405	0.782105	0.823829
20	F	-0.743060	1.851905	-0.677956
21	C	-2.500069	-0.221538	-0.482781
22	H	-1.949144	-0.334975	-1.425945
23	C	-3.493871	0.932089	-0.713038
24	O	-4.063681	1.004195	-1.773055
25	C	-3.227427	-1.549034	-0.233015
26	O	-2.842327	-2.548232	-0.787384
27	C	-3.729857	1.904512	0.414180
28	H	-3.888489	1.326409	1.339150
29	H	-2.768893	2.428155	0.560919
30	C	-4.863708	2.875109	0.137977
31	H	-5.812302	2.336662	0.004794
32	H	-4.979715	3.582146	0.968789
33	H	-4.671102	3.443399	-0.781323
34	C	-4.382645	-1.541354	0.735567
35	H	-3.985516	-1.128362	1.677854
36	H	-5.122960	-0.807219	0.372080
37	C	-5.007464	-2.911615	0.931741

38	H	-4.264070	-3.625266	1.311316
39	H	-5.837296	-2.859655	1.647693
40	H	-5.391585	-3.304509	-0.019136

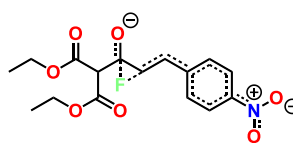
**7d-IM1**



1	C	-1.161510	-1.391380	-0.536341
2	O	-1.411155	-2.051143	0.510749
3	C	0.262368	-0.861638	-0.733319
4	C	1.197612	-1.069226	0.197045
5	H	0.472807	-0.333581	-1.669845
6	H	0.865284	-1.604227	1.092299
7	C	2.605661	-0.654438	0.150715
8	C	3.433057	-0.939234	1.251811
9	C	3.167625	0.019829	-0.950875
10	C	4.771887	-0.567823	1.266981
11	H	3.010774	-1.462106	2.111345
12	C	4.501553	0.398979	-0.953966
13	H	2.551224	0.250537	-1.819981
14	C	5.285552	0.098387	0.159085
15	H	5.416245	-0.785147	2.116994
16	H	4.943271	0.920492	-1.801166
17	N	6.697263	0.496657	0.160935
18	O	7.361838	0.226382	1.135692
19	O	7.124394	1.075432	-0.812563
20	F	-1.290715	-2.226105	-1.785290
21	C	-2.204150	-0.256240	-0.889239
22	H	-2.112529	0.027224	-1.945574
23	C	-2.063120	0.984420	-0.034466
24	O	-1.368204	1.115670	0.937640
25	C	-3.577900	-0.853130	-0.698666
26	O	-4.164494	-1.521301	-1.509596
27	C	-2.861123	3.181727	0.249492
28	H	-1.841637	3.592252	0.294784
29	H	-3.167889	2.949142	1.280174
30	C	-5.348705	-1.140120	0.827173
31	H	-5.259361	-2.235972	0.792032
32	H	-6.076971	-0.843083	0.058490
33	C	-3.822751	4.130322	-0.425599
34	H	-4.831910	3.697811	-0.458969
35	H	-3.866949	5.076549	0.129215
36	H	-3.498601	4.343356	-1.453213
37	C	-5.742044	-0.649210	2.199995
38	H	-6.713242	-1.073630	2.485915
39	H	-4.994857	-0.951379	2.946114
40	H	-5.823601	0.446356	2.209316

41	O	-2.838467	1.968452	-0.506673
42	O	-4.078980	-0.568943	0.506522

**7d-TS (Frequency: 311.4743 i cm<sup>-1</sup>)**

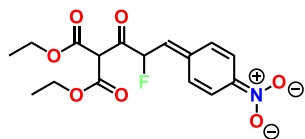


1	C	1.090214	-1.089287	0.326306
2	O	1.348376	-2.198723	-0.076199
3	C	-0.299788	-0.564565	0.473435
4	C	-1.343509	-1.275741	-0.067073
5	H	-0.392995	0.511650	0.624279
6	H	-1.136910	-2.268253	-0.472856
7	C	-2.698183	-0.800639	-0.086566
8	C	-3.684555	-1.464631	-0.862892
9	C	-3.117282	0.332178	0.662861
10	C	-4.989024	-1.012208	-0.924210
11	H	-3.396052	-2.349299	-1.433438
12	C	-4.417085	0.798849	0.602282
13	H	-2.405816	0.820378	1.329697
14	C	-5.348520	0.127489	-0.196756
15	H	-5.738601	-1.520657	-1.528672
16	H	-4.733702	1.666545	1.179076
17	N	-6.713524	0.609226	-0.257208
18	O	-7.511142	-0.001312	-0.941832
19	O	-7.003588	1.604652	0.377325
20	F	0.036673	-0.796489	2.296061
21	C	2.206136	-0.139543	0.769056
22	H	1.948885	0.170119	1.790022
23	C	2.279405	1.069618	-0.142634
24	O	1.561107	1.261227	-1.089211
25	C	3.527548	-0.880156	0.793249
26	O	3.994465	-1.415292	1.761991
27	C	3.467739	3.051362	-0.583416
28	H	2.546097	3.650476	-0.597072
29	H	3.664106	2.716045	-1.611995
30	C	5.330819	-1.602922	-0.537048
31	H	5.155872	-2.656816	-0.276525
32	H	6.045025	-1.192782	0.191237
33	C	4.633281	3.812617	-0.000969
34	H	5.537137	3.188726	0.006320
35	H	4.831236	4.706952	-0.605771
36	H	4.414388	4.128201	1.027836
37	C	5.811307	-1.440614	-1.958558
38	H	6.760213	-1.975536	-2.093658
39	H	5.075960	-1.849607	-2.664190
40	H	5.972109	-0.379599	-2.192940
41	O	3.247291	1.893944	0.236115



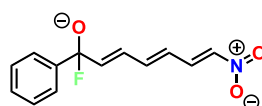
42 O 4.091821 -0.893693 -0.410419

**7d-IM2**



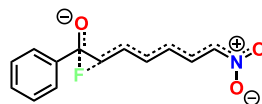
1	C	1.040844	-0.984565	0.099605
2	O	1.141995	-2.096367	-0.346581
3	C	-0.276696	-0.223218	0.101572
4	C	-1.414737	-1.054452	0.540126
5	H	-0.409309	0.170143	-0.922728
6	H	-1.199218	-1.993289	1.053077
7	C	-2.721911	-0.676560	0.325649
8	C	-3.832185	-1.519222	0.731329
9	C	-3.091784	0.577588	-0.306788
10	C	-5.133194	-1.173473	0.501852
11	H	-3.604281	-2.464868	1.228248
12	C	-4.397117	0.915237	-0.538577
13	H	-2.306612	1.284154	-0.580830
14	C	-5.447715	0.049807	-0.146245
15	H	-5.950434	-1.825790	0.808003
16	H	-4.653326	1.860869	-1.015509
17	N	-6.785222	0.407014	-0.377234
18	O	-7.683392	-0.356045	-0.016605
19	O	-7.037110	1.475523	-0.937542
20	F	-0.079897	0.931290	0.897336
21	C	2.238185	-0.248941	0.703296
22	H	2.001425	0.026384	1.739646
23	C	2.520513	1.013528	-0.095457
24	O	2.039909	1.258528	-1.169912
25	C	3.444609	-1.170071	0.711750
26	O	3.751393	-1.874294	1.633871
27	C	3.799967	2.982877	-0.153161
28	H	2.908437	3.595749	-0.347472
29	H	4.226604	2.693775	-1.124323
30	C	5.236149	-1.976872	-0.585238
31	H	4.899906	-3.016853	-0.467130
32	H	5.941399	-1.757356	0.228778
33	C	4.802487	3.695209	0.720834
34	H	5.677656	3.057781	0.904555
35	H	5.138331	4.614474	0.223962
36	H	4.352676	3.964368	1.685750
37	C	5.837396	-1.722971	-1.945732
38	H	6.712259	-2.369737	-2.090651
39	H	5.107803	-1.939503	-2.737314
40	H	6.157809	-0.676485	-2.037715
41	O	3.389433	1.789200	0.533381
42	O	4.095977	-1.116284	-0.443193

**8a-IM1**



1	C	4.771545	1.577660	0.998096
2	C	3.858624	0.528678	1.112491
3	C	3.359111	-0.106680	-0.030054
4	C	3.792770	0.320190	-1.286087
5	C	4.704993	1.369903	-1.406707
6	C	5.195892	2.002839	-0.263398
7	H	5.159777	2.063324	1.895708
8	H	3.536120	0.181015	2.095863
9	H	3.401228	-0.204582	-2.159166
10	H	5.037986	1.694825	-2.394672
11	H	5.910185	2.823284	-0.353631
12	C	2.324590	-1.255471	0.037096
13	O	2.251995	-2.004287	-0.986093
14	C	0.998907	-0.668715	0.546555
15	C	-0.144665	-0.844724	-0.133349
16	H	1.008354	-0.084287	1.474594
17	H	-0.090629	-1.435640	-1.053628
18	F	2.765810	-1.997039	1.272824
19	C	-1.418865	-0.305214	0.289239
20	C	-2.583068	-0.477610	-0.381654
21	H	-1.429922	0.282482	1.214827
22	H	-2.597195	-1.059924	-1.307621
23	C	-3.819613	0.090727	0.089975
24	C	-4.998855	-0.048997	-0.540119
25	H	-3.805041	0.673718	1.015491
26	H	-5.184146	-0.592568	-1.463360
27	N	-6.191792	0.557605	0.001892
28	O	-6.126113	1.195784	1.032582
29	O	-7.218963	0.387623	-0.624686

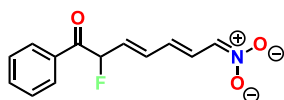
**8a-TS (Frequency: 226.0900 i cm<sup>-1</sup>)**



1	C	4.851992	1.825753	0.131800
2	C	3.680087	1.130844	0.424258
3	C	3.490023	-0.161659	-0.080278
4	C	4.487144	-0.753117	-0.862484
5	C	5.656914	-0.054211	-1.158765
6	C	5.838305	1.238397	-0.664788
7	H	5.004037	2.828256	0.535524
8	H	2.919017	1.528561	1.094660
9	H	4.329500	-1.766344	-1.235906
10	H	6.428393	-0.517601	-1.775913

11	H	6.753195	1.787312	-0.894662
12	C	2.230335	-0.948366	0.163436
13	O	2.255954	-2.164749	0.154332
14	C	0.942960	-0.198741	0.237797
15	C	-0.252130	-0.852246	0.141994
16	H	0.976443	0.885309	0.124659
17	H	-0.251989	-1.945372	0.150580
18	F	1.748274	-0.016976	2.088384
19	C	-1.489853	-0.153534	0.072323
20	C	-2.729564	-0.727324	-0.013523
21	H	-1.438765	0.942771	0.079168
22	H	-2.823512	-1.817214	-0.018684
23	C	-3.911555	0.064480	-0.096256
24	C	-5.170277	-0.428328	-0.181214
25	H	-3.805181	1.153645	-0.090775
26	H	-5.452416	-1.477763	-0.197922
27	N	-6.292124	0.454266	-0.259443
28	O	-6.119809	1.660856	-0.253321
29	O	-7.395471	-0.061145	-0.330498

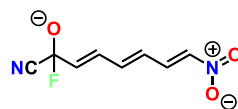
**8a-IM2**



1	C	5.112647	1.600192	-0.227381
2	C	3.804095	1.159008	-0.037128
3	C	3.499484	-0.203162	-0.163243
4	C	4.518013	-1.113168	-0.476868
5	C	5.824817	-0.672126	-0.657163
6	C	6.122396	0.687472	-0.534291
7	H	5.345228	2.661543	-0.132529
8	H	3.026097	1.877689	0.219176
9	H	4.260641	-2.168305	-0.577498
10	H	6.614240	-1.385850	-0.896393
11	H	7.146105	1.036652	-0.678307
12	C	2.107658	-0.738815	-0.019576
13	O	1.845078	-1.884441	-0.302973
14	C	1.010286	0.212574	0.481804
15	C	-0.281498	-0.460839	0.751630
16	H	0.877402	1.015979	-0.263030
17	H	-0.245867	-1.381568	1.341345
18	F	1.521933	0.813398	1.641159
19	C	-1.460857	0.024169	0.301622
20	C	-2.762005	-0.544963	0.520396
21	H	-1.438663	0.943149	-0.300401
22	H	-2.829302	-1.461601	1.116002
23	C	-3.899205	0.025765	0.011806
24	C	-5.217918	-0.442150	0.164155
25	H	-3.798631	0.942463	-0.578754

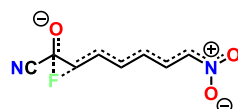
26	H	-5.492132	-1.338291	0.714217
27	N	-6.277321	0.222736	-0.393002
28	O	-6.106075	1.268169	-1.049172
29	O	-7.425099	-0.236896	-0.232583

**8b-IM1**



1	C	3.669116	-0.339225	0.135598
2	O	3.722142	-1.483919	-0.378813
3	C	2.295976	0.272542	0.415697
4	C	1.182115	-0.343917	-0.000755
5	H	2.257632	1.223576	0.958144
6	H	1.302267	-1.288889	-0.540411
7	F	4.328435	-0.235727	1.447573
8	C	4.488944	0.732138	-0.647167
9	N	5.104163	1.454081	-1.308000
10	C	-0.154744	0.167566	0.231169
11	C	-1.280670	-0.453076	-0.187705
12	H	-0.242980	1.113192	0.777965
13	H	-1.210787	-1.397625	-0.735116
14	C	-2.590815	0.096730	0.066152
15	C	-3.732317	-0.485612	-0.333339
16	H	-2.663660	1.040218	0.614573
17	H	-3.832370	-1.418093	-0.883789
18	N	-5.008057	0.129726	-0.037210
19	O	-5.039992	1.179053	0.570445
20	O	-5.995199	-0.460178	-0.426751

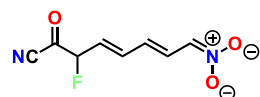
**8b-TS (Frequency: 379.0603 i cm<sup>-1</sup>)**



1	C	-3.660607	0.437397	-0.238593
2	O	-3.872763	1.621927	-0.210605
3	C	-2.332958	-0.211188	-0.098665
4	C	-1.198580	0.563248	0.001221
5	H	-2.254057	-1.255256	-0.407184
6	H	-1.308891	1.638823	0.158735
7	F	-3.200265	-0.640879	1.502193
8	C	-4.804939	-0.499456	-0.446627
9	N	-5.714585	-1.176386	-0.655502
10	C	0.093229	-0.009682	-0.053285
11	C	1.285312	0.666827	0.048891
12	H	0.145199	-1.095768	-0.203926
13	H	1.281689	1.749428	0.205700
14	C	2.528654	-0.011181	-0.046130
15	C	3.751080	0.574879	0.042719

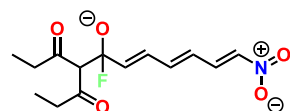
16	H	2.513724	-1.094244	-0.203301
17	H	3.947508	1.632511	0.196898
18	N	4.937694	-0.204781	-0.067624
19	O	4.864076	-1.410688	-0.243431
20	O	6.002225	0.388200	0.021291

**8b-IM2**



1	C	-3.485626	0.644264	-0.239029
2	O	-3.228446	1.806425	-0.348474
3	C	-2.451596	-0.477611	-0.253451
4	C	-1.242748	-0.155854	0.540206
5	H	-2.185596	-0.641184	-1.312372
6	H	-1.395530	0.159177	1.576816
7	F	-3.111902	-1.615450	0.197701
8	C	-4.908269	0.208920	-0.100437
9	N	-6.021028	-0.074263	0.001036
10	C	0.004353	-0.237315	0.015608
11	C	1.235354	0.052197	0.686348
12	H	0.094769	-0.551320	-1.033240
13	H	1.192783	0.371157	1.732855
14	C	2.448275	-0.059769	0.051424
15	C	3.712002	0.197137	0.603551
16	H	2.455999	-0.380784	-0.995491
17	H	3.883972	0.525112	1.625048
18	N	4.857157	0.048077	-0.140483
19	O	4.805941	-0.323345	-1.326241
20	O	5.952172	0.292967	0.396950

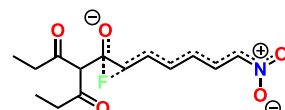
**8c-IM1**



1	C	1.510690	-0.859136	-0.198585
2	O	1.601802	-0.631429	-1.439727
3	C	0.109022	-0.852136	0.410673
4	C	-0.962009	-0.513053	-0.321050
5	H	0.001572	-1.134688	1.463776
6	H	-0.791017	-0.242589	-1.368196
7	F	1.961380	-2.251822	0.169389
8	C	2.472512	-0.014113	0.744574
9	H	2.210183	-0.193006	1.795498
10	C	2.183271	1.452049	0.483713
11	O	1.417721	2.046585	1.213799
12	C	3.921565	-0.463579	0.608453
13	O	4.598518	-0.567315	1.610376
14	C	2.814834	2.133023	-0.707700

15	H	2.813357	1.415633	-1.539764
16	H	2.167948	2.981365	-0.971504
17	C	4.224259	2.642016	-0.384949
18	H	4.903497	1.832005	-0.081170
19	H	4.663720	3.132490	-1.263769
20	H	4.191072	3.374207	0.434107
21	C	4.488433	-0.824438	-0.746328
22	H	3.876910	-1.668038	-1.099587
23	H	4.266626	-0.017764	-1.458118
24	C	5.970514	-1.153293	-0.693969
25	H	6.163332	-1.984737	-0.003013
26	H	6.341350	-1.434623	-1.688510
27	H	6.555054	-0.291418	-0.340068
28	C	-2.312814	-0.494238	0.201403
29	C	-3.405193	-0.161583	-0.524996
30	H	-2.444761	-0.768660	1.254445
31	H	-3.296795	0.115657	-1.577663
32	C	-4.726380	-0.161116	0.052358
33	C	-5.840070	0.160169	-0.626556
34	H	-4.834634	-0.437663	1.105135
35	H	-5.905648	0.455434	-1.670999
36	N	-7.127330	0.134508	0.030441
37	O	-7.197284	-0.179763	1.200475
38	O	-8.087591	0.437899	-0.648730

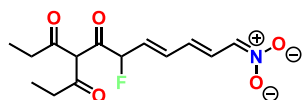
**8c-TS (Frequency: 339.6679 i cm<sup>-1</sup>)**



1	C	1.370564	0.366281	-0.337456
2	O	1.530807	0.458724	-1.534355
3	C	0.021028	0.144286	0.266765
4	C	-1.096955	0.108957	-0.532653
5	H	-0.089189	0.338419	1.334455
6	H	-0.965393	0.056716	-1.616332
7	F	0.839705	-1.556420	0.633085
8	C	2.538012	0.439662	0.641943
9	H	2.160767	0.552461	1.663563
10	C	3.446756	1.649936	0.397350
11	O	3.533299	2.505337	1.246534
12	C	3.368229	-0.860040	0.659566
13	O	3.921533	-1.168876	1.687218
14	C	4.267020	1.720488	-0.870852
15	H	3.756215	1.185360	-1.680530
16	H	4.342345	2.782356	-1.144215
17	C	5.672960	1.157630	-0.624232
18	H	5.650220	0.094310	-0.344256
19	H	6.283513	1.252321	-1.531508
20	H	6.167462	1.710553	0.186133

21	C	3.493153	-1.674466	-0.603899
22	H	2.478187	-2.069753	-0.764064
23	H	3.691316	-1.000705	-1.451222
24	C	4.525919	-2.782219	-0.487953
25	H	4.286387	-3.448216	0.351361
26	H	4.557678	-3.379501	-1.408368
27	H	5.531543	-2.374466	-0.308432
28	C	-2.400826	0.096958	0.018307
29	C	-3.579767	0.045159	-0.685354
30	H	-2.473292	0.144226	1.112660
31	H	-3.557102	-0.009497	-1.777664
32	C	-4.835020	0.060507	-0.021688
33	C	-6.047337	0.011042	-0.632032
34	H	-4.837845	0.115394	1.071425
35	H	-6.227421	-0.045711	-1.702205
36	N	-7.246209	0.031198	0.137394
37	O	-7.190924	0.093186	1.355282
38	O	-8.301179	-0.015866	-0.476829

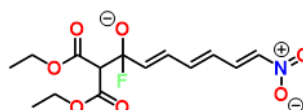
**8c-IM2**



1	C	-1.394137	-0.823593	0.090006
2	O	-1.213849	-1.459335	-0.916698
3	C	-0.217574	-0.254982	0.887075
4	C	0.904379	0.219521	0.043010
5	H	0.120603	-1.056519	1.566598
6	H	0.656282	0.828927	-0.832309
7	F	-0.739995	0.763211	1.700622
8	C	-2.774287	-0.585564	0.687854
9	H	-2.736399	-0.822808	1.760152
10	C	-3.827871	-1.511873	0.066494
11	O	-4.340488	-2.364683	0.747728
12	C	-3.231297	0.886392	0.603248
13	O	-4.048209	1.290818	1.390299
14	C	-4.236047	-1.292002	-1.372454
15	H	-3.399771	-0.873351	-1.946677
16	H	-4.472088	-2.280884	-1.789281
17	C	-5.475285	-0.391165	-1.454383
18	H	-5.280402	0.620901	-1.071153
19	H	-5.802434	-0.297002	-2.497682
20	H	-6.299613	-0.821848	-0.869871
21	C	-2.658683	1.741054	-0.500600
22	H	-1.577434	1.823419	-0.295005
23	H	-2.736471	1.180393	-1.447309
24	C	-3.306327	3.111407	-0.591703
25	H	-3.203855	3.649473	0.359520
26	H	-2.837715	3.707631	-1.384327

27	H	-4.379395	3.023963	-0.811984
28	C	2.195541	-0.075061	0.327973
29	C	3.353031	0.341553	-0.406638
30	H	2.390589	-0.703756	1.207604
31	H	3.206248	0.970540	-1.290871
32	C	4.620512	-0.027086	-0.029776
33	C	5.821828	0.317218	-0.669710
34	H	4.733568	-0.655355	0.859980
35	H	5.890512	0.931925	-1.562988
36	N	7.032341	-0.118370	-0.191532
37	O	7.099901	-0.830884	0.826272
38	O	8.067477	0.213973	-0.797806

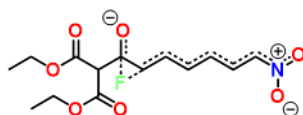
**8d-IM1**



1	C	-1.889526	0.327436	1.546585
2	O	-1.712716	1.300466	2.318374
3	C	-0.650397	-0.390133	1.012905
4	C	0.566891	0.151106	1.171751
5	H	-0.789789	-1.322506	0.457715
6	H	0.633833	1.092865	1.726340
7	F	-2.644998	-0.797477	2.192475
8	C	-2.888868	0.635950	0.301205
9	H	-3.565114	1.392038	0.715843
10	C	-3.711954	-0.559741	-0.083848
11	O	-4.910359	-0.629604	0.043324
12	C	-2.114675	1.230550	-0.843610
13	O	-1.910044	0.707839	-1.912104
14	C	-3.676797	-2.783808	-0.841213
15	H	-4.459751	-2.575012	-1.584846
16	H	-4.177578	-3.134005	0.073920
17	C	-0.766060	3.041982	-1.489708
18	H	-1.324318	3.198350	-2.424518
19	H	0.058836	2.348108	-1.710988
20	C	1.778367	-0.440953	0.642295
21	C	3.010139	0.104499	0.773169
22	H	1.675743	-1.386801	0.097786
23	H	3.133632	1.048855	1.311543
24	C	4.180930	-0.525419	0.215560
25	C	5.421625	-0.020320	0.316012
26	H	4.058005	-1.469602	-0.322862
27	H	5.712541	0.901450	0.814023
28	N	6.542399	-0.715973	-0.274699
29	O	6.357613	-1.762778	-0.860094
30	O	7.631904	-0.194672	-0.145437
31	C	-2.667625	-3.785176	-1.351094
32	H	-1.901865	-3.986242	-0.589325

33	H	-3.168409	-4.730238	-1.598751
34	H	-2.171559	-3.405459	-2.254654
35	C	-0.268001	4.341055	-0.902888
36	H	0.405559	4.839005	-1.612480
37	H	-1.107446	5.015447	-0.686170
38	H	0.281488	4.155424	0.030058
39	O	-2.979926	-1.572900	-0.548142
40	O	-1.630214	2.432306	-0.527763

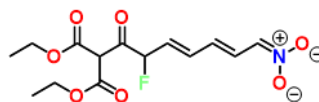
**8d-TS (Frequency: 315.7478 i cm<sup>-1</sup>)**



1	C	-1.784044	-0.285504	-1.612573
2	O	-1.752780	-0.698282	-2.746899
3	C	-0.558466	0.136623	-0.872194
4	C	0.686330	-0.124830	-1.390913
5	H	-0.670925	0.354139	0.189747
6	H	0.764249	-0.476759	-2.422651
7	F	-1.319780	1.862261	-1.323183
8	C	-3.122894	-0.236194	-0.859707
9	H	-3.912516	-0.452897	-1.590089
10	C	-3.405828	1.138791	-0.274503
11	O	-4.156307	1.939564	-0.759337
12	C	-3.212520	-1.287522	0.237903
13	O	-4.181250	-1.444126	0.931189
14	C	-2.611099	2.669823	1.304660
15	H	-3.603968	3.085022	1.529732
16	H	-2.176103	3.218124	0.457611
17	C	-2.066627	-3.027031	1.345859
18	H	-2.878157	-3.742439	1.151103
19	H	-2.262786	-2.552984	2.318008
20	C	1.861569	0.092845	-0.632038
21	C	3.151682	-0.121462	-1.052823
22	H	1.722941	0.458742	0.393823
23	H	3.336767	-0.480872	-2.069297
24	C	4.257259	0.115721	-0.194108
25	C	5.561610	-0.067051	-0.525961
26	H	4.053999	0.476300	0.819102
27	H	5.938650	-0.417486	-1.483038
28	N	6.594044	0.204794	0.417000
29	O	6.312245	0.607867	1.534326
30	O	7.744163	0.015618	0.050992
31	C	-1.706797	2.677092	2.513408
32	H	-0.718941	2.269742	2.256944
33	H	-1.574645	3.705296	2.874959
34	H	-2.135267	2.074912	3.326334
35	C	-0.704985	-3.675588	1.290162
36	H	-0.635612	-4.459690	2.055039

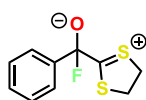
37	H	-0.533383	-4.131043	0.305716
38	H	0.083709	-2.934089	1.476589
39	O	-2.755674	1.312659	0.874481
40	O	-2.104077	-2.011076	0.332370

**8d-IM2**



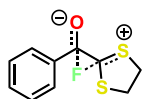
1	C	1.649772	-0.136201	-1.681073
2	O	1.384572	0.160275	-2.813537
3	C	0.658349	-0.849622	-0.752506
4	C	-0.704667	-0.970159	-1.305840
5	H	0.654406	-0.344750	0.224249
6	H	-0.797389	-1.306109	-2.342305
7	F	1.261068	-2.112298	-0.549025
8	C	3.032197	0.207996	-1.101867
9	H	3.729173	0.325769	-1.939947
10	C	3.572641	-0.880689	-0.184430
11	O	4.336716	-1.739291	-0.525402
12	C	2.981023	1.529704	-0.337933
13	O	3.958603	2.130770	0.009931
14	C	3.317016	-1.837077	1.951339
15	H	4.397341	-1.878265	2.149502
16	H	3.023007	-2.774991	1.459342
17	C	1.546573	3.126067	0.647751
18	H	2.018725	3.949364	0.093729
19	H	2.068902	3.021187	1.609107
20	C	-1.800611	-0.659445	-0.572329
21	C	-3.168805	-0.725532	-0.995925
22	H	-1.639340	-0.310390	0.457168
23	H	-3.379622	-1.067354	-2.014630
24	C	-4.200025	-0.374939	-0.161326
25	C	-5.572627	-0.396676	-0.460142
26	H	-3.952765	-0.038634	0.851040
27	H	-5.990746	-0.699503	-1.416225
28	N	-6.508071	-0.021000	0.470178
29	O	-6.166979	0.346515	1.609599
30	O	-7.712086	-0.054270	0.153838
31	C	2.513620	-1.574406	3.201026
32	H	1.440941	-1.540833	2.966460
33	H	2.686702	-2.377419	3.928912
34	H	2.806133	-0.619543	3.657965
35	C	0.061298	3.327427	0.820952
36	H	-0.123531	4.251899	1.382825
37	H	-0.434910	3.406478	-0.155528
38	H	-0.381240	2.488337	1.374693
39	O	3.060643	-0.762438	1.035452
40	O	1.734352	1.912656	-0.100201

**9-IM1**



1	C	3.893563	-0.890078	0.317612
2	C	3.188963	-1.048362	-0.877291
3	C	1.987124	-0.368157	-1.075574
4	C	1.483315	0.469738	-0.075673
5	C	2.193115	0.631562	1.114205
6	C	3.395917	-0.046521	1.312469
7	H	4.834253	-1.421430	0.471255
8	H	3.581381	-1.698811	-1.660806
9	H	1.438657	-0.475785	-2.012999
10	H	1.786298	1.304850	1.870133
11	H	3.948991	0.084142	2.244209
12	C	0.150149	1.211200	-0.227055
13	O	-0.044164	2.243630	0.464902
14	C	-1.057266	0.189987	-0.047357
15	C	-3.520838	-0.614094	0.095859
16	C	-2.659459	-1.800565	0.479409
17	S	-0.956247	-1.480626	-0.127378
18	S	-2.530853	0.911982	0.311189
19	H	-3.827259	-0.649168	-0.958134
20	H	-4.410396	-0.537112	0.732390
21	H	-3.014979	-2.733058	0.025192
22	H	-2.578532	-1.929112	1.567169
23	F	0.006778	1.421833	-1.670914

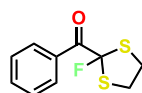
**9-TS (Frequency: 349.8528 i cm<sup>-1</sup>)**



1	C	-4.035580	-0.771015	-0.258131
2	C	-3.149681	-1.261071	0.703121
3	C	-1.899034	-0.668555	0.872188
4	C	-1.528595	0.418377	0.072295
5	C	-2.422854	0.916041	-0.879625
6	C	-3.672493	0.321021	-1.047343
7	H	-5.013493	-1.237468	-0.387468
8	H	-3.438410	-2.104039	1.332765
9	H	-1.209383	-1.018795	1.639494
10	H	-2.126383	1.776186	-1.481684
11	H	-4.365309	0.711487	-1.794261
12	C	-0.185252	1.104209	0.165654
13	O	-0.065130	2.297916	-0.069077
14	C	1.047521	0.225955	-0.007046
15	C	3.547910	-0.458881	-0.068113
16	F	0.315288	0.648172	1.813651

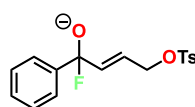
17	C	2.786114	-1.603617	-0.702409
18	S	1.026367	-1.461012	-0.207389
19	S	2.517764	1.046079	-0.194816
20	H	3.742013	-0.632116	0.998495
21	H	4.494742	-0.265139	-0.586364
22	H	3.152495	-2.579039	-0.360321
23	H	2.812741	-1.563795	-1.799174

**9-IM2**



1	C	-4.219960	-0.659465	0.037827
2	C	-3.994152	0.647599	-0.400772
3	C	-2.699481	1.153071	-0.430831
4	C	-1.618334	0.359533	-0.020517
5	C	-1.850688	-0.950424	0.424410
6	C	-3.149718	-1.454914	0.447064
7	H	-5.234953	-1.059016	0.061149
8	H	-4.830145	1.270528	-0.720857
9	H	-2.500683	2.168435	-0.775010
10	H	-1.028378	-1.581981	0.759356
11	H	-3.325481	-2.474634	0.791095
12	C	-0.259880	0.979111	-0.110372
13	O	-0.090394	2.091717	-0.543235
14	C	0.954112	0.147335	0.355374
15	C	3.529080	-0.293035	0.243988
16	C	3.026139	-1.085500	-0.948250
17	S	1.210587	-1.259149	-0.792779
18	S	2.448377	1.162466	0.401409
19	H	3.488875	-0.884511	1.168005
20	H	4.553389	0.069293	0.087537
21	H	3.450408	-2.097977	-0.972186
22	H	3.251452	-0.570542	-1.890422
23	F	0.672504	-0.342919	1.612402

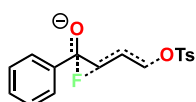
**10-IM1**



1	C	-3.436700	-0.054892	-1.815479
2	C	-2.557569	-1.028899	-1.339541
3	C	-2.233142	-1.096341	0.020669
4	C	-2.814236	-0.177052	0.895036
5	C	-3.711739	0.784573	0.429830
6	C	-4.020573	0.853809	-0.929685
7	H	-3.677086	-0.010974	-2.879679
8	H	-2.130531	-1.752338	-2.037291
9	H	-2.540759	-0.253532	1.948751

10	H	-4.170222	1.488548	1.127595
11	H	-4.715250	1.611075	-1.298576
12	C	-1.280858	-2.167106	0.610281
13	O	-1.073093	-2.092606	1.861351
14	C	-0.035001	-2.300124	-0.275872
15	C	1.182717	-2.082709	0.217137
16	H	1.256842	-1.812685	1.275122
17	C	2.433707	-2.173968	-0.597641
18	H	3.269810	-2.589276	-0.018960
19	H	2.281041	-2.776914	-1.500135
20	O	2.864830	-0.890210	-1.129173
21	S	3.178847	0.307361	-0.114032
22	O	3.583206	-0.250337	1.165499
23	O	4.078850	1.173813	-0.846961
24	C	1.628953	1.137672	0.065305
25	C	1.024342	1.676395	-1.071220
26	C	1.085022	1.310798	1.334095
27	C	-0.139251	2.421456	-0.919471
28	H	1.462781	1.520003	-2.058201
29	C	-0.073522	2.073559	1.466015
30	H	1.572371	0.865619	2.202144
31	C	-0.689982	2.653954	0.350920
32	H	-0.621311	2.849841	-1.800537
33	H	-0.503431	2.226755	2.457700
34	C	-1.885494	3.551548	0.509536
35	H	-2.411163	3.351445	1.451669
36	H	-1.564100	4.604931	0.518204
37	H	-2.590637	3.422234	-0.321742
38	H	-0.164067	-2.575477	-1.329135
39	F	-2.011803	-3.434261	0.220265

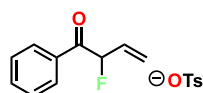
10-TS (Frequency: 289.5923 i cm<sup>-1</sup>)



1	C	-3.912092	-0.452609	-1.514385
2	C	-2.688145	-0.966064	-1.084602
3	C	-2.309787	-0.846204	0.257823
4	C	-3.175849	-0.220316	1.162688
5	C	-4.401244	0.284968	0.735638
6	C	-4.769905	0.171915	-0.606836
7	H	-4.205322	-0.554414	-2.560507
8	H	-2.041621	-1.515250	-1.767603
9	H	-2.867920	-0.143665	2.206630
10	H	-5.069842	0.772162	1.447351
11	H	-5.728457	0.568618	-0.945893
12	C	-1.003702	-1.383509	0.784194
13	O	-0.835976	-1.467897	1.983460
14	C	0.055865	-1.816566	-0.203004

15	C	1.328570	-2.067098	0.293945
16	H	1.449150	-2.211304	1.367572
17	C	2.500979	-2.139997	-0.568113
18	H	3.346790	-2.667078	-0.109188
19	H	2.309816	-2.554875	-1.566134
20	O	3.132233	-0.801115	-1.012277
21	S	3.292627	0.385649	0.007392
22	O	3.608613	-0.112650	1.338135
23	O	4.220880	1.311522	-0.626024
24	C	1.699284	1.159701	0.025945
25	C	1.192026	1.654093	-1.176437
26	C	0.985247	1.262630	1.212394
27	C	-0.068957	2.237585	-1.182490
28	H	1.773644	1.567567	-2.095814
29	C	-0.272673	1.863767	1.190673
30	H	1.401448	0.848899	2.131028
31	C	-0.821626	2.346701	-0.002298
32	H	-0.483874	2.614950	-2.119657
33	H	-0.848374	1.938500	2.115568
34	C	-2.198571	2.948571	-0.044198
35	H	-2.620874	3.054405	0.963188
36	H	-2.181461	3.936619	-0.526447
37	H	-2.873427	2.303464	-0.627907
38	H	-0.006169	-1.324723	-1.181461
39	F	-0.875340	-3.163171	-0.666774

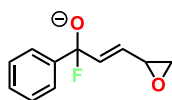
10-IM2



1	C	3.493113	-0.903226	-1.855300
2	C	2.479282	-0.099887	-1.336545
3	C	2.671428	0.567319	-0.119850
4	C	3.889668	0.437767	0.558760
5	C	4.907320	-0.350316	0.030798
6	C	4.705848	-1.027450	-1.174503
7	H	3.337370	-1.432392	-2.796246
8	H	1.536112	-0.004727	-1.874793
9	H	4.016199	0.958507	1.509075
10	H	5.856366	-0.444985	0.560020
11	H	5.498802	-1.653469	-1.586790
12	C	1.590669	1.363178	0.536743
13	O	1.654941	1.674832	1.704143
14	C	0.378526	1.782468	-0.303673
15	C	-0.412564	2.870184	0.353518
16	H	0.167577	3.704450	0.758443
17	C	-1.742031	2.854411	0.429683
18	H	-2.282476	3.680826	0.897390
19	H	-2.334940	2.027809	0.027562

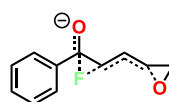
20	O	-3.287310	0.420393	-1.605331
21	S	-3.646003	-0.398436	-0.425050
22	O	-4.261097	0.386656	0.665154
23	O	-4.390425	-1.623362	-0.774511
24	C	-2.065391	-0.959150	0.214554
25	C	-1.241314	-1.726772	-0.611649
26	C	-1.633427	-0.577644	1.480467
27	C	0.021465	-2.102525	-0.164125
28	H	-1.588031	-2.013720	-1.606379
29	C	-0.364094	-0.959345	1.919077
30	H	-2.290820	0.031101	2.102261
31	C	0.481234	-1.724142	1.107335
32	H	0.674186	-2.689971	-0.814478
33	H	-0.016027	-0.641986	2.904650
34	C	1.843796	-2.144148	1.589916
35	H	2.256570	-1.404060	2.289444
36	H	1.789082	-3.110709	2.115042
37	H	2.544019	-2.255610	0.749338
38	H	-0.255952	0.896743	-0.487503
39	F	0.853108	2.228299	-1.532567

#### 11-IMI



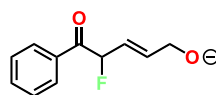
1	C	-3.194370	-1.140209	-1.066787
2	C	-2.030002	-0.381449	-1.200685
3	C	-1.465480	0.261790	-0.098762
4	C	-2.091483	0.142659	1.147488
5	C	-3.255370	-0.613826	1.288351
6	C	-3.809673	-1.260149	0.180308
7	H	-3.626770	-1.637540	-1.937688
8	H	-1.532278	-0.255605	-2.163411
9	H	-1.665088	0.664482	2.006563
10	H	-3.737903	-0.696420	2.264488
11	H	-4.720592	-1.851712	0.289254
12	C	-0.160381	1.068817	-0.305970
13	O	0.101632	1.402117	-1.504018
14	C	0.969570	0.377161	0.474327
15	C	2.115716	0.048718	-0.120105
16	H	0.804543	0.147498	1.534258
17	H	2.225262	0.295749	-1.182399
18	C	3.256816	-0.601865	0.556377
19	C	4.643497	-0.360841	0.119357
20	H	5.459280	-0.446785	0.844586
21	H	4.820963	0.321607	-0.718880
22	O	3.981276	-1.561501	-0.204013
23	H	3.098434	-0.885325	1.603800
24	F	-0.406907	2.263810	0.586697

#### 11-TS (Frequency: 94.1027 i cm<sup>-1</sup>)



1	C	-3.651834	0.450855	1.097542
2	C	-2.420459	-0.187194	1.215067
3	C	-1.529332	-0.218727	0.134383
4	C	-1.905703	0.367760	-1.079939
5	C	-3.147965	0.990955	-1.204650
6	C	-4.017316	1.042236	-0.114881
7	H	-4.332705	0.486093	1.949552
8	H	-2.122769	-0.669672	2.147277
9	H	-1.238914	0.310197	-1.941330
10	H	-3.438583	1.436060	-2.157419
11	H	-4.984407	1.538559	-0.211008
12	C	-0.219800	-0.944337	0.305995
13	O	-0.132593	-1.818186	1.151655
14	C	0.945232	-0.517006	-0.534724
15	C	2.083162	-0.240101	0.240237
16	H	0.703237	0.274430	-1.254805
17	H	2.249439	-0.810212	1.158631
18	C	3.138683	0.652930	-0.231386
19	C	4.528649	0.646367	0.260586
20	H	5.361932	0.943717	-0.389364
21	H	4.797725	-0.074225	1.043835
22	O	3.657075	1.681975	0.660859
23	H	2.999484	1.039958	-1.250936
24	F	0.998868	-1.738629	-1.569323

#### 11-IM2

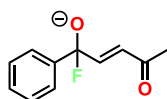


1	C	-3.602489	-0.164257	-0.245915
2	C	-2.545611	0.733709	-0.381203
3	C	-1.236695	0.351170	-0.060249
4	C	-0.994174	-0.960135	0.375445
5	C	-2.052954	-1.858526	0.504456
6	C	-3.358003	-1.463597	0.201511
7	H	-4.619130	0.148620	-0.490201
8	H	-2.715130	1.752656	-0.732410
9	H	0.030390	-1.291505	0.553652
10	H	-1.856253	-2.880641	0.832654
11	H	-4.182132	-2.171476	0.305322
12	C	-0.162592	1.399591	-0.191769
13	O	-0.332853	2.353539	-0.934246
14	C	1.122296	1.199797	0.559490
15	C	2.005969	0.440700	-0.303623



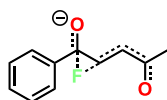
16	H	0.939795	0.670379	1.508884
17	H	1.931142	0.590266	-1.384971
18	C	2.671467	-0.745917	0.187032
19	C	3.358766	-1.719675	-0.668098
20	H	4.258037	-2.244256	-0.317146
21	H	3.345692	-1.548966	-1.753896
22	O	2.139004	-2.128951	-0.099596
23	H	3.002491	-0.726707	1.234851
24	F	1.575556	2.514197	0.961281

### 12-IMI



1	C	3.673121	1.204970	-0.501457
2	C	3.158436	0.324338	-1.454581
3	C	2.017872	-0.427038	-1.166348
4	C	1.378745	-0.307577	0.068401
5	C	1.902867	0.572635	1.021882
6	C	3.043345	1.325420	0.739842
7	H	4.565271	1.793697	-0.722748
8	H	3.650992	0.221857	-2.423800
9	H	1.599339	-1.135554	-1.882982
10	H	1.417179	0.649563	1.996578
11	H	3.448036	2.005297	1.492348
12	C	0.102476	-1.146265	0.316451
13	O	-0.047740	-2.169251	-0.418380
14	C	-1.091717	-0.177028	0.397387
15	C	-2.173655	-0.351837	-0.367511
16	H	-2.188182	-1.210487	-1.045021
17	H	-1.016136	0.664174	1.095679
18	F	0.235723	-1.489093	1.778093
19	C	-3.369855	0.519390	-0.373100
20	O	-4.311037	0.267017	-1.101731
21	C	-3.396891	1.724131	0.541729
22	H	-3.290098	1.411806	1.590178
23	H	-2.559621	2.398586	0.313240
24	H	-4.346531	2.253944	0.408408

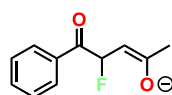
### 12-TS (Frequency: 205.5505 i cm<sup>-1</sup>)



1	C	4.028000	0.752218	-0.477193
2	C	3.782674	-0.603269	-0.703790
3	C	2.520942	-1.133952	-0.439783
4	C	1.495031	-0.311135	0.038213
5	C	1.746956	1.046012	0.275309
6	C	3.011902	1.572347	0.018985

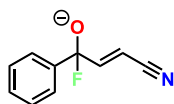
7	H	5.015551	1.169468	-0.681692
8	H	4.576613	-1.246579	-1.086578
9	H	2.312095	-2.192104	-0.605832
10	H	0.946856	1.637878	0.719297
11	H	3.211105	2.627201	0.215626
12	C	0.142613	-0.929711	0.264915
13	O	0.050519	-2.109012	0.540527
14	C	-1.066582	-0.077270	0.035353
15	C	-2.297398	-0.656257	-0.084727
16	H	-2.418340	-1.715808	0.150977
17	H	-0.888546	0.919502	-0.365760
18	F	-0.589123	0.603426	1.790465
19	C	-3.498960	0.085105	-0.416205
20	O	-4.593921	-0.455869	-0.532450
21	C	-3.377989	1.590227	-0.604670
22	H	-2.891000	2.046875	0.267919
23	H	-2.759738	1.821059	-1.485024
24	H	-4.378391	2.014835	-0.746190

### 12-IM2



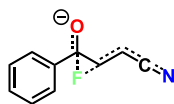
1	C	-4.133028	-0.716945	-0.217356
2	C	-3.920179	0.663238	-0.251897
3	C	-2.625746	1.166533	-0.163292
4	C	-1.531577	0.300569	-0.036206
5	C	-1.752770	-1.082649	0.003608
6	C	-3.049444	-1.586640	-0.089633
7	H	-5.146506	-1.115175	-0.288711
8	H	-4.766059	1.345222	-0.349987
9	H	-2.436067	2.240113	-0.194176
10	H	-0.913496	-1.765204	0.130410
11	H	-3.214714	-2.664463	-0.058087
12	C	-0.155689	0.910979	0.021437
13	O	-0.024388	2.112091	-0.044098
14	C	1.044651	-0.033316	0.161879
15	C	2.339414	0.619493	0.171352
16	H	2.395339	1.649770	0.529022
17	H	0.964017	-0.821963	-0.603954
18	F	0.718864	-0.750749	1.392282
19	C	3.533418	-0.018158	-0.192175
20	O	4.670032	0.508712	-0.174746
21	C	3.447541	-1.480407	-0.667656
22	H	2.863666	-2.107945	0.020548
23	H	2.972209	-1.548188	-1.659637
24	H	4.467128	-1.878024	-0.745573

### 13-IMI



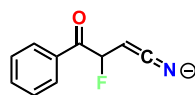
1	C	-3.405637	-1.099755	-0.135919
2	C	-2.857818	-0.522783	-1.282899
3	C	-1.644419	0.163216	-1.207499
4	C	-0.967649	0.279614	0.006920
5	C	-1.524642	-0.295028	1.154948
6	C	-2.736671	-0.982392	1.085071
7	H	-4.353967	-1.637345	-0.191316
8	H	-3.380600	-0.606681	-2.237865
9	H	-1.195088	0.636590	-2.082009
10	H	-1.007031	-0.185069	2.110085
11	H	-3.165915	-1.424510	1.986374
12	C	0.383549	1.029980	0.024682
13	O	0.620544	1.790289	-0.962549
14	C	1.491450	0.011604	0.366396
15	C	2.562314	-0.074968	-0.429222
16	H	2.611933	0.595015	-1.292731
17	H	1.381618	-0.628893	1.247517
18	F	0.321108	1.764898	1.330754
19	C	3.640402	-0.989247	-0.196292
20	N	4.515636	-1.725277	-0.019082

**13-TS (Frequency: 181.8347 i cm<sup>-1</sup>)**



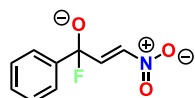
1	C	-3.666130	0.666490	0.470082
2	C	-3.373995	-0.691966	0.603436
3	C	-2.084122	-1.153176	0.345113
4	C	-1.078441	-0.258675	-0.036574
5	C	-1.377125	1.101736	-0.182219
6	C	-2.668855	1.559586	0.070801
7	H	-4.675465	1.029760	0.671094
8	H	-4.153148	-1.392009	0.909185
9	H	-1.837763	-2.212035	0.439531
10	H	-0.591538	1.757527	-0.556082
11	H	-2.903685	2.618054	-0.053362
12	C	0.302667	-0.808945	-0.259834
13	O	0.457111	-1.968259	-0.587441
14	C	1.470588	0.071643	0.056926
15	C	2.708070	-0.489319	0.176220
16	H	2.870109	-1.518839	-0.146276
17	H	1.268878	1.045686	0.501219
18	F	0.974695	0.760613	-1.692366
19	C	3.828367	0.259182	0.619563
20	N	4.746761	0.861867	0.997776

**13-IM2**



1	C	-3.726614	-0.667270	-0.337276
2	C	-3.467803	0.705284	-0.366083
3	C	-2.166918	1.168402	-0.192823
4	C	-1.112055	0.267157	0.002410
5	C	-1.378179	-1.108107	0.034885
6	C	-2.682783	-1.570665	-0.133503
7	H	-4.745724	-1.033273	-0.472561
8	H	-4.283111	1.412596	-0.524948
9	H	-1.941946	2.235587	-0.211002
10	H	-0.567411	-1.811643	0.221458
11	H	-2.885906	-2.642009	-0.101780
12	C	0.274812	0.829297	0.158525
13	O	0.434385	2.020590	0.301980
14	C	1.454025	-0.148561	0.130689
15	C	2.749138	0.476933	0.059621
16	H	2.904251	1.437337	0.550402
17	H	1.304069	-0.907877	-0.652469
18	F	1.187115	-0.917019	1.367031
19	C	3.843235	-0.190184	-0.484185
20	N	4.762217	-0.739426	-0.965969

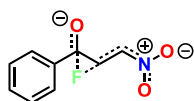
**14-IMI**



1	C	-3.699013	-1.159629	-0.406807
2	C	-3.179235	-0.339161	-1.409316
3	C	-2.010547	0.388561	-1.179085
4	C	-1.351846	0.304823	0.047618
5	C	-1.879608	-0.515274	1.051074
6	C	-3.046942	-1.245036	0.825961
7	H	-4.612530	-1.730242	-0.583565
8	H	-3.688924	-0.265406	-2.372112
9	H	-1.583897	1.047890	-1.936511
10	H	-1.375764	-0.565772	2.018522
11	H	-3.454466	-1.879473	1.615486
12	C	-0.053208	1.121009	0.239747
13	O	0.151473	2.063522	-0.582396
14	C	1.107357	0.120511	0.421037
15	C	2.185879	0.234579	-0.345493
16	H	2.321805	1.002358	-1.103379
17	H	1.044534	-0.680793	1.162009
18	F	-0.178718	1.591438	1.656810
19	N	3.310003	-0.679079	-0.222112

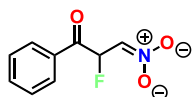
20	O	3.263174	-1.580143	0.586954
21	O	4.254186	-0.478411	-0.957730

**14-TS (Frequency: 182.0771 i cm<sup>-1</sup>)**



1	C	4.011596	0.695508	-0.520718
2	C	3.704049	-0.643741	-0.762753
3	C	2.428064	-1.127249	-0.473486
4	C	1.452075	-0.275085	0.051677
5	C	1.767133	1.065729	0.303291
6	C	3.043021	1.546855	0.017556
7	H	5.009290	1.076405	-0.745722
8	H	4.459624	-1.312435	-1.178361
9	H	2.170509	-2.172220	-0.653220
10	H	1.010036	1.688067	0.778241
11	H	3.288973	2.589666	0.225072
12	C	0.081040	-0.848819	0.294903
13	O	-0.063528	-2.039648	0.504400
14	C	-1.094322	0.030321	0.017224
15	C	-2.318344	-0.515305	-0.121976
16	H	-2.557492	-1.562769	0.033514
17	H	-0.940285	1.075778	-0.241681
18	F	-0.398970	0.374047	1.910972
19	N	-3.447457	0.299491	-0.440592
20	O	-3.309172	1.501275	-0.589413
21	O	-4.522751	-0.263456	-0.560832

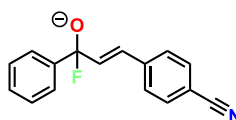
**14-IM2**



1	C	-4.140129	-0.624197	-0.182586
2	C	-3.882719	0.746496	-0.100306
3	C	-2.569511	1.201046	-0.033607
4	C	-1.502478	0.292875	-0.040490
5	C	-1.766750	-1.080941	-0.119768
6	C	-3.082814	-1.534620	-0.194008
7	H	-5.168952	-0.983642	-0.237809
8	H	-4.708693	1.459015	-0.090955
9	H	-2.344818	2.266885	0.021841
10	H	-0.947671	-1.799182	-0.110338
11	H	-3.283654	-2.604785	-0.258275
12	C	-0.109387	0.850596	-0.006243
13	O	0.080013	2.042540	-0.087758
14	C	1.053260	-0.138789	0.124167
15	C	2.353955	0.508882	0.222953
16	H	2.501399	1.518624	0.588487

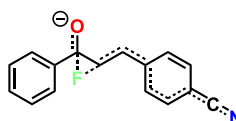
17	H	1.047410	-0.839851	-0.725412
18	F	0.723452	-0.937154	1.257029
19	N	3.450730	-0.146581	-0.201231
20	O	3.365128	-1.320071	-0.643918
21	O	4.569638	0.416945	-0.157431

**15-IM1**



1	C	4.832535	1.859439	-0.723855
2	C	4.468232	0.854186	-1.621263
3	C	3.554784	-0.128570	-1.235728
4	C	2.992988	-0.119555	0.041937
5	C	3.366987	0.888066	0.938588
6	C	4.280570	1.872296	0.559564
7	H	5.547166	2.629123	-1.021209
8	H	4.901051	0.835848	-2.623741
9	H	3.261617	-0.934749	-1.910130
10	H	2.945823	0.883946	1.945790
11	H	4.569250	2.650740	1.268855
12	C	1.962614	-1.217682	0.400397
13	O	2.007047	-2.275103	-0.301877
14	C	0.583720	-0.549002	0.549614
15	C	-0.473064	-1.017832	-0.121343
16	H	-0.282821	-1.892960	-0.751676
17	C	-1.848526	-0.501115	-0.092771
18	C	-2.839875	-1.165622	-0.835390
19	C	-2.224261	0.635677	0.647715
20	C	-4.157167	-0.724562	-0.843347
21	H	-2.564205	-2.047664	-1.415990
22	C	-3.534784	1.088578	0.649144
23	H	-1.477237	1.175199	1.230771
24	C	-4.510668	0.408447	-0.098053
25	H	-4.914111	-1.252525	-1.423984
26	H	-3.811981	1.970823	1.226774
27	H	0.512426	0.318826	1.214695
28	F	2.279749	-1.472555	1.852048
29	C	-5.871801	0.876081	-0.098702
30	N	-6.964971	1.252033	-0.098942

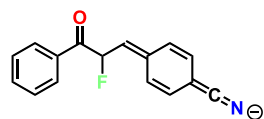
**15-TS (Frequency: 287.3125 i cm<sup>-1</sup>)**



1	C	5.341940	1.373373	-0.669440
2	C	5.333351	0.010516	-0.973677
3	C	4.216670	-0.762537	-0.662348
4	C	3.097615	-0.176161	-0.059912

5	C	3.112962	1.188752	0.253626
6	C	4.235159	1.958070	-0.050124
7	H	6.216369	1.980353	-0.910462
8	H	6.199135	-0.448466	-1.453671
9	H	4.192503	-1.830214	-0.886430
10	H	2.255203	1.598915	0.786143
11	H	4.251227	3.019036	0.204833
12	C	1.908819	-1.051512	0.225455
13	O	2.060683	-2.246526	0.384724
14	C	0.553512	-0.415995	0.235587
15	C	-0.557667	-1.220416	0.167075
16	H	-0.426771	-2.301286	0.252052
17	C	-1.892207	-0.693748	0.048962
18	C	-2.981862	-1.523428	-0.315679
19	C	-2.177913	0.671673	0.309378
20	C	-4.262559	-1.019389	-0.459275
21	H	-2.797895	-2.583885	-0.499454
22	C	-3.453921	1.185576	0.158155
23	H	-1.375271	1.310131	0.680489
24	C	-4.513673	0.347325	-0.234755
25	H	-5.082744	-1.677172	-0.750865
26	H	-3.648601	2.239193	0.364487
27	H	0.494658	0.604062	-0.147605
28	F	0.984717	0.273859	1.921572
29	C	-5.838575	0.875195	-0.384001
30	N	-6.907949	1.301863	-0.506517

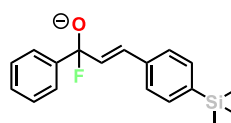
**15-IM2**



1	C	-5.569594	-1.225743	-0.249277
2	C	-5.567745	0.167968	-0.344902
3	C	-4.364915	0.864391	-0.281716
4	C	-3.153633	0.179254	-0.116392
5	C	-3.162692	-1.218639	-0.016589
6	C	-4.367916	-1.915902	-0.086885
7	H	-6.510993	-1.775148	-0.301140
8	H	-6.506463	0.709249	-0.471072
9	H	-4.339817	1.951715	-0.362508
10	H	-2.231338	-1.763667	0.131109
11	H	-4.368534	-3.004045	-0.010855
12	C	-1.889163	0.992340	-0.093310
13	O	-1.925907	2.183859	-0.299975
14	C	-0.570411	0.261660	0.186051
15	C	0.596612	1.139170	0.248276
16	H	0.424641	2.208045	0.375940
17	C	1.891527	0.653397	0.142775
18	C	3.038720	1.534342	0.126221

19	C	2.206876	-0.756079	0.047190
20	C	4.321599	1.071933	-0.019915
21	H	2.863458	2.608790	0.221330
22	C	3.495031	-1.209321	-0.108274
23	H	1.399089	-1.485434	0.129885
24	C	4.595242	-0.316413	-0.153744
25	H	5.153140	1.780515	-0.036283
26	H	3.681390	-2.283621	-0.180741
27	H	-0.453235	-0.541792	-0.565300
28	F	-0.815255	-0.462680	1.402959
29	C	5.924366	-0.793572	-0.304172
30	N	7.012826	-1.183439	-0.429890

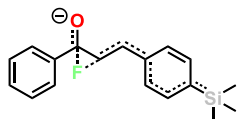
**16-IM1**



1	C	-5.926918	2.058535	0.718205
2	C	-5.640334	1.031374	1.618957
3	C	-4.795436	-0.013624	1.240602
4	C	-4.224808	-0.046147	-0.032576
5	C	-4.522469	0.983334	-0.933144
6	C	-5.367075	2.029984	-0.561706
7	H	-6.587728	2.877049	1.009660
8	H	-6.080605	1.044787	2.618333
9	H	-4.564373	-0.839025	1.915977
10	H	-4.097183	0.947394	-1.938102
11	H	-5.596040	2.825307	-1.274119
12	C	-3.271440	-1.214978	-0.381658
13	O	-3.381684	-2.254936	0.340319
14	C	-1.853375	-0.645444	-0.558348
15	C	-0.822804	-1.161160	0.118125
16	H	-1.067116	-2.000910	0.778021
17	C	0.587641	-0.740441	0.070975
18	C	1.532378	-1.427074	0.851248
19	C	1.047236	0.323769	-0.722790
20	C	2.877984	-1.066712	0.837420
21	H	1.196625	-2.257804	1.476618
22	C	2.393504	0.679708	-0.731957
23	H	0.341769	0.881449	-1.341682
24	C	3.343679	-0.004406	0.045507
25	H	3.577643	-1.631667	1.461585
26	H	2.708601	1.514040	-1.364375
27	H	-1.729791	0.197154	-1.248056
28	F	-3.630992	-1.474153	-1.825432
29	Si	5.175973	0.460506	0.047174
30	C	5.453168	1.902629	-1.128256
31	H	4.874866	2.786518	-0.819313
32	H	6.517916	2.180617	-1.138962

33	H	5.160385	1.640812	-2.156325
34	C	5.682592	0.941025	1.796594
35	H	5.498148	0.113831	2.498697
36	H	6.754209	1.189284	1.836574
37	H	5.112414	1.816208	2.142269
38	C	6.184305	-1.031147	-0.505863
39	H	5.914363	-1.327417	-1.530515
40	H	7.260570	-0.801327	-0.485086
41	H	6.007129	-1.891863	0.156693

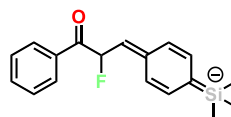
**16-TS (Frequency: 279.9668 i cm<sup>-1</sup>)**



1	C	6.448270	1.638720	-0.646393
2	C	6.516143	0.307705	-1.064226
3	C	5.461176	-0.559636	-0.790248
4	C	4.325595	-0.100894	-0.112043
5	C	4.265460	1.232120	0.313876
6	C	5.326564	2.096485	0.047482
7	H	7.274484	2.319652	-0.858038
8	H	7.393749	-0.052151	-1.603599
9	H	5.496755	-1.604737	-1.101644
10	H	3.399952	1.552784	0.892911
11	H	5.281731	3.131926	0.388932
12	C	3.205582	-1.075109	0.137373
13	O	3.436059	-2.268166	0.133492
14	C	1.824303	-0.519490	0.349270
15	C	0.753301	-1.395410	0.228767
16	H	0.956880	-2.468060	0.224551
17	C	-0.613228	-0.951254	0.164541
18	C	-1.660857	-1.829928	-0.216082
19	C	-0.998361	0.377904	0.477018
20	C	-2.975933	-1.397708	-0.317087
21	H	-1.413139	-2.869872	-0.446277
22	C	-2.318321	0.801491	0.357346
23	H	-0.240123	1.066482	0.855880
24	C	-3.350301	-0.065239	-0.045607
25	H	-3.738441	-2.123051	-0.622885
26	H	-2.553643	1.840739	0.607802
27	H	1.680112	0.500519	-0.022902
28	F	2.212664	0.028001	1.945707
29	Si	-5.136651	0.488217	-0.207242
30	C	-5.285652	2.297923	0.295938
31	H	-4.667108	2.942381	-0.347155
32	H	-6.330350	2.632785	0.207641
33	H	-4.967330	2.448098	1.338822
34	C	-5.711125	0.279987	-1.993132
35	H	-5.608167	-0.767713	-2.315093

36	H	-6.768060	0.567802	-2.103423
37	H	-5.110506	0.904196	-2.671847
38	C	-6.240695	-0.569627	0.899069
39	H	-5.959283	-0.455682	1.956796
40	H	-7.297562	-0.281123	0.789903
41	H	-6.150817	-1.634933	0.636541

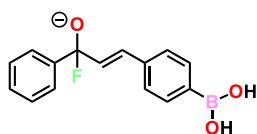
**16-IM2**



1	C	-6.607730	1.539748	0.462680
2	C	-6.687122	0.181828	0.781192
3	C	-5.572548	-0.634707	0.615007
4	C	-4.367383	-0.105387	0.134372
5	C	-4.295807	1.256362	-0.188323
6	C	-5.413612	2.073477	-0.023281
7	H	-7.479898	2.182756	0.592001
8	H	-7.620216	-0.237531	1.160391
9	H	-5.611731	-1.697221	0.858260
10	H	-3.372897	1.668517	-0.594100
11	H	-5.352776	3.132110	-0.279635
12	C	-3.193052	-1.039159	0.000919
13	O	-3.344270	-2.226304	0.189578
14	C	-1.837839	-0.434493	-0.369205
15	C	-0.729368	-1.353219	-0.310007
16	H	-0.946632	-2.421580	-0.338396
17	C	0.607945	-0.919068	-0.226040
18	C	1.692507	-1.841102	-0.040383
19	C	1.005473	0.456112	-0.317873
20	C	3.005133	-1.424801	0.081587
21	H	1.457671	-2.908261	0.016785
22	C	2.328431	0.851515	-0.178283
23	H	0.247700	1.212306	-0.536443
24	C	3.383562	-0.061064	0.028458
25	H	3.775952	-2.191519	0.227789
26	H	2.553903	1.921017	-0.254838
27	H	-1.668766	0.488782	0.213049
28	F	-2.124192	0.128180	-1.712146
29	Si	5.164292	0.464185	0.202572
30	C	5.305481	2.333722	-0.012704
31	H	4.717368	2.867946	0.749227
32	H	6.354766	2.651951	0.084111
33	H	4.944671	2.648252	-1.003985
34	C	5.840747	-0.009477	1.904019
35	H	5.752371	-1.094762	2.068009
36	H	6.903275	0.263322	2.000586
37	H	5.279740	0.499167	2.702816
38	C	6.242526	-0.389840	-1.094920

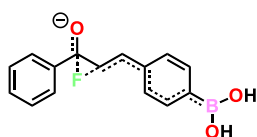
39	H	5.926549	-0.110275	-2.111483
40	H	7.301983	-0.114789	-0.974427
41	H	6.164697	-1.484645	-1.006310

**17-IM1**



1	C	-4.654421	2.037919	-0.277979
2	C	-3.790129	1.069394	-0.789514
3	C	-3.472562	-0.069454	-0.040164
4	C	-4.042331	-0.225405	1.224172
5	C	-4.906790	0.740737	1.742381
6	C	-5.213723	1.877424	0.992398
7	H	-4.899064	2.920030	-0.873409
8	H	-3.364453	1.181734	-1.788559
9	H	-3.794365	-1.132457	1.778127
10	H	-5.346477	0.606978	2.733100
11	H	-5.889765	2.634776	1.393581
12	C	-2.496906	-1.159374	-0.546702
13	O	-2.584643	-2.291030	0.025051
14	C	-1.092148	-0.539571	-0.641296
15	C	-0.050444	-1.109594	-0.028004
16	H	-0.988423	0.388869	-1.214095
17	H	-0.273612	-2.030557	0.521755
18	C	1.346598	-0.645046	-0.009190
19	C	2.292369	-1.356563	0.747263
20	C	1.788650	0.487309	-0.717563
21	C	3.624372	-0.952368	0.797948
22	H	1.966862	-2.239512	1.302351
23	C	3.119627	0.884964	-0.663421
24	H	1.079834	1.059198	-1.319168
25	C	4.067682	0.176522	0.094584
26	H	4.339254	-1.523177	1.395143
27	H	3.439474	1.767124	-1.223054
28	O	6.432513	-0.102104	0.911683
29	O	5.931661	1.733651	-0.568130
30	B	5.570186	0.630980	0.149601
31	H	6.862861	1.977452	-0.510025
32	H	7.345001	0.209621	0.918443
33	F	-2.853709	-1.222276	-2.013389

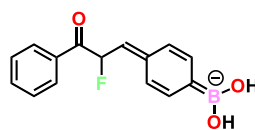
**17-TS (Frequency: 294.0330 i cm<sup>-1</sup>)**



1	C	5.793506	0.128383	-1.054046
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2	C	4.704088	-0.682302	-0.743402
3	C	3.584857	-0.145739	-0.095927
4	C	3.574588	1.208420	0.261727
5	C	4.670041	2.015999	-0.041225
6	C	5.776087	1.480343	-0.703965
7	H	6.658633	-0.292316	-1.569009
8	H	4.700405	-1.742397	-1.001885
9	H	2.719323	1.587707	0.820336
10	H	4.664885	3.068279	0.247690
11	H	6.629508	2.116896	-0.943958
12	C	2.427091	-1.062019	0.195886
13	O	2.613950	-2.260295	0.270841
14	C	1.063591	-0.448667	0.342713
15	C	-0.035605	-1.288969	0.268205
16	H	0.962150	0.557616	-0.075185
17	H	0.130355	-2.366296	0.335682
18	C	-1.386361	-0.806774	0.157112
19	C	-2.455504	-1.679877	-0.172235
20	C	-1.729118	0.554907	0.370936
21	C	-3.754701	-1.216322	-0.318144
22	H	-2.235224	-2.739844	-0.325351
23	C	-3.031793	1.006783	0.209363
24	H	-0.950621	1.243586	0.705430
25	C	-4.084766	0.141918	-0.143377
26	H	-4.547311	-1.922703	-0.580519
27	H	-3.252669	2.064288	0.380254
28	F	1.476871	0.181012	1.933291
29	O	-6.519680	-0.243085	-0.657915
30	O	-5.796733	1.989734	-0.117200
31	B	-5.545435	0.657319	-0.314703
32	H	-6.716344	2.253797	-0.234538
33	H	-7.404051	0.128344	-0.752573

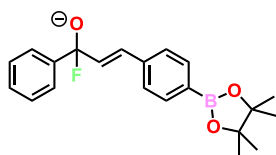
**17-IM2**



1	C	5.984570	-0.009591	0.673782
2	C	4.828705	0.749862	0.520674
3	C	3.627064	0.146532	0.125931
4	C	3.600161	-1.232519	-0.121674
5	C	4.758599	-1.993047	0.033153
6	C	5.949606	-1.384976	0.431408
7	H	6.915147	0.468053	0.983873
8	H	4.832418	1.824298	0.708053
9	H	2.679039	-1.706440	-0.458315
10	H	4.731717	-3.065967	-0.162172
11	H	6.853919	-1.983744	0.551978

12	C	2.407772	1.022469	0.009220
13	O	2.502265	2.215435	0.194604
14	C	1.075568	0.353427	-0.340823
15	C	-0.066323	1.241685	-0.320476
16	H	0.936222	-0.540360	0.293498
17	H	0.121196	2.313671	-0.392288
18	C	-1.384668	0.777105	-0.206283
19	C	-2.496172	1.680575	-0.069769
20	C	-1.743515	-0.616645	-0.215596
21	C	-3.792941	1.235583	0.083546
22	H	-2.288185	2.754773	-0.076830
23	C	-3.050901	-1.036148	-0.049350
24	H	-0.963016	-1.361474	-0.388936
25	C	-4.132140	-0.139908	0.110264
26	H	-4.593755	1.974510	0.190598
27	H	-3.260973	-2.110782	-0.060499
28	O	-6.589887	0.305087	0.439654
29	O	-5.848165	-1.978904	0.278304
30	B	-5.586468	-0.626094	0.283103
31	H	-6.777974	-2.207980	0.384635
32	H	-7.470977	-0.068887	0.548785
33	F	1.367951	-0.250953	-1.646938

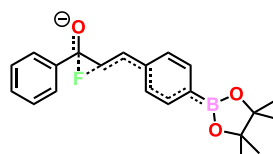
#### 18-IM1



1	C	-6.507118	2.257483	-0.307920
2	C	-5.723887	1.212289	-0.798797
3	C	-5.493816	0.069627	-0.023632
4	C	-6.069095	-0.011572	1.245196
5	C	-6.852954	1.031227	1.742599
6	C	-7.072429	2.170874	0.966943
7	H	-6.683891	3.142211	-0.923134
8	H	-5.294707	1.267813	-1.801154
9	H	-5.890277	-0.921823	1.819940
10	H	-7.297780	0.955443	2.737131
11	H	-7.685265	2.988138	1.351776
12	C	-4.610015	-1.105497	-0.507799
13	O	-4.784777	-2.214868	0.087039
14	C	-3.160159	-0.604456	-0.619807
15	C	-2.166113	-1.250953	-0.003276
16	H	-2.983152	0.300536	-1.211641
17	H	-2.463183	-2.139272	0.564806
18	C	-0.733965	-0.910691	-0.009829
19	C	0.157943	-1.699524	0.736041
20	C	-0.207335	0.173087	-0.736924
21	C	1.521670	-1.419032	0.755956

22	H	-0.235222	-2.545277	1.304761
23	C	1.154174	0.449765	-0.713203
24	H	-0.874161	0.802239	-1.328954
25	C	2.047438	-0.339372	0.031890
26	H	2.195205	-2.048917	1.341942
27	H	1.541436	1.295861	-1.285904
28	C	5.797828	-0.314612	0.372613
29	C	5.518874	1.094251	-0.256490
30	O	4.480414	-0.718327	0.804862
31	O	4.151894	0.960545	-0.701976
32	C	6.262438	-1.338491	-0.659182
33	H	7.287406	-1.130728	-0.994933
34	H	6.239387	-2.336942	-0.201506
35	H	5.598457	-1.343826	-1.535657
36	C	6.734951	-0.300091	1.567345
37	H	6.878155	-1.325910	1.934066
38	H	7.716801	0.102107	1.278258
39	H	6.330196	0.306596	2.386372
40	C	6.400214	1.443614	-1.442737
41	H	6.140618	2.446048	-1.810278
42	H	7.458531	1.449877	-1.144012
43	H	6.267645	0.729066	-2.264076
44	C	5.543986	2.216513	0.777253
45	H	6.566936	2.419656	1.121887
46	H	5.141668	3.129329	0.317043
47	H	4.921659	1.964441	1.648029
48	B	3.572772	-0.028973	0.046239
49	F	-4.975151	-1.169694	-1.972534

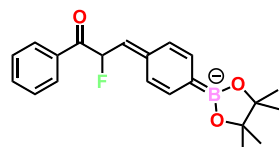
#### 18-TS (Frequency: 304.8923 i cm<sup>-1</sup>)



1	C	-7.741880	0.606741	1.089223
2	C	-6.744923	-0.334315	0.841825
3	C	-5.591319	0.026744	0.135814
4	C	-5.454076	1.335000	-0.345253
5	C	-6.457227	2.272856	-0.104647
6	C	-7.597069	1.913197	0.617282
7	H	-8.633959	0.323432	1.650076
8	H	-6.841115	-1.361864	1.196037
9	H	-4.577460	1.572368	-0.947478
10	H	-6.353563	3.289052	-0.488602
11	H	-8.377643	2.651648	0.808348
12	C	-4.534778	-1.022534	-0.080068
13	O	-4.839078	-2.198569	-0.049008
14	C	-3.119692	-0.564665	-0.282231
15	C	-2.108302	-1.497774	-0.146474

16	H	-2.913003	0.464887	0.022783
17	H	-2.380275	-2.554553	-0.105410
18	C	-0.714035	-1.144367	-0.123257
19	C	0.277436	-2.082980	0.263457
20	C	-0.254999	0.147866	-0.493117
21	C	1.619953	-1.740372	0.314138
22	H	-0.037871	-3.093814	0.535060
23	C	1.089397	0.482967	-0.423887
24	H	-0.979910	0.869020	-0.875635
25	C	2.066684	-0.445590	-0.016604
26	H	2.353361	-2.491258	0.621464
27	H	1.404053	1.489821	-0.712919
28	F	-3.508892	-0.040723	-1.942750
29	C	5.819702	-0.303781	0.172157
30	C	5.439119	1.214092	0.091088
31	O	4.552984	-0.914916	0.485049
32	O	4.063363	1.156819	-0.333013
33	C	6.271986	-0.867457	-1.172515
34	H	7.266576	-0.493052	-1.450728
35	H	6.317946	-1.962690	-1.098716
36	H	5.560305	-0.603608	-1.968179
37	C	6.825464	-0.647820	1.257162
38	H	7.039099	-1.725489	1.231771
39	H	7.768435	-0.106423	1.092111
40	H	6.441032	-0.395449	2.252911
41	C	6.243239	2.016015	-0.917663
42	H	5.916821	3.065115	-0.896965
43	H	7.313765	1.984033	-0.667719
44	H	6.104886	1.631493	-1.935483
45	C	5.461408	1.898032	1.455731
46	H	6.488746	2.035321	1.819745
47	H	4.987639	2.885038	1.363538
48	H	4.899485	1.312371	2.197683
49	B	3.563601	-0.067340	0.044769

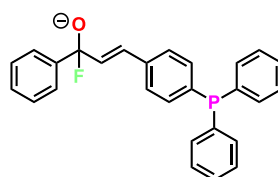
**18-IM2**



1	C	-7.984830	0.423898	0.672433
2	C	-6.894941	-0.439201	0.614040
3	C	-5.643352	0.021809	0.184122
4	C	-5.497971	1.364493	-0.190310
5	C	-6.589745	2.229509	-0.128069
6	C	-7.832087	1.762209	0.302059
7	H	-8.955524	0.056333	1.008396
8	H	-6.990155	-1.486328	0.903783
9	H	-4.537065	1.729346	-0.550448

10	H	-6.470316	3.273454	-0.421169
11	H	-8.684358	2.442163	0.347924
12	C	-4.501081	-0.958744	0.175473
13	O	-4.680464	-2.100396	0.535853
14	C	-3.130051	-0.458208	-0.290637
15	C	-2.074876	-1.453864	-0.233300
16	H	-2.877150	0.462310	0.266796
17	H	-2.367425	-2.503431	-0.188045
18	C	-0.720181	-1.110591	-0.215401
19	C	0.312950	-2.101658	-0.045349
20	C	-0.238882	0.240885	-0.362815
21	C	1.647681	-1.767998	0.020834
22	H	0.009249	-3.148581	0.046953
23	C	1.104158	0.550192	-0.281048
24	H	-0.957240	1.036861	-0.572485
25	C	2.107048	-0.429077	-0.082042
26	H	2.384875	-2.565550	0.160769
27	H	1.409467	1.596093	-0.391699
28	C	5.855107	-0.312463	0.037774
29	C	5.473370	1.193241	0.236551
30	O	4.601688	-0.973031	0.272979
31	O	4.095987	1.209254	-0.170038
32	C	6.272319	-0.623333	-1.398273
33	H	7.259002	-0.200871	-1.633181
34	H	6.319595	-1.713925	-1.524145
35	H	5.538151	-0.224088	-2.113130
36	C	6.893484	-0.837438	1.015287
37	H	7.106601	-1.892729	0.793941
38	H	7.831732	-0.270786	0.923194
39	H	6.537454	-0.767900	2.050523
40	C	6.264923	2.166123	-0.621371
41	H	5.940222	3.194052	-0.407026
42	H	7.339350	2.091408	-0.397875
43	H	6.110795	1.971930	-1.689928
44	C	5.520587	1.618498	1.702847
45	H	6.553634	1.693227	2.069410
46	H	5.042341	2.603062	1.799925
47	H	4.972684	0.904135	2.334447
48	B	3.589385	-0.067514	0.004241
49	F	-3.406924	0.055676	-1.625037

**19-IM1**

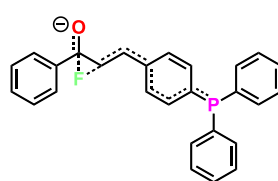


1	C	-7.501796	2.025543	0.094347
2	C	-7.380946	1.046584	1.082215



3	C	-6.510858	-0.029126	0.896251
4	C	-5.751260	-0.140314	-0.269269
5	C	-5.881682	0.841773	-1.258116
6	C	-6.750791	1.918590	-1.079002
7	H	-8.181939	2.867613	0.235372
8	H	-7.970286	1.121897	1.998571
9	H	-6.405804	-0.818585	1.642262
10	H	-5.305564	0.743617	-2.180183
11	H	-6.848899	2.676157	-1.859360
12	C	-4.784147	-1.341576	-0.403485
13	O	-5.043211	-2.346957	0.329025
14	C	-3.342492	-0.806917	-0.357938
15	C	-2.454206	-1.306316	0.506777
16	H	-2.824399	-2.106946	1.156887
17	C	-1.046045	-0.910714	0.672632
18	C	-0.271225	-1.533722	1.664100
19	C	-0.426484	0.071859	-0.119296
20	C	1.063716	-1.188900	1.860136
21	H	-0.732121	-2.296607	2.295429
22	C	0.909933	0.410092	0.066914
23	H	-0.997091	0.577471	-0.900099
24	C	1.678535	-0.219554	1.057104
25	H	1.637531	-1.684415	2.647936
26	H	1.361796	1.171949	-0.571893
27	P	3.460733	0.124914	1.363510
28	C	4.272715	-1.113806	0.263255
29	C	3.587986	-1.911997	-0.661051
30	C	5.664051	-1.250940	0.378926
31	C	4.283821	-2.821636	-1.460077
32	H	2.504329	-1.824039	-0.762303
33	C	6.359770	-2.149913	-0.427538
34	H	6.209020	-0.644204	1.107315
35	C	5.668986	-2.939736	-1.348782
36	H	3.738217	-3.438531	-2.176035
37	H	7.442832	-2.240773	-0.330588
38	H	6.210299	-3.649929	-1.975733
39	C	3.698349	1.677647	0.395368
40	C	4.176850	1.721131	-0.919931
41	C	3.365191	2.880292	1.035952
42	C	4.310568	2.943008	-1.582510
43	H	4.444134	0.796325	-1.435365
44	C	3.487355	4.098738	0.370228
45	H	3.002697	2.861570	2.067338
46	C	3.963196	4.132255	-0.941967
47	H	4.684719	2.963138	-2.607438
48	H	3.218205	5.025325	0.879812
49	H	4.066482	5.085364	-1.462913
50	H	-3.083044	0.000186	-1.052267
51	F	-4.896777	-1.655412	-1.877006

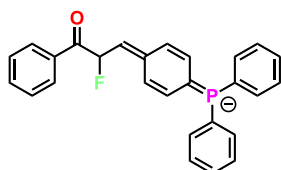
19-TS (Frequency: 287.5810 i cm<sup>-1</sup>)



1	C	-7.723073	-1.780068	0.932312
2	C	-8.023382	-0.844452	-0.060133
3	C	-7.064727	0.090231	-0.445026
4	C	-5.796126	0.086967	0.146951
5	C	-5.501857	-0.846444	1.148920
6	C	-6.465826	-1.774865	1.539577
7	H	-8.473251	-2.511950	1.236781
8	H	-9.006820	-0.845041	-0.532866
9	H	-7.281321	0.833447	-1.213945
10	H	-4.530947	-0.787558	1.639781
11	H	-6.238202	-2.494441	2.327723
12	C	-4.790004	1.101741	-0.324391
13	O	-5.171060	2.127686	-0.852385
14	C	-3.333690	0.776388	-0.160032
15	C	-2.415923	1.519450	-0.880073
16	H	-2.755448	2.433266	-1.371758
17	C	-1.021760	1.170856	-0.953537
18	C	-0.154647	1.770036	-1.900387
19	C	-0.438433	0.214548	-0.080707
20	C	1.181652	1.405463	-1.997527
21	H	-0.559571	2.522097	-2.582150
22	C	0.896926	-0.149791	-0.185762
23	H	-1.053677	-0.207449	0.716277
24	C	1.738907	0.435959	-1.146384
25	H	1.812713	1.880970	-2.754255
26	H	1.303424	-0.889592	0.509472
27	P	3.523022	0.068993	-1.313544
28	C	4.281744	1.077526	0.034980
29	C	3.543255	1.851523	0.937374
30	C	5.682148	1.081998	0.127911
31	C	4.191460	2.603464	1.920398
32	H	2.453187	1.866120	0.874244
33	C	6.328427	1.821374	1.116510
34	H	6.273175	0.494432	-0.580459
35	C	5.582394	2.586849	2.015837
36	H	3.602940	3.202799	2.617209
37	H	7.417766	1.807571	1.180656
38	H	6.086452	3.172714	2.786078
39	C	3.612023	-1.624565	-0.579030
40	C	4.000671	-1.898761	0.737917
41	C	3.256980	-2.694829	-1.414161
42	C	4.027129	-3.213430	1.209565

43	H	4.281186	-1.081855	1.405905
44	C	3.273033	-4.005441	-0.941068
45	H	2.960827	-2.497168	-2.448086
46	C	3.661594	-4.268341	0.374361
47	H	4.331308	-3.411297	2.238848
48	H	2.989017	-4.825210	-1.603054
49	H	3.681555	-5.294151	0.745613
50	H	-3.108712	-0.278957	0.018686
51	F	-3.426201	1.099394	1.585018

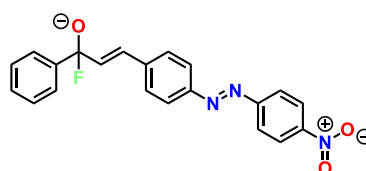
### 19-IM2



1	C	7.824824	1.299947	1.631792
2	C	8.163589	0.631342	0.452856
3	C	7.174611	-0.005521	-0.290463
4	C	5.839227	0.016375	0.133926
5	C	5.506960	0.684663	1.320002
6	C	6.498080	1.324946	2.062852
7	H	8.597707	1.801758	2.216319
8	H	9.200513	0.609812	0.114454
9	H	7.415910	-0.529047	-1.216327
10	H	4.477113	0.686380	1.674169
11	H	6.232969	1.842958	2.985553
12	C	4.816872	-0.667167	-0.734398
13	O	5.163379	-1.222981	-1.752600
14	C	3.352294	-0.625274	-0.286459
15	C	2.425155	-1.250383	-1.209051
16	H	2.829491	-1.939614	-1.950739
17	C	1.049697	-0.993255	-1.180363
18	C	0.152204	-1.527495	-2.169415
19	C	0.415918	-0.178958	-0.173989
20	C	-1.198632	-1.242244	-2.172719
21	H	0.568630	-2.164917	-2.954366
22	C	-0.936985	0.100308	-0.197354
23	H	1.019752	0.208236	0.649856
24	C	-1.794838	-0.417137	-1.192500
25	H	-1.828290	-1.667629	-2.961315
26	H	-1.358300	0.728878	0.594368
27	P	-3.584499	-0.148145	-1.241415
28	C	-4.249265	-1.155009	0.161774
29	C	-3.442384	-1.933341	0.999241
30	C	-5.639392	-1.175923	0.356302
31	C	-4.010679	-2.702674	2.018162
32	H	-2.359999	-1.934736	0.853227
33	C	-6.206676	-1.932996	1.379400

34	H	-6.285390	-0.585647	-0.300335
35	C	-5.391103	-2.701268	2.214224
36	H	-3.368200	-3.304527	2.663541
37	H	-7.288822	-1.931009	1.521795
38	H	-5.833063	-3.300853	3.011667
39	C	-3.722559	1.556207	-0.529758
40	C	-4.088539	1.844061	0.790867
41	C	-3.426978	2.625124	-1.390582
42	C	-4.152443	3.166069	1.239645
43	H	-4.322134	1.031441	1.481643
44	C	-3.481982	3.943047	-0.942508
45	H	-3.144305	2.418062	-2.426585
46	C	-3.848307	4.218129	0.377365
47	H	-4.437215	3.371480	2.273174
48	H	-3.244799	4.759609	-1.626772
49	H	-3.897613	5.249547	0.730014
50	H	3.078442	0.417651	-0.042443
51	F	3.404005	-1.241250	1.037560

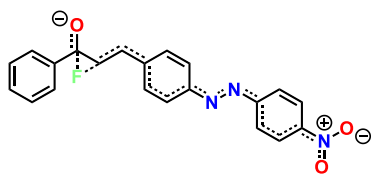
### 20-IM1



1	C	7.905936	2.199764	-1.252430
2	C	7.615257	1.033475	-1.962487
3	C	6.867911	0.018769	-1.362249
4	C	6.399768	0.154713	-0.054258
5	C	6.699570	1.324216	0.653784
6	C	7.447746	2.341349	0.059768
7	H	8.491128	2.995078	-1.717779
8	H	7.976217	0.914749	-2.986319
9	H	6.638022	-0.910631	-1.885981
10	H	6.353516	1.422297	1.684378
11	H	7.680731	3.247244	0.623250
12	C	5.549013	-0.992146	0.543492
13	O	5.702038	-2.134809	0.009793
14	C	4.102914	-0.485544	0.684152
15	C	3.086503	-1.174048	0.153876
16	H	3.361901	-2.104260	-0.354604
17	C	1.659698	-0.827119	0.190977
18	C	0.728156	-1.712185	-0.389998
19	C	1.173145	0.353983	0.780268
20	C	-0.631498	-1.441925	-0.385404
21	H	1.095234	-2.630952	-0.851977
22	C	-0.186000	0.633460	0.788703
23	H	1.867716	1.061482	1.234508
24	C	-1.097665	-0.258937	0.208909

25	H	-1.346897	-2.129583	-0.835169
26	H	-0.572401	1.547124	1.242657
27	H	3.949078	0.457934	1.219592
28	F	5.972514	-0.966096	1.990551
29	N	-2.455950	0.118174	0.270616
30	N	-3.263362	-0.675190	-0.237679
31	C	-4.622471	-0.271632	-0.163651
32	C	-5.548959	-1.158791	-0.722565
33	C	-5.051323	0.930386	0.421796
34	C	-6.906486	-0.859151	-0.703467
35	H	-5.182345	-2.082928	-1.169398
36	C	-6.403090	1.239077	0.446001
37	H	-4.313019	1.606088	0.850150
38	C	-7.305239	0.337152	-0.117751
39	H	-7.648649	-1.530823	-1.130531
40	H	-6.769556	2.162086	0.891657
41	N	-8.740367	0.666235	-0.091545
42	O	-9.508842	-0.124133	-0.587332
43	O	-9.069804	1.708473	0.424548

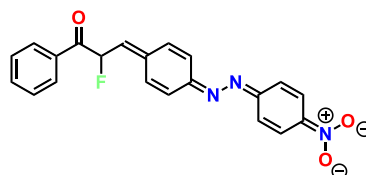
**20-TS (Frequency: 295.0557 i cm<sup>-1</sup>)**



1	C	8.497509	1.962721	-0.857957
2	C	8.622877	0.628419	-1.249692
3	C	7.634670	-0.291639	-0.904489
4	C	6.510173	0.118953	-0.179691
5	C	6.392252	1.455509	0.222008
6	C	7.386535	2.371889	-0.116907
7	H	9.270987	2.684611	-1.125836
8	H	9.492570	0.306231	-1.824568
9	H	7.717096	-1.339745	-1.196706
10	H	5.541478	1.722599	0.848599
11	H	7.300245	3.410776	0.206034
12	C	5.458125	-0.908864	0.133049
13	O	5.762429	-2.082228	0.221845
14	C	4.039320	-0.450691	0.238777
15	C	3.031492	-1.377020	0.204768
16	H	3.300858	-2.435454	0.224496
17	C	1.635290	-1.026580	0.202565
18	C	0.644677	-1.999064	-0.103709
19	C	1.188278	0.280736	0.519422
20	C	-0.698278	-1.683987	-0.133178
21	H	0.966972	-3.017892	-0.329987
22	C	-0.156929	0.601951	0.481672
23	H	1.920085	1.024247	0.837240

24	C	-1.120238	-0.367757	0.152648
25	H	-1.448247	-2.436167	-0.376930
26	H	-0.503413	1.607671	0.726769
27	H	3.835134	0.581336	-0.046893
28	F	4.552095	0.195433	1.979201
29	N	-2.450458	0.054398	0.152142
30	N	-3.310562	-0.807385	-0.122059
31	C	-4.642484	-0.333340	-0.117572
32	C	-5.634482	-1.295736	-0.349903
33	C	-5.000606	1.009649	0.095432
34	C	-6.976145	-0.935817	-0.366276
35	H	-5.327309	-2.328554	-0.514674
36	C	-6.336393	1.380098	0.078395
37	H	-4.216891	1.744467	0.270600
38	C	-7.302154	0.399783	-0.151274
39	H	-7.763625	-1.666202	-0.542024
40	H	-6.643450	2.412130	0.238696
41	N	-8.717783	0.793162	-0.168574
42	O	-9.542426	-0.070930	-0.359704
43	O	-8.982588	1.959977	0.009518

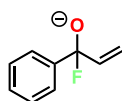
**20-IM2**



1	C	8.908356	1.655393	0.011455
2	C	9.024701	0.263132	0.010051
3	C	7.881791	-0.526465	-0.061656
4	C	6.613193	0.066343	-0.121189
5	C	6.501880	1.463536	-0.116507
6	C	7.649203	2.252667	-0.055500
7	H	9.803461	2.277124	0.064523
8	H	10.008913	-0.204135	0.062420
9	H	7.949922	-1.614971	-0.074323
10	H	5.523130	1.940424	-0.154664
11	H	7.558815	3.339555	-0.057238
12	C	5.428347	-0.842911	-0.234458
13	O	5.565434	-2.022146	-0.463335
14	C	4.030088	-0.231330	-0.077667
15	C	2.955342	-1.250925	0.033563
16	H	3.261539	-2.292724	0.133494
17	C	1.630514	-0.922819	0.019558
18	C	0.603187	-1.955233	0.123582
19	C	1.147521	0.449181	-0.089315
20	C	-0.720364	-1.665059	0.100849
21	H	0.937542	-2.991561	0.216824
22	C	-0.181403	0.729127	-0.114310

23	H	1.874675	1.261782	-0.127880
24	C	-1.185402	-0.299468	-0.022020
25	H	-1.472346	-2.450056	0.174667
26	H	-0.535226	1.759441	-0.196313
27	H	3.863705	0.441567	-0.939844
28	F	4.063947	0.606680	1.046452
29	N	-2.459943	0.075741	-0.047385
30	N	-3.367282	-0.854892	0.039389
31	C	-4.649778	-0.389383	0.012088
32	C	-5.689820	-1.356259	0.100964
33	C	-5.030258	0.980990	-0.095248
34	C	-7.019824	-0.992320	0.085106
35	H	-5.399532	-2.404283	0.183421
36	C	-6.359805	1.348477	-0.111769
37	H	-4.246329	1.732093	-0.163075
38	C	-7.355943	0.365060	-0.021682
39	H	-7.812458	-1.735823	0.153610
40	H	-6.653788	2.394243	-0.193328
41	N	-8.743462	0.754619	-0.038528
42	O	-9.592325	-0.114921	0.046101
43	O	-9.014595	1.938132	-0.136526

21

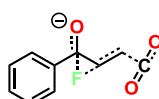


1	C	-3.052998	0.078223	-0.336568
2	C	-2.361144	1.259132	-0.062147
3	C	-0.988842	1.221227	0.192091
4	C	-0.290408	0.013186	0.172068
5	C	-0.992544	-1.167938	-0.095340
6	C	-2.364273	-1.137487	-0.349263
7	H	-4.125997	0.103129	-0.535773
8	H	-2.895222	2.211634	-0.043722
9	H	-0.422062	2.124346	0.424369
10	H	-0.453901	-2.117420	-0.086202
11	H	-2.902210	-2.065828	-0.552777
12	C	1.236589	0.041272	0.427472
13	O	1.679367	1.068800	1.029895
14	C	1.955052	-0.361664	-0.872202
15	H	1.645664	-1.297349	-1.352835
16	C	2.907010	0.400922	-1.403436
17	H	3.430945	0.137232	-2.324910
18	F	1.424560	-1.228127	1.231341
19	H	3.176164	1.325760	-0.885428

22a

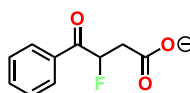
1	C	0.000000	0.000000	0.000000
2	O	-0.000000	-0.000000	1.156108
3	O	0.000000	-0.000000	-1.156108

22-TS (Frequency: 464.1381 i cm<sup>-1</sup>)

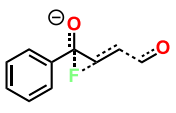
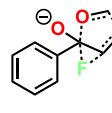
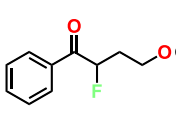
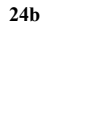


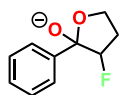
1	C	3.708541	0.672981	0.491745
2	C	3.022454	1.438329	-0.453815
3	C	1.738289	1.067374	-0.846605
4	C	1.125023	-0.059589	-0.287280
5	C	1.818612	-0.828552	0.655371
6	C	3.108257	-0.462589	1.039236
7	H	4.715394	0.960324	0.799678
8	H	3.491291	2.324717	-0.884254
9	H	1.186794	1.648104	-1.587833
10	H	1.344090	-1.733033	1.035155
11	H	3.651215	-1.069329	1.765861
12	C	-0.275044	-0.394995	-0.726366
13	O	-0.673155	-0.012555	-1.806772
14	C	-1.148220	-1.180745	0.223524
15	H	-0.817174	-1.142015	1.266481
16	C	-2.517509	-1.139673	0.004422
17	H	-3.199818	-1.565900	0.742739
18	F	-0.285964	-2.615925	-0.148804
19	H	-2.883803	-1.040395	-1.019953
20	C	-2.836515	1.249732	0.563212
21	O	-1.750155	1.632107	0.778545
22	O	-3.998896	1.253848	0.433316

22b



1	C	4.021506	-0.095232	-0.430797
2	C	3.470190	-1.234731	0.161148
3	C	2.109749	-1.275804	0.448200
4	C	1.288756	-0.181377	0.146114
5	C	1.846900	0.959718	-0.445271
6	C	3.210622	0.999457	-0.732321
7	H	5.088386	-0.060757	-0.657219
8	H	4.104768	-2.090126	0.396901
9	H	1.655843	-2.154478	0.908292
10	H	1.222758	1.824625	-0.670104
11	H	3.642150	1.889492	-1.191959
12	C	-0.172017	-0.287477	0.463434
13	O	-0.632558	-1.285739	0.966280
14	C	-1.055799	0.925313	0.154655
15	H	-0.950230	1.171768	-0.910883
16	C	-2.504119	0.683621	0.473007
17	H	-3.047548	1.637580	0.389186

18	F	-0.541381	1.988429	0.896949	7	H	4.148091	-1.947270	-0.229751					
19	H	-2.624891	0.314660	1.500678	8	H	1.686994	-2.263642	-0.538114					
20	C	-3.132562	-0.339276	-0.515279	9	H	1.026871	1.855515	0.519934					
21	O	-2.462732	-0.588808	-1.541370	10	H	3.457075	2.165224	0.858313					
22	O	-4.244480	-0.794689	-0.196758	11	H	5.025079	0.273733	0.475320					
<b>23a (24a): HCHO</b>														
1	C	0.526155	0.000031	-0.000087	12	C	-0.260935	-0.504090	-0.201158					
2	H	1.116399	0.942584	0.000175	13	O	-0.669200	-1.629368	-0.372406					
3	H	1.116380	-0.942720	0.000175	14	C	-1.224487	0.685530	-0.137219					
4	O	-0.673714	-0.000006	0.000021	15	C	-2.654248	0.344782	-0.465151					
<b>23-TS (Frequency: 299.2943 i cm<sup>-1</sup>)</b>														
														
1	C	2.965350	1.447546	0.314584	16	H	-1.170651	1.106819	0.885401					
2	C	1.660399	1.170521	0.714774	17	H	-3.142615	1.252530	-0.853404					
3	C	1.004764	0.024198	0.249029	18	H	-2.701347	-0.430808	-1.244325					
4	C	1.676630	-0.856082	-0.608950	19	C	-3.470926	-0.148366	0.771964					
5	C	2.986248	-0.582153	-1.001269	20	H	-2.797464	-0.942314	1.247808					
6	C	3.629386	0.570412	-0.545993	21	H	-3.344782	0.719901	1.514652					
7	H	3.467546	2.347754	0.672403	22	O	-4.706885	-0.512949	0.500009					
8	H	1.124440	1.839646	1.389750	23	F	-0.716497	1.659770	-0.996982					
9	H	1.169886	-1.769337	-0.919924	<b>24-TS (Frequency: 312.3541 i cm<sup>-1</sup>)</b>									
10	H	3.510780	-1.274156	-1.662091										
11	H	4.652496	0.784501	-0.859823	1	C	-2.862599	-1.211987	0.376953					
12	C	-0.415582	-0.210000	0.690425	2	C	-1.529703	-1.033967	0.740552					
13	O	-0.836373	0.356466	1.680007	3	C	-0.815895	0.078345	0.281416					
14	C	-1.291934	-1.103166	-0.159264	4	C	-1.452216	1.025781	-0.529319					
15	C	-2.668731	-1.006632	0.064721	5	C	-2.790775	0.853426	-0.881009					
16	H	-0.986683	-1.124352	-1.213063	6	C	-3.494516	-0.266795	-0.434811					
17	H	-3.358272	-1.453941	-0.654702	7	H	-3.412620	-2.087488	0.725927					
18	H	-3.023725	-0.894981	1.091563	8	H	-1.015594	-1.756688	1.376019					
19	C	-2.850522	1.401881	-0.471137	9	H	-0.889534	1.909300	-0.832113					
20	H	-2.826447	1.453670	0.637525	10	H	-3.289799	1.598706	-1.502651					
21	H	-1.834902	1.362853	-0.932010	11	H	-4.539802	-0.402755	-0.717729					
22	O	-3.843635	1.650005	-1.131222	12	C	0.624830	0.217784	0.689353					
23	F	-0.514567	-2.495842	0.286510	13	O	1.005683	-0.271840	1.730847					
<b>23b</b>														
														
1	C	3.461383	-1.116519	-0.061750	14	C	1.550772	0.961943	-0.243081					
2	C	2.093307	-1.296837	-0.238282	15	C	2.908267	0.681957	-0.119076					
3	C	1.204685	-0.233704	-0.029487	16	H	1.168980	1.058373	-1.266087					
4	C	1.703148	1.015352	0.364790	17	H	3.611408	1.064950	-0.862342					
5	C	3.073698	1.192246	0.548449	18	H	3.303419	0.430253	0.867334					
6	C	3.952691	0.130090	0.333872	19	C	2.603735	-1.548900	-1.063824					
<b>24b</b>														
														
7	H	4.148091	-1.947270	-0.229751	20	H	2.431150	-1.009676	-2.020674					
8	H	1.686994	-2.263642	-0.538114	21	H	3.677409	-1.661181	-0.799592					
9	H	1.026871	1.855515	0.519934	22	O	1.728686	-2.206445	-0.522910					
10	H	3.457075	2.165224	0.858313	23	F	0.958737	2.459663	0.273941					
11	H	5.025079	0.273733	0.475320										
12	C	-0.260935	-0.504090	-0.201158										
13	O	-0.669200	-1.629368	-0.372406										
14	C	-1.224487	0.685530	-0.137219										
15	C	-2.654248	0.344782	-0.465151										
16	H	-1.170651	1.106819	0.885401										
17	H	-3.142615	1.252530	-0.853404										
18	H	-2.701347	-0.430808	-1.244325										
19	C	-3.470926	-0.148366	0.771964										
20	H	-2.797464	-0.942314	1.247808										
21	H	-3.344782	0.719901	1.514652										
22	O	-4.706885	-0.512949	0.500009										
23	F	-0.716497	1.659770	-0.996982										

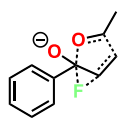


1	C	-2.971005	-1.175588	-0.032890
2	C	-1.588146	-1.261729	0.125302
3	C	-0.788819	-0.112627	0.089800
4	C	-1.408994	1.127290	-0.101024
5	C	-2.793779	1.218885	-0.260540
6	C	-3.580624	0.067101	-0.227055
7	H	-3.580283	-2.081801	-0.008782
8	H	-1.102552	-2.228591	0.268921
9	H	-0.793958	2.030108	-0.120104
10	H	-3.260533	2.194446	-0.412733
11	H	-4.662632	0.135687	-0.353451
12	C	0.713615	-0.199010	0.388148
13	O	0.996031	-0.214032	1.649559
14	C	1.558272	0.824143	-0.431272
15	C	2.929198	0.176100	-0.396002
16	H	1.176724	0.949418	-1.458037
17	H	3.606887	0.511957	-1.191667
18	H	3.360533	0.422035	0.583053
19	C	2.571330	-1.323493	-0.477858
20	H	2.874671	-1.760639	-1.443048
21	H	3.086147	-1.891447	0.318049
22	O	1.171170	-1.416107	-0.360479
23	F	1.567899	2.079277	0.160611

**25a: CH<sub>3</sub>CHO**

1	C	0.231110	0.397966	0.000021
2	H	0.306483	1.511575	0.000053
3	O	1.229332	-0.276152	-0.000011
4	C	-1.163344	-0.149301	0.000014
5	H	-1.701931	0.226727	0.882484
6	H	-1.700799	0.224266	-0.884210
7	H	-1.145001	-1.245340	0.001548

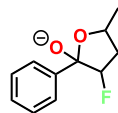
**25-TS (Frequency: 303.6057 i cm<sup>-1</sup>)**



1	C	-3.027135	-1.443888	0.489081
2	C	-1.743806	-1.060069	0.870153
3	C	-1.143467	0.069276	0.301518
4	C	-1.851013	0.826372	-0.639819
5	C	-3.141054	0.448349	-1.012226
6	C	-3.727876	-0.688651	-0.454513
7	H	-3.484830	-2.332672	0.926638
8	H	-1.179381	-1.633337	1.607243
9	H	-1.390632	1.730043	-1.038590

10	H	-3.693356	1.046417	-1.738991
11	H	-4.734590	-0.985949	-0.753313
12	C	0.253024	0.425492	0.737750
13	O	0.662726	0.031529	1.808586
14	C	1.092518	1.288991	-0.186811
15	C	2.475186	1.259773	0.040287
16	H	0.791654	1.189740	-1.238942
17	H	3.140523	1.748491	-0.676576
18	H	2.828148	1.182197	1.071797
19	C	2.549504	-1.038005	-0.939732
20	H	2.737338	-0.447685	-1.864156
21	O	1.482911	-1.619692	-0.782092
22	F	0.266379	2.648447	0.132363
23	C	3.788543	-1.421703	-0.165568
24	H	4.184460	-2.356959	-0.598843
25	H	4.562039	-0.647386	-0.223213
26	H	3.529581	-1.619242	0.883005

**25b**

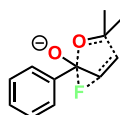


1	C	-2.940725	-1.074378	-0.980389
2	C	-1.563836	-0.904761	-0.831586
3	C	-1.050165	-0.068586	0.167368
4	C	-1.942511	0.585214	1.017832
5	C	-3.321999	0.422811	0.873502
6	C	-3.825837	-0.407741	-0.128448
7	H	-3.328193	-1.732523	-1.761076
8	H	-0.868657	-1.434539	-1.486335
9	H	-1.508237	1.215255	1.795370
10	H	-4.008238	0.942921	1.545581
11	H	-4.903345	-0.539013	-0.244805
12	C	0.459957	0.192280	0.353487
13	O	0.789175	0.765429	1.465412
14	C	1.074862	0.897680	-0.899279
15	C	2.532338	0.514710	-0.759583
16	H	0.634005	0.532931	-1.842322
17	H	3.127345	0.630106	-1.675568
18	H	2.947395	1.150708	0.035291
19	C	2.430623	-0.948635	-0.279886
20	H	2.627147	-1.626925	-1.130785
21	O	1.087446	-1.146599	0.124074
22	F	0.879841	2.265677	-0.853126
23	C	3.393404	-1.277398	0.851913
24	H	3.272277	-2.323039	1.170264
25	H	4.439721	-1.124406	0.545846
26	H	3.160591	-0.620386	1.701204

**26a: CH<sub>3</sub>COCH<sub>3</sub>**

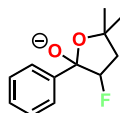
1	C	-0.000002	0.184031	-0.000001
2	O	-0.000023	1.393815	0.000000
3	C	-1.283522	-0.611343	-0.001848
4	H	-2.141759	0.062445	-0.101994
5	H	-1.277117	-1.345482	-0.820076
6	H	-1.363276	-1.176402	0.938922
7	C	1.283539	-0.611312	0.001848
8	H	1.277167	-1.345440	0.820087
9	H	1.363307	-1.176385	-0.938913
10	H	2.141767	0.062492	0.101972

**26-TS (Frequency: 289.1746 i cm<sup>-1</sup>)**



1	C	3.237980	-1.450118	-0.407284
2	C	1.992425	-1.032729	-0.868944
3	C	1.368751	0.090080	-0.312756
4	C	2.016435	0.805882	0.700930
5	C	3.269968	0.394833	1.154981
6	C	3.879256	-0.735007	0.607311
7	H	3.712582	-2.334014	-0.836707
8	H	1.474799	-1.574021	-1.662301
9	H	1.542781	1.702898	1.099159
10	H	3.775486	0.961052	1.939037
11	H	4.856565	-1.058428	0.969825
12	C	0.012979	0.481137	-0.839810
13	O	-0.332200	0.098666	-1.938075
14	C	-0.862263	1.377464	0.024521
15	C	-2.233398	1.383397	-0.312511
16	H	-0.666063	1.207004	1.093522
17	H	-2.919312	1.920584	0.349113
18	H	-2.490533	1.373715	-1.375836
19	C	-2.387565	-0.992348	0.515130
20	O	-1.247587	-1.370822	0.787971
21	F	-0.019194	2.692248	-0.173637
22	C	-3.030721	-1.431889	-0.785117
23	H	-3.281121	-2.504461	-0.692456
24	H	-3.944593	-0.869954	-1.010342
25	H	-2.307153	-1.310737	-1.600729
26	C	-3.317861	-0.572801	1.638620
27	H	-4.202748	-0.037162	1.277226
28	H	-3.643372	-1.488249	2.164933
29	H	-2.772192	0.051381	2.358700

**26b**

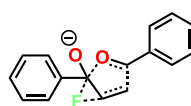


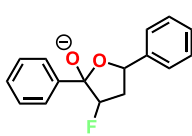
1	C	2.975869	-1.522585	0.554991
2	C	1.632114	-1.167314	0.432433
3	C	1.263030	0.026254	-0.200156
4	C	2.265341	0.850991	-0.712730
5	C	3.612529	0.504335	-0.589796
6	C	3.972186	-0.684943	0.045892
7	H	3.250178	-2.458900	1.045792
8	H	0.848896	-1.823953	0.817314
9	H	1.942738	1.764318	-1.214617
10	H	4.386384	1.161181	-0.993345
11	H	5.023882	-0.961387	0.142548
12	C	-0.202798	0.495366	-0.328036
13	O	-0.403294	1.444205	-1.185949
14	C	-0.821270	0.796001	1.076462
15	C	-2.298449	0.632758	0.791252
16	H	-0.462075	0.091787	1.845698
17	H	-2.919785	0.469408	1.683266
18	H	-2.624167	1.549422	0.281086
19	C	-2.316184	-0.574162	-0.181037
20	O	-0.964271	-0.762480	-0.584383
21	F	-0.506481	2.072351	1.506720
22	C	-3.179489	-0.292759	-1.409203
23	H	-3.160001	-1.155202	-2.092986
24	H	-4.224730	-0.090127	-1.128366
25	H	-2.757304	0.580349	-1.923286
26	C	-2.766406	-1.849245	0.525750
27	H	-3.827544	-1.791435	0.810874
28	H	-2.628765	-2.713413	-0.141057
29	H	-2.167699	-2.015196	1.434334

**27a: C<sub>6</sub>H<sub>5</sub>CHO**

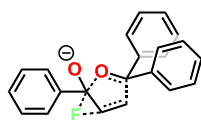
1	C	-1.992921	0.469356	0.000031
2	H	-2.282762	1.545993	0.000047
3	O	-2.831323	-0.398388	-0.000083
4	C	-0.531603	0.215403	0.000046
5	C	-0.048865	-1.099742	0.000036
6	C	0.358203	1.293764	0.000044
7	C	1.322141	-1.331397	0.000038
8	H	-0.765952	-1.922431	0.000064
9	C	1.732723	1.059993	-0.000037
10	H	-0.030193	2.315126	0.000082
11	C	2.211311	-0.250967	-0.000058
12	H	1.705593	-2.352560	0.000058
13	H	2.431115	1.897637	-0.000064
14	H	3.286851	-0.435118	-0.000116

**27-TS (Frequency: 307.7336 i cm<sup>-1</sup>)**



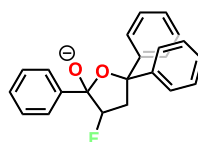
1	C	-3.937551	-1.991078	0.118110	12	C	-0.813326	0.289160	0.397966
2	C	-2.739391	-1.432744	0.556503	13	O	-0.433397	0.092525	1.619738
3	C	-2.450947	-0.086972	0.302646	14	C	-0.650603	1.773611	-0.065409
4	C	-3.384809	0.703949	-0.377049	15	C	0.850640	1.872413	-0.217671
5	C	-4.590224	0.147143	-0.804491	16	H	-1.178003	1.972426	-1.013714
6	C	-4.865371	-1.200032	-0.564038	17	H	1.206761	2.740912	-0.787138
7	H	-4.151671	-3.044316	0.307094	18	H	1.271407	1.889751	0.797370
8	H	-2.001547	-2.030702	1.093642	19	C	1.169781	0.528436	-0.909309
9	H	-3.165091	1.761486	-0.522882	20	H	1.227954	0.693322	-2.001679
10	H	-5.321107	0.768543	-1.324665	21	O	0.080835	-0.327117	-0.639413
11	H	-5.806116	-1.634742	-0.906369	22	F	-1.145573	2.648751	0.880208
12	C	-1.133122	0.458505	0.782805	23	C	2.486289	-0.070653	-0.456749
13	O	-0.568792	-0.072904	1.715108	24	C	2.544330	-0.748529	0.768195
14	C	-0.561800	1.668066	0.071716	25	C	3.646769	0.063486	-1.221772
15	C	0.807080	1.888672	0.239156	26	C	3.752733	-1.278995	1.216180
16	H	-0.938351	1.781744	-0.953254	27	H	1.614657	-0.822643	1.342307
17	H	1.314006	2.636942	-0.374474	28	C	4.858900	-0.466174	-0.770780
18	H	1.272492	1.617319	1.188618	29	H	3.602496	0.582720	-2.182940
19	C	1.282805	-0.114432	-1.235423	30	C	4.913728	-1.139931	0.448730
20	H	1.218400	0.678969	-2.010208	31	H	3.794833	-1.806428	2.171488
21	O	0.411907	-0.965571	-1.120372	32	H	5.759926	-0.357912	-1.377491
22	F	-1.633506	2.709788	0.774576	33	H	5.857926	-1.559239	0.800874
23	C	2.639491	-0.267384	-0.624957	<b>28a: C<sub>6</sub>H<sub>5</sub>COC<sub>6</sub>H<sub>5</sub></b>				
24	C	2.891031	-1.332978	0.245058	1	C	-0.000058	1.098741	0.000188
25	C	3.678817	0.605053	-0.966536	2	O	-0.000215	2.313103	0.000416
26	C	4.163364	-1.510741	0.786608	3	C	1.297750	0.347215	0.025924
27	H	2.070368	-2.011219	0.485169	4	C	2.426973	0.974436	-0.517199
28	C	4.951758	0.425075	-0.431239	5	C	1.430112	-0.905938	0.637879
29	H	3.477507	1.433953	-1.650521	6	C	3.667029	0.344416	-0.477706
30	C	5.195757	-0.632430	0.450572	7	H	2.311920	1.959361	-0.971832
31	H	4.354842	-2.339996	1.470076	8	C	2.677422	-1.527116	0.693542
32	H	5.758940	1.108829	-0.699587	9	H	0.563442	-1.388976	1.091678
33	H	6.192633	-0.773127	0.871658	10	C	3.792763	-0.907857	0.128908
<b>27b</b>					11	H	4.540004	0.830310	-0.915535
					12	H	2.778171	-2.497458	1.181272
1	C	-3.959764	-0.885770	-1.512156	13	H	4.765653	-1.400418	0.165761
2	C	-2.666448	-0.427427	-1.259122	14	C	-1.297678	0.347077	-0.025993
3	C	-2.214879	-0.253745	0.054518	15	C	-1.429913	-0.906093	-0.637585
4	C	-3.080828	-0.551860	1.107387	16	C	-2.427195	0.974560	0.516656
5	C	-4.377870	-1.006990	0.861689	17	C	-2.677262	-1.527498	-0.693122
6	C	-4.821503	-1.175444	-0.450687	18	H	-0.563294	-1.389488	-1.091157
7	H	-4.298215	-1.023496	-2.541259	19	C	-3.667087	0.344587	0.477096
8	H	-1.985023	-0.211818	-2.084696	20	H	-2.311970	1.959621	0.971043
9	H	-2.692781	-0.420699	2.118306	21	C	-3.792656	-0.908112	-0.129070
10	H	-5.045323	-1.234618	1.695738	22	H	-2.777624	-2.498029	-1.180554
11	H	-5.833656	-1.533823	-0.647699	23	H	-4.540214	0.830408	0.914692
					24	H	-4.765561	-1.400653	-0.165813
					<b>28-TS (Frequency: 262.9348 i cm<sup>-1</sup>)</b>				





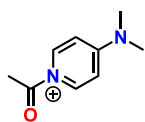
1	C	-4.327040	-1.523657	-1.548279
2	C	-3.185845	-1.752195	-0.784079
3	C	-2.767319	-0.811834	0.164535
4	C	-3.516286	0.355679	0.354878
5	C	-4.665600	0.579317	-0.403488
6	C	-5.068956	-0.355001	-1.358591
7	H	-4.641155	-2.255097	-2.294728
8	H	-2.591370	-2.657679	-0.914284
9	H	-3.207606	1.060783	1.126401
10	H	-5.251561	1.486303	-0.245996
11	H	-5.964599	-0.173855	-1.955354
12	C	-1.510653	-1.100130	0.941786
13	O	-1.103675	-2.240406	1.019711
14	C	-0.810571	0.064285	1.624324
15	C	0.530045	-0.170826	1.987892
16	H	-0.973404	1.011918	1.088585
17	H	1.123881	0.662849	2.368336
18	H	0.800373	-1.173276	2.329129
19	C	1.085104	0.017170	-0.580688
20	O	0.112918	-0.458653	-1.161588
21	F	-1.892634	0.259728	2.766300
22	C	2.313285	-0.845492	-0.422274
23	C	2.129747	-2.188234	-0.059580
24	C	3.592468	-0.404828	-0.774000
25	C	3.211411	-3.059554	-0.012064
26	H	1.121227	-2.512419	0.206920
27	C	4.679962	-1.284504	-0.733124
28	H	3.747733	0.625259	-1.099002
29	C	4.494540	-2.608735	-0.346718
30	H	3.061106	-4.098306	0.287907
31	H	5.673321	-0.928534	-1.011737
32	H	5.343423	-3.293611	-0.310245
33	C	1.183406	1.511999	-0.402708
34	C	2.158356	2.147546	0.380390
35	C	0.234018	2.299358	-1.064961
36	C	2.186225	3.535050	0.486984
37	H	2.882603	1.546091	0.931497
38	C	0.257784	3.690660	-0.956121
39	H	-0.524141	1.793907	-1.664796
40	C	1.236357	4.313126	-0.182988
41	H	2.948415	4.015108	1.103004
42	H	-0.490357	4.289666	-1.478344
43	H	1.259265	5.400629	-0.095733

28b



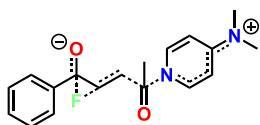
1	C	-4.910038	-0.924170	-0.856305
2	C	-3.689316	-1.370616	-0.344648
3	C	-2.625021	-0.488279	-0.159248
4	C	-2.799388	0.858307	-0.501748
5	C	-4.015495	1.311434	-1.012778
6	C	-5.077212	0.419824	-1.190980
7	H	-5.734374	-1.626890	-0.995944
8	H	-3.519300	-2.414465	-0.077926
9	H	-1.964505	1.552454	-0.375858
10	H	-4.136704	2.363572	-1.278762
11	H	-6.029248	0.773400	-1.591322
12	C	-1.314206	-1.034504	0.444986
13	O	-1.241490	-2.320229	0.533531
14	C	-0.933681	-0.296769	1.768149
15	C	0.566999	-0.461292	1.777939
16	H	-1.229891	0.765832	1.758994
17	H	1.094896	0.134443	2.531065
18	H	0.762591	-1.528971	1.941597
19	C	0.916030	-0.086644	0.316057
20	O	-0.240325	-0.413306	-0.429498
21	F	-1.533960	-0.889644	2.859674
22	C	2.091126	-0.929665	-0.202900
23	C	1.820903	-2.273878	-0.502520
24	C	3.390186	-0.446360	-0.375211
25	C	2.833690	-3.113311	-0.958249
26	H	0.792891	-2.623445	-0.357028
27	C	4.406832	-1.291375	-0.833938
28	H	3.622215	0.597471	-0.159852
29	C	4.133471	-2.624792	-1.127127
30	H	2.611278	-4.157539	-1.187420
31	H	5.416216	-0.897370	-0.965976
32	H	4.926416	-3.281957	-1.488517
33	C	1.194223	1.413710	0.163536
34	C	1.959090	2.138068	1.086079
35	C	0.703365	2.083789	-0.963664
36	C	2.217941	3.496430	0.892973
37	H	2.374387	1.642543	1.965586
38	C	0.959550	3.440942	-1.159458
39	H	0.106185	1.519864	-1.680063
40	C	1.716572	4.154681	-0.229619
41	H	2.814384	4.041420	1.626708
42	H	0.563748	3.944384	-2.043485
43	H	1.915243	5.217154	-0.379091

29a



1	C	2.893029	-0.166585	0.000227
2	C	3.653452	1.123287	-0.000598
3	H	3.415771	1.716719	-0.893752
4	H	3.415385	1.718264	0.891411
5	H	4.718036	0.873673	-0.000138
6	O	3.382309	-1.255174	0.001041
7	N	1.436325	-0.068938	-0.000069
8	C	0.777424	1.127179	-0.000873
9	C	0.714783	-1.230024	0.000571
10	C	-0.580986	1.200701	-0.000840
11	H	1.385983	2.028182	-0.001662
12	C	-0.644674	-1.233519	0.000403
13	H	1.308134	-2.142642	0.001359
14	C	-1.370584	0.003793	-0.000194
15	H	-1.038394	2.186071	-0.001797
16	H	-1.154219	-2.193273	0.001253
17	N	-2.696054	0.039714	-0.000121
18	C	-3.396783	1.320794	0.002147
19	H	-3.136647	1.903538	0.896604
20	H	-3.143613	1.903214	-0.894572
21	H	-4.473299	1.134554	0.006553
22	C	-3.466112	-1.201032	-0.001727
23	H	-3.237644	-1.798167	-0.895336
24	H	-3.246173	-1.795608	0.895807
25	H	-4.530982	-0.956134	-0.007422

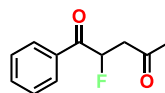
29-TS (Frequency: 324.1923 i cm<sup>-1</sup>)



1	C	6.017410	0.961054	1.019583
2	C	5.825205	-0.059918	0.086617
3	C	4.572974	-0.253061	-0.494389
4	C	3.503460	0.581692	-0.144216
5	C	3.705950	1.612808	0.781809
6	C	4.956178	1.799942	1.366292
7	H	6.998369	1.105729	1.475435
8	H	6.658767	-0.705478	-0.194372
9	H	4.411631	-1.012863	-1.257855
10	H	2.864025	2.258307	1.036974
11	H	5.105486	2.599437	2.093532
12	C	2.120185	0.401892	-0.704520
13	O	1.318394	1.315437	-0.619639
14	C	1.743422	-0.940018	-1.284045
15	C	0.394023	-1.179334	-1.514168

16	H	2.325092	-1.777272	-0.881272
17	H	0.065429	-2.186301	-1.776519
18	C	-0.505183	-1.793403	0.901808
19	C	0.561012	-1.082155	1.683048
20	H	0.708525	-0.035807	1.407547
21	H	0.257255	-1.126611	2.742118
22	H	1.497643	-1.637738	1.565226
23	H	-0.234446	-0.346664	-1.839977
24	F	2.751418	-0.687596	-2.635616
25	O	-0.609596	-2.986421	0.829326
26	N	-1.716421	-0.990601	0.597467
27	C	-1.662077	0.337163	0.313253
28	C	-2.911451	-1.631882	0.587957
29	C	-2.792178	1.059651	0.059940
30	H	-0.670423	0.784774	0.233108
31	C	-4.084185	-0.976413	0.340286
32	H	-2.865662	-2.699824	0.795424
33	C	-4.075871	0.428057	0.077399
34	H	-2.680451	2.114999	-0.172907
35	H	-5.006949	-1.549905	0.357221
36	N	-5.198651	1.110808	-0.148231
37	C	-5.145942	2.544554	-0.405119
38	H	-4.673485	3.074779	0.433955
39	H	-4.583509	2.760165	-1.325139
40	H	-6.165415	2.920506	-0.523371
41	C	-6.484530	0.425081	-0.144265
42	H	-6.515680	-0.354893	-0.918487
43	H	-6.679593	-0.036580	0.834465
44	H	-7.274637	1.151762	-0.350343

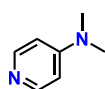
29b



1	C	4.120698	0.058065	-0.482675
2	C	3.240833	1.083757	-0.829970
3	C	1.884784	0.973309	-0.528770
4	C	1.404679	-0.172782	0.120053
5	C	2.293689	-1.200587	0.464147
6	C	3.646949	-1.085201	0.166377
7	H	5.182061	0.149709	-0.718393
8	H	3.612154	1.975582	-1.335846
9	H	1.209757	1.787820	-0.791063
10	H	1.900565	-2.085714	0.965638
11	H	4.336078	-1.885809	0.437647
12	C	-0.039297	-0.366457	0.442451
13	O	-0.457231	-1.399838	0.911474
14	C	-1.000462	0.801770	0.168109
15	C	-2.419669	0.552445	0.651360

16	H	-0.982178	1.037345	-0.909849
17	H	-2.876149	1.523524	0.878710
18	C	-3.340187	-0.158165	-0.329839
19	C	-2.805770	-1.353290	-1.075124
20	H	-2.488212	-2.119783	-0.354532
21	H	-3.582121	-1.744783	-1.741388
22	H	-1.914871	-1.082416	-1.662263
23	H	-2.387053	-0.046575	1.575346
24	F	-0.492612	1.902667	0.834569
25	O	-4.479519	0.221076	-0.467954

**29c**

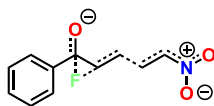


1	N	-2.660833	-0.000007	0.000222
2	C	-1.950601	1.131412	0.000077
3	C	-1.950580	-1.131422	0.000085
4	C	-0.564008	1.199376	-0.000165
5	H	-2.521349	2.066170	0.000175
6	C	-0.563988	-1.199364	-0.000224
7	H	-2.521328	-2.066178	0.000195
8	C	0.189368	0.000007	-0.000266
9	H	-0.081306	2.174612	-0.000246
10	H	-0.081288	-2.174606	-0.000541
11	N	1.548972	0.000007	-0.000417
12	C	2.267976	1.257125	0.000178
13	H	2.031342	1.860499	-0.891316
14	H	2.030590	1.860054	0.891776
15	H	3.343863	1.055760	0.000444
16	C	2.267960	-1.257126	0.000236
17	H	2.030345	-1.860151	0.891695
18	H	2.031556	-1.860412	-0.891364
19	H	3.343835	-1.055791	0.001024

**30a: CH<sub>2</sub>CHNO<sub>2</sub>**

1	C	1.861319	0.060745	0.000254
2	H	1.824119	1.150853	0.000981
3	H	2.826240	-0.445995	0.000135
4	C	0.742874	-0.649048	-0.000384
5	H	0.639270	-1.731598	-0.000902
6	N	-0.558356	0.028035	0.000002
7	O	-0.593996	1.235796	-0.000249
8	O	-1.531790	-0.690757	0.000318

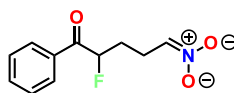
**30-TS (Frequency: 204.6118 i cm<sup>-1</sup>)**



1	C	0.139353	0.864856	0.697718
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2	C	0.216602	2.244858	0.131268
3	H	-0.533743	2.887911	0.605310
4	C	0.240968	2.274283	-1.267953
5	H	0.825501	1.545231	-1.831336
6	H	-0.135877	3.145287	-1.808815
7	O	-0.798398	0.510303	1.394819
8	F	1.532198	2.810095	0.947077
9	C	-2.042256	0.468746	-1.767613
10	H	-2.611454	1.321594	-1.401365
11	H	-1.487488	0.566412	-2.697640
12	C	-2.074581	-0.698597	-1.123004
13	H	-1.544589	-1.608848	-1.391440
14	N	-2.842592	-0.847886	0.095915
15	O	-3.565253	0.052085	0.462045
16	O	-2.737279	-1.911764	0.678748
17	C	1.190448	-0.140109	0.312749
18	C	2.476130	0.243474	-0.089300
19	C	0.869321	-1.500367	0.406573
20	C	3.420092	-0.729176	-0.419549
21	H	2.709243	1.307651	-0.111454
22	C	1.811814	-2.469366	0.069239
23	H	-0.134367	-1.776606	0.737561
24	C	3.089087	-2.083557	-0.345950
25	H	4.422782	-0.430038	-0.729993
26	H	1.554041	-3.528047	0.131268
27	H	3.829875	-2.841449	-0.607169

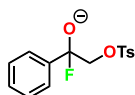
**30b**



1	C	0.084856	0.198951	1.075543
2	C	-0.780193	1.330789	0.505905
3	H	-1.774421	1.208805	0.958557
4	C	-0.913819	1.423589	-1.007709
5	H	-0.039085	1.953932	-1.411984
6	H	-1.795420	2.047662	-1.199150
7	O	-0.299094	-0.427704	2.037242
8	F	-0.225364	2.520962	0.978910
9	C	-1.074990	0.059989	-1.711099
10	H	-1.641998	0.234122	-2.643891
11	H	-0.081649	-0.300019	-2.019865
12	C	-1.684283	-1.026931	-0.884607
13	H	-1.215985	-1.996969	-0.738920
14	N	-2.860133	-0.866652	-0.289056
15	O	-3.489762	0.232384	-0.415352
16	O	-3.364270	-1.786485	0.419343
17	C	1.422891	-0.077051	0.463617
18	C	2.176626	0.929904	-0.151514

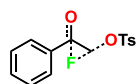
19	C	1.936234	-1.376820	0.552785
20	C	3.429073	0.630275	-0.686991
21	H	1.793930	1.950301	-0.184616
22	C	3.178263	-1.677008	0.000958
23	H	1.340185	-2.143160	1.051282
24	C	3.925088	-0.672294	-0.619858
25	H	4.020691	1.417222	-1.156580
26	H	3.568971	-2.694055	0.055790
27	H	4.900518	-0.905851	-1.049464

**31**



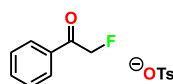
1	C	2.699350	-0.139055	-0.384960
2	H	3.631465	-0.276978	-0.944894
3	H	2.924504	0.000771	0.679546
4	F	3.041256	2.084796	-0.787728
5	O	1.984919	-1.383323	-0.553744
6	S	1.036754	-1.968226	0.587461
7	O	1.062926	-3.402688	0.375693
8	O	1.427510	-1.431882	1.881090
9	C	-0.569292	-1.371559	0.162348
10	C	-1.021462	-1.521288	-1.148103
11	C	-1.379619	-0.844408	1.162272
12	C	-2.315660	-1.117954	-1.455853
13	H	-0.361066	-1.924545	-1.917116
14	C	-2.676566	-0.458477	0.835203
15	H	-0.991280	-0.728100	2.174439
16	C	-3.160610	-0.582823	-0.472262
17	H	-2.680291	-1.219130	-2.479981
18	H	-3.320926	-0.037178	1.609605
19	C	1.954270	1.043634	-1.044505
20	O	1.697596	0.897822	-2.274955
21	C	0.813685	1.606939	-0.165899
22	C	0.956879	1.852635	1.203983
23	C	-0.394456	1.932505	-0.783702
24	C	-0.091585	2.405491	1.940844
25	H	1.899846	1.620619	1.703459
26	C	-1.442859	2.494615	-0.055776
27	H	-0.476515	1.728248	-1.852247
28	C	-1.294516	2.732093	1.311740
29	H	0.032829	2.590895	3.009805
30	H	-2.382681	2.744452	-0.553866
31	H	-2.114297	3.166667	1.887206
32	C	-4.544445	-0.108604	-0.822960
33	H	-4.528778	0.968789	-1.051322
34	H	-4.934311	-0.630096	-1.706506
35	H	-5.240175	-0.257847	0.013159

**31-TS (Frequency: 657.3899 i cm<sup>-1</sup>)**



1	C	-2.696433	0.310479	0.439556
2	H	-3.577583	0.090548	1.031160
3	H	-2.764725	0.284702	-0.641955
4	F	-3.273045	2.124087	0.352767
5	O	-2.069669	-1.329043	0.607724
6	S	-1.253741	-1.951280	-0.539288
7	O	-1.334271	-3.404259	-0.427627
8	O	-1.621782	-1.361824	-1.829104
9	C	0.425116	-1.479250	-0.195223
10	C	0.936570	-1.677517	1.086544
11	C	1.218068	-0.964901	-1.216684
12	C	2.265362	-1.351124	1.341117
13	H	0.296532	-2.073931	1.876907
14	C	2.546882	-0.648128	-0.946153
15	H	0.787020	-0.808723	-2.206108
16	C	3.088876	-0.832915	0.331703
17	H	2.673439	-1.500276	2.343028
18	H	3.174158	-0.239746	-1.741664
19	C	-1.596627	1.038447	1.149553
20	O	-1.511650	1.008882	2.359671
21	C	-0.531587	1.692347	0.315936
22	C	-0.756365	2.094948	-1.005298
23	C	0.725425	1.886954	0.895870
24	C	0.278618	2.665024	-1.743862
25	H	-1.761938	2.007612	-1.414187
26	C	1.758334	2.461057	0.157819
27	H	0.878121	1.572827	1.929590
28	C	1.537389	2.844844	-1.165834
29	H	0.100057	2.984875	-2.771835
30	H	2.739873	2.605495	0.613118
31	H	2.346245	3.290683	-1.747529
32	C	4.513326	-0.444378	0.622095
33	H	4.574543	0.627807	0.866558
34	H	4.914094	-1.003649	1.477315
35	H	5.158673	-0.619890	-0.248823

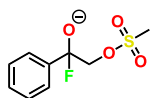
**31-IM**



1	C	2.650258	-1.405728	0.797974
2	H	3.304586	-1.253664	1.666414
3	H	2.838126	-0.637850	0.035382
4	F	2.885045	-2.655538	0.256334

5	O	2.327174	1.585853	0.783929
6	S	1.625436	1.810758	-0.500216
7	O	1.734264	3.197670	-0.991183
8	O	1.968568	0.804479	-1.534106
9	C	-0.113155	1.554816	-0.144946
10	C	-0.591664	1.718546	1.150551
11	C	-0.983501	1.219410	-1.182981
12	C	-1.952468	1.544624	1.408004
13	H	0.110106	1.954302	1.951314
14	C	-2.336957	1.048340	-0.915235
15	H	-0.586807	1.072090	-2.189013
16	C	-2.842335	1.204520	0.384383
17	H	-2.328360	1.664940	2.426819
18	H	-3.017561	0.772764	-1.724728
19	C	1.203453	-1.311176	1.262016
20	O	0.940599	-0.927021	2.379668
21	C	0.136833	-1.736574	0.305273
22	C	0.399897	-1.932499	-1.056466
23	C	-1.159869	-1.925310	0.797973
24	C	-0.628920	-2.320901	-1.911948
25	H	1.400255	-1.756508	-1.449767
26	C	-2.183547	-2.323281	-0.056545
27	H	-1.344063	-1.755135	1.859890
28	C	-1.917304	-2.520960	-1.413423
29	H	-0.425632	-2.467207	-2.973833
30	H	-3.191251	-2.479859	0.332000
31	H	-2.719052	-2.830635	-2.086250
32	C	-4.301901	0.965547	0.665241
33	H	-4.528156	-0.111772	0.628711
34	H	-4.584923	1.335843	1.659022
35	H	-4.937402	1.456302	-0.085202

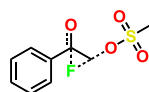
32



1	C	0.690896	1.722979	0.305960
2	H	1.122203	2.723729	0.171793
3	H	0.794962	1.401588	1.348653
4	F	-1.359947	2.523111	0.987750
5	C	-0.774919	1.766354	-0.182324
6	O	-0.968186	2.348237	-1.290962
7	C	-1.415449	0.369665	-0.021161
8	C	-1.944519	-0.249737	-1.153496
9	C	-1.452038	-0.308202	1.202930
10	C	-2.483558	-1.535438	-1.079153
11	H	-1.911682	0.312389	-2.088182
12	C	-1.987696	-1.594349	1.284477
13	H	-1.056763	0.176149	2.098105

14	C	-2.500429	-2.213807	0.141033
15	H	-2.888519	-2.013155	-1.973636
16	H	-2.007790	-2.117498	2.242504
17	H	-2.914586	-3.221695	0.203628
18	O	1.448576	0.832264	-0.544987
19	S	2.144853	-0.491561	0.025701
20	O	3.492741	-0.506326	-0.510231
21	O	1.961387	-0.560623	1.466849
22	C	1.221977	-1.778993	-0.757398
23	H	1.740320	-2.713248	-0.510785
24	H	0.198197	-1.775086	-0.366603
25	H	1.243822	-1.595429	-1.837013

32-TS (Frequency: 660.7201 i cm<sup>-1</sup>)



1	C	0.637577	1.755106	0.311342
2	H	1.207057	2.659269	0.123343
3	H	0.746086	1.251806	1.263900
4	F	-0.743489	2.774471	1.135607
5	C	-0.530413	1.518895	-0.589213
6	O	-0.649217	2.105343	-1.644015
7	C	-1.455007	0.397853	-0.212347
8	C	-2.098556	-0.298710	-1.239931
9	C	-1.642041	0.007745	1.118292
10	C	-2.893567	-1.405176	-0.945616
11	H	-1.949309	0.031450	-2.269304
12	C	-2.441647	-1.095241	1.411686
13	H	-1.190957	0.612606	1.904255
14	C	-3.058643	-1.808533	0.381012
15	H	-3.382679	-1.956736	-1.749978
16	H	-2.591317	-1.397832	2.449263
17	H	-3.676754	-2.677253	0.613739
18	O	1.763184	0.699057	-0.553840
19	S	2.204931	-0.638631	0.073468
20	O	3.608778	-0.880645	-0.246591
21	O	1.833140	-0.697206	1.490880
22	C	1.247527	-1.866854	-0.781393
23	H	1.575741	-2.844100	-0.409000
24	H	0.185908	-1.701802	-0.562704
25	H	1.450263	-1.772456	-1.853931

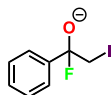
32-IM



1	O	0.549951	-1.098456	0.910856
2	S	0.159872	-0.000020	-0.000066

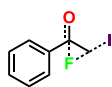
3	O	0.551140	1.338237	0.494508
4	O	0.547441	-0.240727	-1.407146
5	C	-1.633698	0.000820	0.001568
6	H	-1.981919	0.802335	-0.660505
7	H	-1.982166	-0.973503	-0.360841
8	H	-1.979946	0.174144	1.027243

**33**



1	C	-0.885506	1.159936	-0.631341
2	H	-1.617229	1.970809	-0.548123
3	H	-0.581314	1.008958	-1.672325
4	F	0.815276	2.670306	-0.383557
5	C	0.287876	1.448797	0.352499
6	O	-0.035810	1.703278	1.545670
7	C	1.436376	0.439267	0.142267
8	C	2.108555	0.304620	-1.077637
9	C	1.808750	-0.375375	1.211657
10	C	3.124223	-0.639805	-1.228172
11	H	1.840301	0.959962	-1.909018
12	C	2.823751	-1.323425	1.067659
13	H	1.280689	-0.235720	2.156803
14	C	3.482298	-1.460149	-0.155187
15	H	3.643868	-0.734346	-2.183849
16	H	3.103700	-1.958108	1.911056
17	H	4.275685	-2.200619	-0.272546
18	I	-1.964427	-0.637606	-0.084638

**33-TS (Frequency: 461.0191 i cm<sup>-1</sup>)**



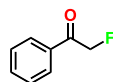
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2	H	1.420967	2.102822	0.092042
3	H	0.438360	1.198720	1.389738
4	F	-0.708891	2.814373	0.375030
5	C	-0.330566	1.047417	-0.717745

6	O	-0.106228	1.266480	-1.889882
7	C	-1.544842	0.265209	-0.291744
8	C	-2.201966	0.501915	0.920833
9	C	-2.006602	-0.738980	-1.147782
10	C	-3.302193	-0.275480	1.277879
11	H	-1.859310	1.339340	1.528029
12	C	-3.102896	-1.521274	-0.785157
13	H	-1.490889	-0.901187	-2.096081
14	C	-3.749786	-1.291697	0.429984
15	H	-3.821434	-0.082702	2.218262
16	H	-3.453515	-2.311542	-1.451001
17	H	-4.609012	-1.901461	0.714603
18	I	2.150028	-0.583420	0.172989

**33-IM: I<sup>-</sup>**

1	I	0.000000	0.000000	0.000000
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**34**



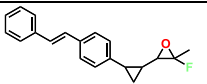
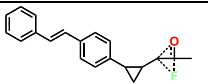
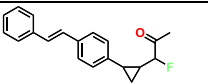
1	C	-2.444009	-0.361750	0.198232
2	H	-3.385284	0.115610	-0.104124
3	H	-2.538580	-0.729492	1.233013
4	F	-2.178243	-1.423813	-0.630061
5	C	-1.345205	0.691788	0.145309
6	O	-1.656943	1.859479	0.205862
7	C	0.083713	0.262719	0.065573
8	C	1.042836	1.248126	-0.205626
9	C	0.490902	-1.058460	0.295775
10	C	2.392780	0.918025	-0.256253
11	H	0.706098	2.272112	-0.372848
12	C	1.845893	-1.383695	0.256206
13	H	-0.243703	-1.835447	0.505187
14	C	2.794805	-0.399961	-0.023494
15	H	3.135502	1.686479	-0.474240
16	H	2.161665	-2.410924	0.442021
17	H	3.853747	-0.660606	-0.059689

## 2. Thermodynamics Data

In this section, all the thermodynamics data of the calculated reactions is presented in table. The symbol of the table is shown below.

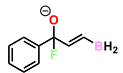
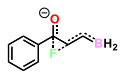
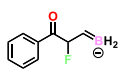
Structure		The structure of below calculation results
ZPE (M05-2X/Gas)	a.u.	The SPE at the level of M05-2X/6-31G* without solvent
ZPE (M05-2X/SMD)	a.u.	The SPE at the level of M05-2X/6-31G* with solvent by SMD model
Solvation delta G	kJ/mol	The Solvation delta G is calculated by <b>Eq. (1)</b> shown in article
ZPE (M06-2X/IEFPCM)	a.u.	The SPE at the level of M06-2X/def2-SVP with solvent by IEFPCM model
ZPE (double hybrid)	a.u.	The SPE at the level of rev-DSDPBEP86-D3(BJ)/def2-TZVPP
ZPE_corr	a.u.	Zero-point correction
U_corr	a.u.	Thermal correction to Energy
H_corr	a.u.	Thermal correction to Enthalpy
G_corr	a.u.	Thermal correction to Gibbs Free Energy
U(T)	a.u.	Sum of ZPE (double hybrid) and U_corr
H(T)	a.u.	Sum of ZPE (double hybrid) and H_corr
G(T)	a.u.	Sum of ZPE (double hybrid) and G_corr
Electron energy barrier	kJ/mol	The electron energy barrier in the unit of kJ/mol
Delta electron energy	kJ/mol	The delta electron energy in the unit of kJ/mol
Gibbs Free Energy Barrier	kJ/mol	The Gibbs free energy barrier in the unit of kJ/mol
Delta G	kJ/mol	The delta Gibbs free energy in the unit of kJ/mol
Electron energy barrier	kcal/mol	The electron energy barrier in the unit of kcal/mol
Delta electron energy	kcal/mol	The delta electron energy in the unit of kcal/mol
Gibbs Free Energy Barrier	kcal/mol	The Gibbs free energy barrier in the unit of kcal/mol
Delta G	kcal/mol	The delta Gibbs free energy in the unit of kcal/mol

**Table S4:** Thermodynamics data of epoxide-induced 1,2-fluorine migration.

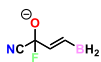
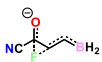

Structure				
ZPE (M05-2X/Gas)	a.u.	-948.47351480	-948.39837210	-948.49408690
ZPE (M05-2X/SMD)	a.u.	-948.50345630	-948.44370570	-948.52548090
Solvation delta G	kJ/mol	-78.61140825	-119.02336680	-82.42494700
ZPE (M06-2X/IEFPCM)	a.u.	-947.49438670	-947.42516120	-947.51531000
ZPE (double hybrid)	a.u.	-947.15594260	-947.09158510	-947.18120980
ZPE_corr	a.u.	0.322474	0.334935	0.337839
U_corr	a.u.	0.357892	0.354583	0.357774
H_corr	a.u.	0.358837	0.355528	0.358718
G_corr	a.u.	0.287012	0.283464	0.285425
U(T)	a.u.	-946.7980506000	-946.7370021000	-946.8234358000
H(T)	a.u.	-946.7971056000	-946.7360571000	-946.8224918000
G(T)	a.u.	-946.8689306000	-946.8081211000	-946.8957848000
Electron energy barrier	kJ/mol	181.7515502497		
Delta electron energy	kJ/mol	-54.9341241501		
Gibbs Free Energy Barrier	kJ/mol	119.2433837001		
Delta G	kJ/mol	-74.3192408501		
Electron energy barrier	kcal/mol	43.4396630616		
Delta electron energy	kcal/mol	-13.1295707816		
Gibbs Free Energy Barrier	kcal/mol	28.4998527008		
Delta G	kcal/mol	-17.7627248686		



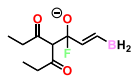
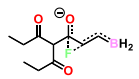
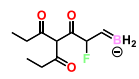
**Table S5:** Thermodynamics data of **3a**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-548.21846319	-548.19654747	-548.21739657
ZPE (M05-2X/SMD)	a.u.	-548.30599311	-548.29130484	-548.31454801
Solvation delta G	kJ/mol	-229.80981021	-248.78547756	-255.07108209
ZPE (M06-2X/IEFPCM)	a.u.	-547.73600948	-547.72112080	-547.74648949
ZPE (double hybrid)	a.u.	-547.50984894	-547.50620451	-547.51255760
ZPE_corr	a.u.	0.156801	0.156623	0.158291
U_corr	a.u.	0.167955	0.167509	0.169104
H_corr	a.u.	0.168899	0.168453	0.170048
G_corr	a.u.	0.119061	0.119294	0.120966
U(T)	a.u.	-547.3418939364	-547.3386955104	-547.3434535982
H(T)	a.u.	-547.3409499364	-547.3377515104	-547.3425095982
G(T)	a.u.	-547.3907879364	-547.3869105104	-547.3915915982
Electron energy barrier	kJ/mol	39.0902135872		
Delta electron energy	kJ/mol	-27.5152741315		
Gibbs Free Energy Barrier	kJ/mol	-8.7954852287		
Delta G	kJ/mol	-27.3712858568		
Electron energy barrier	kcal/mol	9.3427852742		
Delta electron energy	kcal/mol	-6.5763083488		
Gibbs Free Energy Barrier	kcal/mol	-2.1021714218		
Delta G	kcal/mol	-6.5418943252		

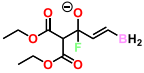
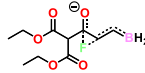
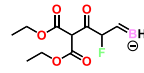
**Table S6:** Thermodynamics data of **3b**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-409.42729193	-409.40361061	-409.42595216
ZPE (M05-2X/SMD)	a.u.	-409.50618400	-409.48064066	-409.50085382
Solvation delta G	kJ/mol	-207.13114029	-202.24238577	-196.65430308
ZPE (M06-2X/IEFPCM)	a.u.	-409.09179385	-409.06709868	-409.09075476
ZPE (double hybrid)	a.u.	-408.95222328	-408.94366527	-408.95578851
ZPE_corr	a.u.	0.073759	0.073326	0.074627
U_corr	a.u.	0.082268	0.081451	0.082926
H_corr	a.u.	0.083212	0.082395	0.083870
G_corr	a.u.	0.040412	0.040536	0.041166
U(T)	a.u.	-408.8699552751	-408.8622142733	-408.8728625098
H(T)	a.u.	-408.8690112751	-408.8612702733	-408.8719185098
G(T)	a.u.	-408.9118112751	-408.9031292733	-408.9146225098
Electron energy barrier	kJ/mol	64.8371583330		
Delta electron energy	kJ/mol	2.7281255439		
Gibbs Free Energy Barrier	kJ/mol	27.6833502134		
Delta G	kJ/mol	3.0959403454		
Electron energy barrier	kcal/mol	15.4964527565		
Delta electron energy	kcal/mol	0.6520376539		
Gibbs Free Energy Barrier	kcal/mol	6.6164794965		
Delta G	kcal/mol	0.7399475013		

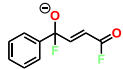
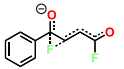
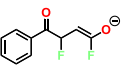
**Table S7:** Thermodynamics data of **3c**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-740.37089590	-740.35066459	-740.35974677
ZPE (M05-2X/SMD)	a.u.	-740.44749930	-740.43174245	-740.44957536
Solvation delta G	kJ/mol	-201.12223720	-212.86992931	-235.84495254
ZPE (M06-2X/IEFPCM)	a.u.	-739.68521629	-739.66883032	-739.68754649
ZPE (double hybrid)	a.u.	-739.46932686	-739.46375113	-739.46377005
ZPE_corr	a.u.	0.236087	0.235990	0.236617
U_corr	a.u.	0.253483	0.253035	0.253840
H_corr	a.u.	0.254427	0.253979	0.254784
G_corr	a.u.	0.190560	0.191103	0.190757
U(T)	a.u.	-739.2158438616	-739.2107161302	-739.2099300512
H(T)	a.u.	-739.2148998616	-739.2097721302	-739.2089860512
G(T)	a.u.	-739.2787668616	-739.2726481302	-739.2730130512
Electron energy barrier	kJ/mol	43.0213484821		
Delta electron energy	kJ/mol	-6.1179479766		
Gibbs Free Energy Barrier	kJ/mol	4.3170373172		
Delta G	kJ/mol	-19.6160859525		
Electron energy barrier	kcal/mol	10.2823490636		
Delta electron energy	kcal/mol	-1.4622246598		
Gibbs Free Energy Barrier	kcal/mol	1.0317966819		
Delta G	kcal/mol	-4.6883570632		

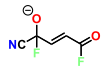
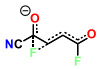
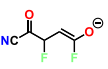
**Table S8:** Thermodynamics data of **3d**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-890.80989338	-890.79223321	-890.81025584
ZPE (M05-2X/SMD)	a.u.	-890.89876429	-890.88541384	-890.90768608
Solvation delta G	kJ/mol	-225.40470581	-236.71987567	-247.87722148
ZPE (M06-2X/IEFPCM)	a.u.	-889.99249981	-889.97784753	-890.00103379
ZPE (double hybrid)	a.u.	-889.76610149	-889.76223442	-889.77099571
ZPE_corr	a.u.	0.247668	0.247509	0.248699
U_corr	a.u.	0.266930	0.266294	0.267546
H_corr	a.u.	0.267874	0.267239	0.268490
G_corr	a.u.	0.197825	0.199015	0.199621
U(T)	a.u.	-889.51843349	-889.51472542	-889.52229671
H(T)	a.u.	-889.49917149	-889.49594042	-889.50344971
G(T)	a.u.	-889.49822749	-889.49499542	-889.50250571
Electron energy barrier	kJ/mol	10.1530039947		
Delta electron energy	kJ/mol	-12.8497807011		
Gibbs Free Energy Barrier	kJ/mol	-2.8293583653		
Delta G	kJ/mol	-33.7049883652		
Electron energy barrier	kcal/mol	2.4266261938		
Delta electron energy	kcal/mol	-3.0711712957		
Gibbs Free Energy Barrier	kcal/mol	-0.6762328789		
Delta G	kcal/mol	-8.0556855557		

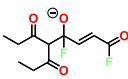
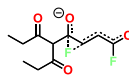
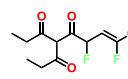
**Table S9:** Thermodynamics data of **4a**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-735.36335651	-735.34613475	-735.36011410
ZPE (M05-2X/SMD)	a.u.	-735.44887544	-735.43605517	-735.45194583
Solvation delta G	kJ/mol	-224.52995597	-236.08606796	-241.10420449
ZPE (M06-2X/IEFPCM)	a.u.	-734.69652771	-734.68296994	-734.70124914
ZPE (double hybrid)	a.u.	-734.49940571	-734.49674211	-734.49590538
ZPE_corr	a.u.	0.148950	0.148396	0.149852
U_corr	a.u.	0.160977	0.160307	0.161872
H_corr	a.u.	0.161921	0.161252	0.162817
G_corr	a.u.	0.108783	0.108851	0.109397
U(T)	a.u.	-734.3384287130	-734.3364351122	-734.3340333828
H(T)	a.u.	-734.3374847130	-734.3354901122	-734.3330883828
G(T)	a.u.	-734.3906227130	-734.3878911122	-734.3865083828
Electron energy barrier	kJ/mol	35.5959330115		
Delta electron energy	kJ/mol	-12.3961039629		
Gibbs Free Energy Barrier	kJ/mol	-4.3842939636		
Delta G	kJ/mol	-5.7720745309		
Electron energy barrier	kcal/mol	8.5076321729		
Delta electron energy	kcal/mol	-2.9627399529		
Gibbs Free Energy Barrier	kcal/mol	-1.0478714062		
Delta G	kcal/mol	-1.3795589223		

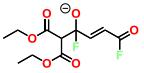
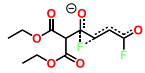
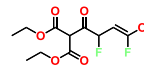
**Table S10:** Thermodynamics data of **4b**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-596.57063294	-596.54532158	-596.56429253
ZPE (M05-2X/SMD)	a.u.	-596.64724936	-596.62063122	-596.63606899
Solvation delta G	kJ/mol	-201.15642909	-197.72544932	-188.44909836
ZPE (M06-2X/IEFPCM)	a.u.	-596.05054767	-596.02414829	-596.04282494
ZPE (double hybrid)	a.u.	-595.94064729	-595.92869249	-595.93537093
ZPE_corr	a.u.	0.065757	0.065009	0.066255
U_corr	a.u.	0.075158	0.074187	0.075671
H_corr	a.u.	0.076102	0.075131	0.076615
G_corr	a.u.	0.029624	0.029556	0.029931
U(T)	a.u.	-595.8654892910	-595.8545054944	-595.8596999309
H(T)	a.u.	-595.8645452910	-595.8535614944	-595.8587559309
G(T)	a.u.	-595.9110232910	-595.8991364944	-595.9054399309
Electron energy barrier	kJ/mol	69.3115669392		
Delta electron energy	kJ/mol	20.2760381171		
Gibbs Free Energy Barrier	kJ/mol	34.6397642963		
Delta G	kJ/mol	27.3664426492		
Electron energy barrier	kcal/mol	16.5658620792		
Delta electron energy	kcal/mol	4.8460894161		
Gibbs Free Energy Barrier	kcal/mol	8.2791023653		
Delta G	kcal/mol	6.5407367708		

**Table S11:** Thermodynamics data of **4c**.

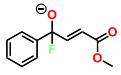
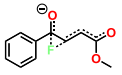
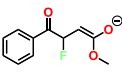
Structure				
ZPE (M05-2X/Gas)	a.u.	-927.51047283	-927.48943228	-927.49774523
ZPE (M05-2X/SMD)	a.u.	-927.58642687	-927.56995195	-927.58353264
Solvation delta G	kJ/mol	-199.41733990	-211.40440146	-225.23485546
ZPE (M06-2X/IEFPCM)	a.u.	-926.64158902	-926.62399960	-926.63855853
ZPE (double hybrid)	a.u.	-926.45512623	-926.44719003	-926.44313094
ZPE_corr	a.u.	0.228632	0.227994	0.228402
U_corr	a.u.	0.246846	0.246078	0.246811
H_corr	a.u.	0.247790	0.247022	0.247755
G_corr	a.u.	0.181024	0.180805	0.179744
U(T)	a.u.	-926.2082802336	-926.2011120265	-926.1963199354
H(T)	a.u.	-926.2073362336	-926.2001680265	-926.1953759354
G(T)	a.u.	-926.2741022336	-926.2663850265	-926.2633869354
Electron energy barrier	kJ/mol	46.1810117079		
Delta electron energy	kJ/mol	7.9565436186		
Gibbs Free Energy Barrier	kJ/mol	8.2744658598		
Delta G	kJ/mol	2.3154999952		
Electron energy barrier	kcal/mol	11.0375266988		
Delta electron energy	kcal/mol	1.9016595647		
Gibbs Free Energy Barrier	kcal/mol	1.9776448040		
Delta G	kcal/mol	0.5534177809		

**Table S12:** Thermodynamics data of **4d**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1077.95448881	-1077.93504835	-1077.95278705
ZPE (M05-2X/SMD)	a.u.	-1078.04187319	-1078.02706914	-1078.04515402
Solvation delta G	kJ/mol	-221.50180817	-233.67470263	-234.58359821
ZPE (M06-2X/IEFPCM)	a.u.	-1076.95268170	-1076.93638945	-1076.95551301
ZPE (double hybrid)	a.u.	-1076.75611113	-1076.74920663	-1076.75433690
ZPE_corr	a.u.	0.239682	0.239046	0.240009
U_corr	a.u.	0.259826	0.259026	0.260154
H_corr	a.u.	0.260770	0.259971	0.261098
G_corr	a.u.	0.187998	0.187691	0.187966
U(T)	a.u.	-1076.51642913	-1076.51016063	-1076.51432790
H(T)	a.u.	-1076.49628513	-1076.49018063	-1076.49418290
G(T)	a.u.	-1076.49534113	-1076.48923563	-1076.49323890
Electron energy barrier	kJ/mol	18.1277526728		
Delta electron energy	kJ/mol	4.6582419154		
Gibbs Free Energy Barrier	kJ/mol	3.8570837171		
Delta G	kJ/mol	-7.5623841295		
Electron energy barrier	kcal/mol	4.3326368721		
Delta electron energy	kcal/mol	1.1133465381		
Gibbs Free Energy Barrier	kcal/mol	0.9218651332		
Delta G	kcal/mol	-1.8074531858		



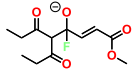
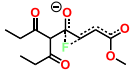
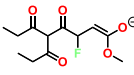
**Table S13:** Thermodynamics data of **5a**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-750.63874463	-750.61920733	-750.62814422
ZPE (M05-2X/SMD)	a.u.	-750.73139296	-750.71409420	-750.72054535
Solvation delta G	kJ/mol	-243.24819567	-249.12546931	-242.59917732
ZPE (M06-2X/IEFPCM)	a.u.	-749.95917229	-749.94190894	-749.95127213
ZPE (double hybrid)	a.u.	-749.72275078	-749.71672366	-749.71178743
ZPE_corr	a.u.	0.189722	0.189383	0.190423
U_corr	a.u.	0.203663	0.203109	0.204301
H_corr	a.u.	0.204607	0.204054	0.205245
G_corr	a.u.	0.146643	0.147479	0.147556
U(T)	a.u.	-749.5190877771	-749.5136146611	-749.5074864268
H(T)	a.u.	-749.5181437771	-749.5126696611	-749.5065424268
G(T)	a.u.	-749.5761077771	-749.5692446611	-749.5642314268
Electron energy barrier	kJ/mol	45.3249490546		
Delta electron energy	kJ/mol	20.7418779566		
Gibbs Free Energy Barrier	kJ/mol	12.1418375729		
Delta G	kJ/mol	31.8303759825		
Electron energy barrier	kcal/mol	10.8329228142		
Delta electron energy	kcal/mol	4.9574278099		
Gibbs Free Energy Barrier	kcal/mol	2.9019688272		
Delta G	kcal/mol	7.6076424432		


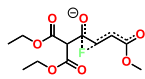
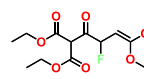
**Table S14:** Thermodynamics data of **5b**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-611.84735073	-611.81770901	-611.83430188
ZPE (M05-2X/SMD)	a.u.	-611.93141632	-611.89761855	-611.90810926
Solvation delta G	kJ/mol	-220.71418817	-209.80248939	-193.78129719
ZPE (M06-2X/IEFPCM)	a.u.	-611.31468521	-611.28208906	-611.29573608
ZPE (double hybrid)	a.u.	-611.16513706	-611.14762112	-611.15326412
ZPE_corr	a.u.	0.106794	0.105905	0.106944
U_corr	a.u.	0.117982	0.116882	0.118163
H_corr	a.u.	0.118926	0.117826	0.119107
G_corr	a.u.	0.068402	0.068088	0.068414
U(T)	a.u.	-611.0471550619	-611.0307391231	-611.0351011198
H(T)	a.u.	-611.0462110619	-611.0297951231	-611.0341571198
G(T)	a.u.	-611.0967350619	-611.0795331231	-611.0848501198
Electron energy barrier	kJ/mol	85.5811970760		
Delta electron energy	kJ/mol	49.7509513169		
Gibbs Free Energy Barrier	kJ/mol	56.0753891713		
Delta G	kJ/mol	58.1368064560		
Electron energy barrier	kcal/mol	20.4543970067		
Delta electron energy	kcal/mol	11.8907627430		
Gibbs Free Energy Barrier	kcal/mol	13.4023396681		
Delta G	kcal/mol	13.8950302237		

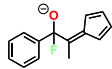
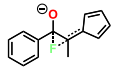
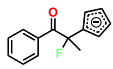
**Table S15:** Thermodynamics data of **5c**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-942.78720055	-942.76201960	-942.76666570
ZPE (M05-2X/SMD)	a.u.	-942.86949187	-942.84675329	-942.85268611
Solvation delta G	kJ/mol	-216.05585541	-222.46828472	-225.84659433
ZPE (M06-2X/IEFPCM)	a.u.	-941.90492964	-941.88171216	-941.88953356
ZPE (double hybrid)	a.u.	-941.67969216	-941.66538964	-941.65971514
ZPE_corr	a.u.	0.269361	0.268795	0.269071
U_corr	a.u.	0.289493	0.288723	0.289260
H_corr	a.u.	0.290437	0.289667	0.290204
G_corr	a.u.	0.218930	0.219048	0.218532
U(T)	a.u.	-941.3901991648	-941.3766666421	-941.3704551426
H(T)	a.u.	-941.3892551648	-941.3757226421	-941.3695111426
G(T)	a.u.	-941.4607621648	-941.4463416421	-941.4411831426
Electron energy barrier	kJ/mol	60.9575016163		
Delta electron energy	kJ/mol	40.4224237930		
Gibbs Free Energy Barrier	kJ/mol	31.4486528316		
Delta G	kJ/mol	41.6139837587		
Electron energy barrier	kcal/mol	14.5691925469		
Delta electron energy	kcal/mol	9.6611911551		
Gibbs Free Energy Barrier	kcal/mol	7.5164084205		
Delta G	kcal/mol	9.9459808219		




**Table S16:** Thermodynamics data of **5d**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1093.23541745	-1093.21703788	-1093.22141565
ZPE (M05-2X/SMD)	a.u.	-1093.32620128	-1093.30693659	-1093.30992541
Solvation delta G	kJ/mol	-230.42706414	-228.10318159	-224.45649336
ZPE (M06-2X/IEFPCM)	a.u.	-1092.21872732	-1092.19926659	-1092.20354215
ZPE (double hybrid)	a.u.	-1091.98342849	-1091.97395352	-1091.97002865
ZPE_corr	a.u.	0.280642	0.280484	0.281110
U_corr	a.u.	0.302395	0.301876	0.302849
H_corr	a.u.	0.303339	0.302820	0.303794
G_corr	a.u.	0.227779	0.228424	0.228627
U(T)	a.u.	-1091.70278649	-1091.69346952	-1091.68891865
H(T)	a.u.	-1091.68103349	-1091.67207752	-1091.66717965
G(T)	a.u.	-1091.68008949	-1091.67113352	-1091.66623465
Electron energy barrier	kJ/mol	24.8765350481		
Delta electron energy	kJ/mol	35.1812843833		
Gibbs Free Energy Barrier	kJ/mol	25.8377831078		
Delta G	kJ/mol	42.3464576677		
Electron energy barrier	kcal/mol	5.9456345717		
Delta electron energy	kcal/mol	8.4085287723		
Gibbs Free Energy Barrier	kcal/mol	6.1753783718		
Delta G	kcal/mol	10.1210462877		

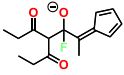
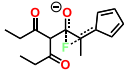
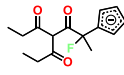
**Table S17:** Thermodynamics data of **6a**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-715.69003479	-715.66822784	-715.70530375
ZPE (M05-2X/SMD)	a.u.	-715.78360009	-715.76647625	-715.80285238
Solvation delta G	kJ/mol	-245.65569778	-257.95121096	-256.11392019
ZPE (M06-2X/IEFPCM)	a.u.	-715.03163569	-715.01404142	-715.05195116
ZPE (double hybrid)	a.u.	-714.73712759	-714.73037847	-714.75074273
ZPE_corr	a.u.	0.220568	0.219353	0.221351
U_corr	a.u.	0.234129	0.233243	0.234825
H_corr	a.u.	0.235073	0.234187	0.235769
G_corr	a.u.	0.179754	0.177338	0.180508
U(T)	a.u.	-714.5029985877	-714.4971354700	-714.5159177308
H(T)	a.u.	-714.5020545877	-714.4961914700	-714.5149737308
G(T)	a.u.	-714.5573735877	-714.5530404700	-714.5702347308
Electron energy barrier	kJ/mol	46.1937611360		
Delta electron energy	kJ/mol	-53.3382612338		
Gibbs Free Energy Barrier	kJ/mol	-0.9189126601		
Delta G	kJ/mol	-44.2251535957		
Electron energy barrier	kcal/mol	11.0405738853		
Delta electron energy	kcal/mol	-12.7481503905		
Gibbs Free Energy Barrier	kcal/mol	-0.2196253968		
Delta G	kcal/mol	-10.5700653909		

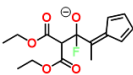
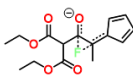
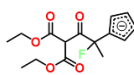
**Table S18:** Thermodynamics data of **6b**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-576.89983504	-576.87294478	-576.90456606
ZPE (M05-2X/SMD)	a.u.	-576.98538943	-576.95822736	-576.98834783
Solvation delta G	kJ/mol	-224.62305357	-223.90941904	-219.96903451
ZPE (M06-2X/IEFPCM)	a.u.	-576.38862738	-576.36169199	-576.39396370
ZPE (double hybrid)	a.u.	-576.18031749	-576.16815301	-576.18488782
ZPE_corr	a.u.	0.137424	0.136327	0.137380
U_corr	a.u.	0.148415	0.147276	0.148438
H_corr	a.u.	0.149359	0.148220	0.149382
G_corr	a.u.	0.100196	0.099428	0.099994
U(T)	a.u.	-576.0319024862	-576.0208770064	-576.0364498156
H(T)	a.u.	-576.0309584862	-576.0199330064	-576.0355058156
G(T)	a.u.	-576.0801214862	-576.0687250064	-576.0848938156
Electron energy barrier	kJ/mol	70.7188716961		
Delta electron energy	kJ/mol	-14.0104976580		
Gibbs Free Energy Barrier	kJ/mol	30.6350924021		
Delta G	kJ/mol	-7.8757318310		
Electron energy barrier	kcal/mol	16.9022159886		
Delta electron energy	kcal/mol	-3.3485893064		
Gibbs Free Energy Barrier	kcal/mol	7.3219628112		
Delta G	kcal/mol	-1.8823450839		

**Table S19:** Thermodynamics data of **6c**.

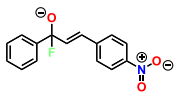
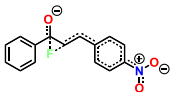
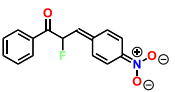
Structure				
ZPE (M05-2X/Gas)	a.u.	-907.83848484	-907.80445320	-907.85476994
ZPE (M05-2X/SMD)	a.u.	-907.92216513	-907.90072191	-907.94274545
Solvation delta G	kJ/mol	-219.70261190	-252.75351123	-230.97971463
ZPE (M06-2X/IEFPCM)	a.u.	-906.97901990	-906.95474003	-907.00042470
ZPE (double hybrid)	a.u.	-906.69438200	-906.67764131	-906.71080801
ZPE_corr	a.u.	0.299891	0.298509	0.299769
U_corr	a.u.	0.319771	0.318620	0.319604
H_corr	a.u.	0.320715	0.319564	0.320548
G_corr	a.u.	0.250720	0.249015	0.251291
U(T)	a.u.	-906.3746109961	-906.3590213090	-906.3912040107
H(T)	a.u.	-906.3736669961	-906.3580773090	-906.3902600107
G(T)	a.u.	-906.4436619961	-906.4286263090	-906.4595170107
Electron energy barrier	kJ/mol	63.7468118126		
Delta electron energy	kJ/mol	-56.1982997746		
Gibbs Free Energy Barrier	kJ/mol	6.4252970143		
Delta G	kJ/mol	-52.9044435941		
Electron energy barrier	kcal/mol	15.2358536837		
Delta electron energy	kcal/mol	-13.4317160073		
Gibbs Free Energy Barrier	kcal/mol	1.5356828428		
Delta G	kcal/mol	-12.6444654862		

**Table S20:** Thermodynamics data of **6d**.

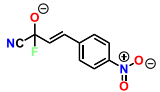
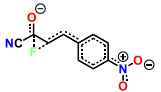
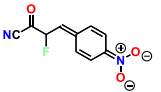
Structure				
ZPE (M05-2X/Gas)	a.u.	-1058.28554858	-1058.25719733	-1058.29263480
ZPE (M05-2X/SMD)	a.u.	-1058.37632514	-1058.36010894	-1058.39588863
Solvation delta G	kJ/mol	-230.40797676	-262.26855053	-263.16704914
ZPE (M06-2X/IEFPCM)	a.u.	-1057.29117601	-1057.26954247	-1057.30594148
ZPE (double hybrid)	a.u.	-1056.99812683	-1056.98795906	-1057.00547784
ZPE_corr	a.u.	0.311097	0.310090	0.311125
U_corr	a.u.	0.332678	0.332009	0.333138
H_corr	a.u.	0.333622	0.332954	0.334082
G_corr	a.u.	0.260325	0.256787	0.257442
U(T)	a.u.	-1056.68702983	-1056.67786906	-1056.69435284
H(T)	a.u.	-1056.66544883	-1056.65595006	-1056.67233984
G(T)	a.u.	-1056.66450483	-1056.65500506	-1056.67139584
Electron energy barrier	kJ/mol	26.6954790848		
Delta electron energy	kJ/mol	-19.3000859444		
Gibbs Free Energy Barrier	kJ/mol	-6.9189286902		
Delta G	kJ/mol	-50.8514283291		
Electron energy barrier	kcal/mol	6.38203726302		
Delta electron energy	kcal/mol	-4.6128312487		
Gibbs Free Energy Barrier	kcal/mol	-1.6536636449		
Delta G	kcal/mol	-12.1537830614		



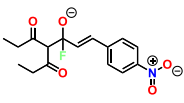
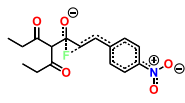
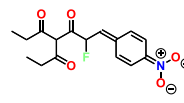
**Table S21:** Thermodynamics data of **7a**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-958.31044238	-958.29389455	-958.31190388
ZPE (M05-2X/SMD)	a.u.	-958.40120515	-958.38134046	-958.39572821
Solvation delta G	kJ/mol	-238.29764476	-229.58923933	-220.08076529
ZPE (M06-2X/IEFPCM)	a.u.	-957.40705933	-957.38798564	-957.40505522
ZPE (double hybrid)	a.u.	-957.09813775	-957.09473543	-957.09692642
ZPE_corr	a.u.	0.231354	0.230869	0.231923
U_corr	a.u.	0.247868	0.247267	0.248413
H_corr	a.u.	0.248812	0.248211	0.249357
G_corr	a.u.	0.183799	0.184531	0.185147
U(T)	a.u.	-956.8502697541	-956.8474684274	-956.8485134187
H(T)	a.u.	-956.8493257541	-956.8465244274	-956.8475694187
G(T)	a.u.	-956.9143387541	-956.9102044274	-956.9117794187
Electron energy barrier	kJ/mol	50.0779757205		
Delta electron energy	kJ/mol	5.2617934306		
Gibbs Free Energy Barrier	kJ/mol	19.5630802052		
Delta G	kJ/mol	24.9364144587		
Electron energy barrier	kcal/mol	11.9689234514		
Delta electron energy	kcal/mol	1.2575988123		
Gibbs Free Energy Barrier	kcal/mol	4.6756883856		
Delta G	kcal/mol	5.9599460943		

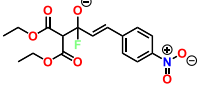
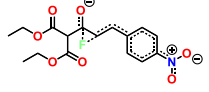
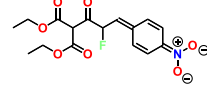
**Table S22:** Thermodynamics data of **7b**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-819.51843190	-819.49080259	-819.50418650
ZPE (M05-2X/SMD)	a.u.	-819.60243625	-819.56425749	-819.57469326
Solvation delta G	kJ/mol	-220.55342092	-192.85583995	-185.11549575
ZPE (M06-2X/IEFPCM)	a.u.	-818.76359573	-818.72718693	-818.74096441
ZPE (double hybrid)	a.u.	-818.53990141	-818.52440278	-818.52502342
ZPE_corr	a.u.	0.148436	0.147102	0.148115
U_corr	a.u.	0.162236	0.160838	0.161985
H_corr	a.u.	0.163180	0.161782	0.162929
G_corr	a.u.	0.105222	0.104295	0.105022
U(T)	a.u.	-818.3776654063	-818.3635647805	-818.3630384209
H(T)	a.u.	-818.3767214063	-818.3626207805	-818.3620944209
G(T)	a.u.	-818.4346794063	-818.4201077805	-818.4200014209
Electron energy barrier	kJ/mol	95.5912833959		
Delta electron energy	kJ/mol	59.4185175322		
Gibbs Free Energy Barrier	kJ/mol	65.9553844339		
Delta G	kJ/mol	73.9749756541		
Electron energy barrier	kcal/mol	22.8468650564		
Delta electron energy	kcal/mol	14.2013665230		
Gibbs Free Energy Barrier	kcal/mol	15.7637152089		
Delta G	kcal/mol	17.6804435120		

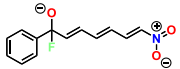
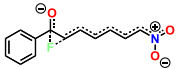
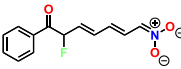
**Table S23:** Thermodynamics data of **7c**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1150.44582947	-1150.42008243	-1150.45157351
ZPE (M05-2X/SMD)	a.u.	-1150.53319156	-1150.50602357	-1150.53026408
Solvation delta G	kJ/mol	-229.36916729	-225.63846307	-206.60209154
ZPE (M06-2X/IEFPCM)	a.u.	-1149.34665881	-1149.31793590	-1149.34458950
ZPE (double hybrid)	a.u.	-1149.04492995	-1149.03230891	-1149.04799946
ZPE_corr	a.u.	0.310811	0.309574	0.310465
U_corr	a.u.	0.333532	0.332353	0.333515
H_corr	a.u.	0.334476	0.333297	0.334459
G_corr	a.u.	0.255624	0.254536	0.254297
U(T)	a.u.	-1148.7113979479	-1148.6999559091	-1148.7144844630
H(T)	a.u.	-1148.7104539479	-1148.6990119091	-1148.7135404630
G(T)	a.u.	-1148.7893059479	-1148.7777729091	-1148.7937024630
Electron energy barrier	kJ/mol	75.4120002048		
Delta electron energy	kJ/mol	5.4329734051		
Gibbs Free Energy Barrier	kJ/mol	34.0106975946		
Delta G	kJ/mol	11.2240253647		
Electron energy barrier	kcal/mol	18.0239006226		
Delta electron energy	kcal/mol	1.2985118081		
Gibbs Free Energy Barrier	kcal/mol	8.1287518151		
Delta G	kcal/mol	2.6826064447		

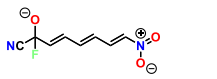
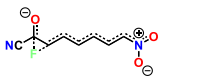
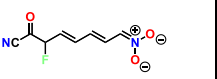
**Table S24:** Thermodynamics data of **7d**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1300.89591909	-1300.87817896	-1300.89844489
ZPE (M05-2X/SMD)	a.u.	-1300.99293952	-1300.97060992	-1300.98670619
Solvation delta G	kJ/mol	-246.80125744	-234.75160396	-223.80416163
ZPE (M06-2X/IEFPCM)	a.u.	-1299.66249716	-1299.63810922	-1299.65613739
ZPE (double hybrid)	a.u.	-1299.35089815	-1299.34604564	-1299.35111701
ZPE_corr	a.u.	0.321569	0.320573	0.321756
U_corr	a.u.	0.346474	0.345497	0.346679
H_corr	a.u.	0.347419	0.346441	0.347623
G_corr	a.u.	0.261145	0.260869	0.261959
U(T)	a.u.	-1299.02932915	-1299.02547264	-1299.02936101
H(T)	a.u.	-1299.00442415	-1299.00054864	-1299.00443801
G(T)	a.u.	-1299.00347915	-1298.99960464	-1299.00349401
Electron energy barrier	kJ/mol	12.7402516152		
Delta electron energy	kJ/mol	-0.5746156170		
Gibbs Free Energy Barrier	kJ/mol	22.2221660999		
Delta G	kJ/mol	22.9580821985		
Electron energy barrier	kcal/mol	3.0449932159		
Delta electron energy	kcal/mol	-0.1373364285		
Gibbs Free Energy Barrier	kcal/mol	5.3112251673		
Delta G	kcal/mol	5.4871133362		

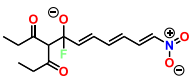
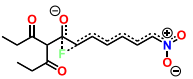
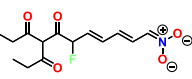
**Table S25:** Thermodynamics data of **8a**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-882.05992673	-882.04545318	-882.07584655
ZPE (M05-2X/SMD)	a.u.	-882.14887858	-882.13309857	-882.16351757
Solvation delta G	kJ/mol	-233.54307955	-230.11296882	-230.18028139
ZPE (M06-2X/IEFPCM)	a.u.	-881.23470376	-881.21890475	-881.25258121
ZPE (double hybrid)	a.u.	-880.97135603	-880.97077692	-880.98254552
ZPE_corr	a.u.	0.216981	0.216385	0.218029
U_corr	a.u.	0.233300	0.232560	0.234258
H_corr	a.u.	0.234244	0.233504	0.235202
G_corr	a.u.	0.169855	0.170090	0.170757
U(T)	a.u.	-880.7380560256	-880.7382169220	-880.7482875181
H(T)	a.u.	-880.7371120256	-880.7372729220	-880.7473435181
G(T)	a.u.	-880.8015010256	-880.8006869220	-880.8117885181
Electron energy barrier	kJ/mol	41.4803007551		
Delta electron energy	kJ/mol	-46.9372397238		
Gibbs Free Energy Barrier	kJ/mol	5.5675397052		
Delta G	kJ/mol	-23.6470134242		
Electron energy barrier	kcal/mol	9.9140298172		
Delta electron energy	kcal/mol	-11.2182695325		
Gibbs Free Energy Barrier	kcal/mol	1.3306739257		
Delta G	kcal/mol	-5.6517718509		

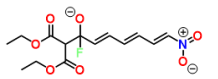
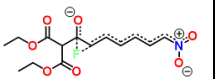
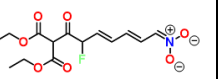
**Table S26:** Thermodynamics data of **8b**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-743.26696293	-743.24463094	-743.26688095
ZPE (M05-2X/SMD)	a.u.	-743.34969492	-743.31744649	-743.34144192
Solvation delta G	kJ/mol	-217.21283449	-191.17722915	-195.75981623
ZPE (M06-2X/IEFPCM)	a.u.	-742.59080178	-742.55981762	-742.58729719
ZPE (double hybrid)	a.u.	-742.41250562	-742.40257380	-742.40911465
ZPE_corr	a.u.	0.134085	0.132869	0.134256
U_corr	a.u.	0.147705	0.146309	0.147860
H_corr	a.u.	0.148649	0.147253	0.148804
G_corr	a.u.	0.091138	0.090470	0.090324
U(T)	a.u.	-742.2648006244	-742.2562647966	-742.2612546501
H(T)	a.u.	-742.2638566244	-742.2553207966	-742.2603106501
G(T)	a.u.	-742.3213676244	-742.3121037966	-742.3187906501
Electron energy barrier	kJ/mol	81.3489094545		
Delta electron energy	kJ/mol	9.2012957941		
Gibbs Free Energy Barrier	kJ/mol	50.3577851798		
Delta G	kJ/mol	28.2188640755		
Electron energy barrier	kcal/mol	19.4428559882		
Delta electron energy	kcal/mol	2.1991624747		
Gibbs Free Energy Barrier	kcal/mol	12.0357995171		
Delta G	kcal/mol	6.7444703813		

**Table S27:** Thermodynamics data of **8c**.


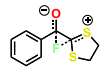
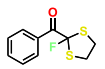
Structure				
ZPE (M05-2X/Gas)	a.u.	-1074.20712402	-1074.18855154	-1074.20765763
ZPE (M05-2X/SMD)	a.u.	-1074.28735515	-1074.26678220	-1074.29330249
Solvation delta G	kJ/mol	-210.64683181	-205.39459783	-224.86057993
ZPE (M06-2X/IEFPCM)	a.u.	-1073.18074965	-1073.15973593	-1073.18708571
ZPE (double hybrid)	a.u.	-1072.92739367	-1072.92089936	-1072.92533220
ZPE_corr	a.u.	0.296843	0.295883	0.296761
U_corr	a.u.	0.319318	0.318212	0.319362
H_corr	a.u.	0.320262	0.319156	0.320307
G_corr	a.u.	0.242169	0.241926	0.241373
U(T)	a.u.	-1072.6080756684	-1072.6026873575	-1072.6059701956
H(T)	a.u.	-1072.6071316684	-1072.6017433575	-1072.6050251956
G(T)	a.u.	-1072.6852246684	-1072.6789733575	-1072.6839591956
Electron energy barrier	kJ/mol	55.1715218604		
Delta electron energy	kJ/mol	-16.6353255299		
Gibbs Free Energy Barrier	kJ/mol	21.6650507520		
Delta G	kJ/mol	-10.8912492788		
Electron energy barrier	kcal/mol	13.1863101961		
Delta electron energy	kcal/mol	-3.9759382242		
Gibbs Free Energy Barrier	kcal/mol	5.1780714034		
Delta G	kcal/mol	-2.6030710513		

**Table S28:** Thermodynamics data of **8d**.

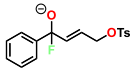
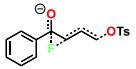
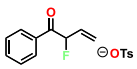
Structure				
ZPE (M05-2X/Gas)	a.u.	-1224.65449847	-1224.64168994	-1224.66222816
ZPE (M05-2X/SMD)	a.u.	-1224.74335238	-1224.72650648	-1224.74916345
Solvation delta G	kJ/mol	-225.36005919	-214.75994425	-220.32272237
ZPE (M06-2X/IEFPCM)	a.u.	-1223.49267773	-1223.47574655	-1223.50002036
ZPE (double hybrid)	a.u.	-1223.23129894	-1223.22885352	-1223.23668449
ZPE_corr	a.u.	0.307209	0.307016	0.308211
U_corr	a.u.	0.331846	0.331204	0.332770
H_corr	a.u.	0.332790	0.332148	0.333714
G_corr	a.u.	0.248030	0.249082	0.248431
U(T)	a.u.	-1222.92408994	-1222.92183752	-1222.92847349
H(T)	a.u.	-1222.89945294	-1222.89764952	-1222.90391449
G(T)	a.u.	-1222.89850894	-1222.89670552	-1222.90297049
Electron energy barrier	kJ/mol	6.4204478471		
Delta electron energy	kJ/mol	-14.1397565362		
Gibbs Free Energy Barrier	kJ/mol	15.3349917830		
Delta G	kJ/mol	-6.6764577252		
Electron energy barrier	kcal/mol	1.5345238640		
Delta electron energy	kcal/mol	-3.3794829197		
Gibbs Free Energy Barrier	kcal/mol	3.6651509998		
Delta G	kcal/mol	-1.5957116934		




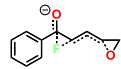
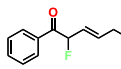
**Table S29:** Thermodynamics data of **9**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1357.74457429	-1357.74133853	-1357.81273772
ZPE (M05-2X/SMD)	a.u.	-1357.78412234	-1357.77664905	-1357.83298395
Solvation delta G	kJ/mol	-103.83340528	-92.70777026	-53.15647686
ZPE (M06-2X/IEFPCM)	a.u.	-1356.95833716	-1356.94925632	-1357.01051035
ZPE (double hybrid)	a.u.	-1356.47835761	-1356.48126075	-1356.53761190
ZPE_corr	a.u.	0.168913	0.168258	0.170567
U_corr	a.u.	0.181480	0.180494	0.182964
H_corr	a.u.	0.182424	0.181438	0.183908
G_corr	a.u.	0.128096	0.128819	0.130577
U(T)	a.u.	-1356.2968776118	-1356.3007667498	-1356.3546479026
H(T)	a.u.	-1356.2959336118	-1356.2998227498	-1356.3537039026
G(T)	a.u.	-1356.3502616118	-1356.3524417498	-1356.4070349026
Electron energy barrier	kJ/mol	23.8417454201		
Delta electron energy	kJ/mol	-136.9807103452		
Gibbs Free Energy Barrier	kJ/mol	5.4016826963		
Delta G	kJ/mol	-98.3813465849		
Electron energy barrier	kcal/mol	5.6983139149		
Delta electron energy	kcal/mol	-32.7391755127		
Gibbs Free Energy Barrier	kcal/mol	1.2910331492		
Delta G	kcal/mol	-23.5137061627		

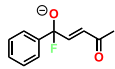
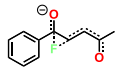
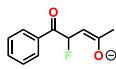
**Table S30:** Thermodynamics data of **10**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1456.18025554	-1456.15891727	-1456.22121279
ZPE (M05-2X/SMD)	a.u.	-1456.28243499	-1456.25395433	-1456.31894241
Solvation delta G	kJ/mol	-268.27214597	-249.51980103	-256.58911731
ZPE (M06-2X/IEFPCM)	a.u.	-1455.05556727	-1455.02741334	-1455.09348801
ZPE (double hybrid)	a.u.	-1454.62700406	-1454.61016369	-1454.66983141
ZPE_corr	a.u.	0.300107	0.297937	0.299045
U_corr	a.u.	0.320842	0.319076	0.320968
H_corr	a.u.	0.321786	0.320020	0.321912
G_corr	a.u.	0.249617	0.245971	0.246350
U(T)	a.u.	-1454.3061620584	-1454.2910876921	-1454.3488634098
H(T)	a.u.	-1454.3052180584	-1454.2901436921	-1454.3479194098
G(T)	a.u.	-1454.3773870584	-1454.3641926921	-1454.4234814098
Electron energy barrier	kJ/mol	73.9181432148		
Delta electron energy	kJ/mol	-99.5609028703		
Gibbs Free Energy Barrier	kJ/mol	53.3941536660		
Delta G	kJ/mol	-109.3376909364		
Electron energy barrier	kcal/mol	17.6668602330		
Delta electron energy	kcal/mol	-23.7956268810		
Gibbs Free Energy Barrier	kcal/mol	12.7615090024		
Delta G	kcal/mol	-26.1323353098		

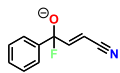
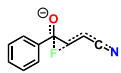
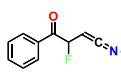
**Table S31:** Thermodynamics data of **11**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-675.36428796	-675.32334719	-675.33387056
ZPE (M05-2X/SMD)	a.u.	-675.46050310	-675.41952465	-675.42343400
Solvation delta G	kJ/mol	-252.61285007	-252.51390810	-235.14880909
ZPE (M06-2X/IEFPCM)	a.u.	-674.76002570	-674.71944557	-674.72503811
ZPE (double hybrid)	a.u.	-674.51840099	-674.48798625	-674.49120860
ZPE_corr	a.u.	0.184936	0.183696	0.184313
U_corr	a.u.	0.197280	0.195860	0.196791
H_corr	a.u.	0.198225	0.196804	0.197735
G_corr	a.u.	0.144480	0.143798	0.144574
U(T)	a.u.	-674.3211209945	-674.2921262543	-674.2944175999
H(T)	a.u.	-674.3201759945	-674.2911822543	-674.2934735999
G(T)	a.u.	-674.3739209945	-674.3441882543	-674.3466345999
Electron energy barrier	kJ/mol	106.5431313149		
Delta electron energy	kJ/mol	91.8599201702		
Gibbs Free Energy Barrier	kJ/mol	78.1622512310		
Delta G	kJ/mol	89.1044698927		
Electron energy barrier	kcal/mol	25.4644195303		
Delta electron energy	kcal/mol	21.9550478418		
Gibbs Free Energy Barrier	kcal/mol	18.6812263936		
Delta G	kcal/mol	21.2964794199		

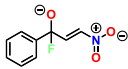
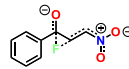
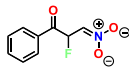
**Table S32:** Thermodynamics data of **12**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-675.41565096	-675.39683417	-675.40284407
ZPE (M05-2X/SMD)	a.u.	-675.50814591	-675.49110688	-675.49802901
Solvation delta G	kJ/mol	-242.84548860	-247.51299485	-249.90805472
ZPE (M06-2X/IEFPCM)	a.u.	-674.80661064	-674.78993452	-674.79921483
ZPE (double hybrid)	a.u.	-674.57280341	-674.56836270	-674.56036238
ZPE_corr	a.u.	0.183831	0.183561	0.184502
U_corr	a.u.	0.196761	0.196354	0.197519
H_corr	a.u.	0.197705	0.197298	0.198463
G_corr	a.u.	0.143012	0.143239	0.143158
U(T)	a.u.	-674.3760424146	-674.3720086954	-674.3628433809
H(T)	a.u.	-674.3750984146	-674.3710646954	-674.3618993809
G(T)	a.u.	-674.4297914146	-674.4251236954	-674.4172043809
Electron energy barrier	kJ/mol	43.7831530601		
Delta electron energy	kJ/mol	19.4176860275		
Gibbs Free Energy Barrier	kJ/mol	7.5875906628		
Delta G	kJ/mol	25.9846909649		
Electron energy barrier	kcal/mol	10.4644247276		
Delta electron energy	kcal/mol	4.6409383431		
Gibbs Free Energy Barrier	kcal/mol	1.8134776919		
Delta G	kcal/mol	6.2104901924		

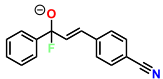
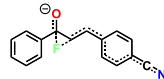
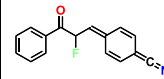
**Table S33:** Thermodynamics data of **13**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-615.03725154	-615.01487205	-615.01941068
ZPE (M05-2X/SMD)	a.u.	-615.12299382	-615.10698718	-615.11476645
Solvation delta G	kJ/mol	-225.11635089	-241.84827119	-250.35658201
ZPE (M06-2X/IEFPCM)	a.u.	-614.48523640	-614.46856040	-614.47618131
ZPE (double hybrid)	a.u.	-614.25651510	-614.24849566	-614.23944199
ZPE_corr	a.u.	0.145017	0.144696	0.145599
U_corr	a.u.	0.156176	0.155738	0.156912
H_corr	a.u.	0.157120	0.156683	0.157856
G_corr	a.u.	0.106797	0.106835	0.106892
U(T)	a.u.	-614.1003391044	-614.0927576628	-614.0825299920
H(T)	a.u.	-614.0993951044	-614.0918126628	-614.0815859920
G(T)	a.u.	-614.1497181044	-614.1416606628	-614.1325499920
Electron energy barrier	kJ/mol	43.7828511276		
Delta electron energy	kJ/mol	23.7741492970		
Gibbs Free Energy Barrier	kJ/mol	4.4228926732		
Delta G	kJ/mol	19.8346479313		
Electron energy barrier	kcal/mol	10.4643525639		
Delta electron energy	kcal/mol	5.6821580538		
Gibbs Free Energy Barrier	kcal/mol	1.0570967192		
Delta G	kcal/mol	4.7405946298		

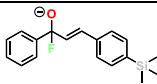
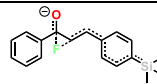
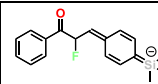
**Table S34:** Thermodynamics data of **14**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-727.27302562	-727.25567090	-727.27318961
ZPE (M05-2X/SMD)	a.u.	-727.35662817	-727.34395271	-727.36520349
Solvation delta G	kJ/mol	-219.49851340	-231.78389216	-241.58243406
ZPE (M06-2X/IEFPCM)	a.u.	-726.61188159	-726.59830028	-726.62275786
ZPE (double hybrid)	a.u.	-726.41458600	-726.41116321	-726.41195593
ZPE_corr	a.u.	0.149758	0.149162	0.150908
U_corr	a.u.	0.161632	0.160906	0.162744
H_corr	a.u.	0.162576	0.161850	0.163688
G_corr	a.u.	0.109794	0.109870	0.110822
U(T)	a.u.	-726.2529539991	-726.2502572051	-726.2492119337
H(T)	a.u.	-726.2520099991	-726.2493132051	-726.2482679337
G(T)	a.u.	-726.3047919991	-726.3012932051	-726.3011339337
Electron energy barrier	kJ/mol	35.6577372813		
Delta electron energy	kJ/mol	-28.5556495106		
Gibbs Free Energy Barrier	kJ/mol	-3.0992951308		
Delta G	kJ/mol	-12.4796699523		
Electron energy barrier	kcal/mol	8.5224037479		
Delta electron energy	kcal/mol	-6.8249640322		
Gibbs Free Energy Barrier	kcal/mol	-0.7407493142		
Delta G	kcal/mol	-2.9827127037		

**Table S35:** Thermodynamics data of **15**.

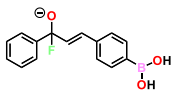
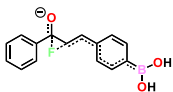
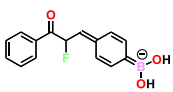
Structure				
ZPE (M05-2X/Gas)	a.u.	-846.07230904	-846.05501664	-846.06606878
ZPE (M05-2X/SMD)	a.u.	-846.16578513	-846.14430410	-846.15245675
Solvation delta G	kJ/mol	-245.42146117	-234.42423148	-226.81161786
ZPE (M06-2X/IEFPCM)	a.u.	-845.27865084	-845.25804910	-845.26851306
ZPE (double hybrid)	a.u.	-844.93895343	-844.93356851	-844.93100564
ZPE_corr	a.u.	0.226959	0.226277	0.227296
U_corr	a.u.	0.242758	0.242050	0.243171
H_corr	a.u.	0.243702	0.242994	0.244116
G_corr	a.u.	0.181130	0.180857	0.181433
U(T)	a.u.	-844.6961954348	-844.6915185131	-844.6878346384
H(T)	a.u.	-844.6952514348	-844.6905745131	-844.6868896384
G(T)	a.u.	-844.7578234348	-844.7527115131	-844.7495726384
Electron energy barrier	kJ/mol	54.0898867485		
Delta electron energy	kJ/mol	26.6167361392		
Gibbs Free Energy Barrier	kJ/mol	24.4185801885		
Delta G	kJ/mol	40.2723094389		
Electron energy barrier	kcal/mol	12.9277931999		
Delta electron energy	kcal/mol	6.3615526145		
Gibbs Free Energy Barrier	kcal/mol	5.8361807334		
Delta G	kcal/mol	9.6253129634		

**Table S36:** Thermodynamics data of **16**.

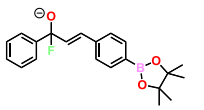
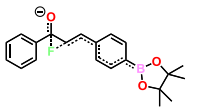
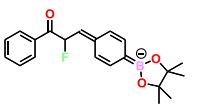
Structure				
ZPE (M05-2X/Gas)	a.u.	-1162.45161459	-1162.43099443	-1162.43481451
ZPE (M05-2X/SMD)	a.u.	-1162.55043209	-1162.52335234	-1162.52410619
Solvation delta G	kJ/mol	-259.44534625	-242.48569270	-234.43530584
ZPE (M06-2X/IEFPCM)	a.u.	-1161.54222877	-1161.51579365	-1161.51790245
ZPE (double hybrid)	a.u.	-1161.02066564	-1161.00832357	-1161.00428222
ZPE_corr	a.u.	0.328730	0.327951	0.328279
U_corr	a.u.	0.350753	0.349821	0.350510
H_corr	a.u.	0.351697	0.350765	0.351454
G_corr	a.u.	0.274905	0.275342	0.274546
U(T)	a.u.	-1160.6699126421	-1160.6585025735	-1160.6537722235
H(T)	a.u.	-1160.6689686421	-1160.6575585735	-1160.6528282235
G(T)	a.u.	-1160.7457606421	-1160.7329815735	-1160.7297362235
Electron energy barrier	kJ/mol	69.4054075602		
Delta electron energy	kJ/mol	63.8687531600		
Gibbs Free Energy Barrier	kJ/mol	50.5110981543		
Delta G	kJ/mol	67.0821514445		
Electron energy barrier	kcal/mol	16.5882905259		
Delta electron energy	kcal/mol	15.2649983652		
Gibbs Free Energy Barrier	kcal/mol	12.0724421975		
Delta G	kcal/mol	16.0330189877		



**Table S37:** Thermodynamics data of **17**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-929.81819706	-929.79684501	-929.80140082
ZPE (M05-2X/SMD)	a.u.	-929.92867656	-929.90267614	-929.90460736
Solvation delta G	kJ/mol	-290.06390887	-277.85963707	-270.96878127
ZPE (M06-2X/IEFPCM)	a.u.	-928.97025152	-928.94472541	-928.94823554
ZPE (double hybrid)	a.u.	-928.62529526	-928.61356112	-928.60940067
ZPE_corr	a.u.	0.252733	0.251804	0.252428
U_corr	a.u.	0.270297	0.269357	0.270245
H_corr	a.u.	0.271242	0.270301	0.271189
G_corr	a.u.	0.204728	0.204174	0.203790
U(T)	a.u.	-928.3549982629	-928.3442041161	-928.3391556709
H(T)	a.u.	-928.3540532629	-928.3432601161	-928.3382116709
G(T)	a.u.	-928.4205672629	-928.4093871161	-928.4056106709
Electron energy barrier	kJ/mol	67.0187939285		
Delta electron energy	kJ/mol	57.8029581157		
Gibbs Free Energy Barrier	kJ/mol	41.5577470714		
Delta G	kJ/mol	58.3636596860		
Electron energy barrier	kcal/mol	16.0178761780		
Delta electron energy	kcal/mol	13.8152385554		
Gibbs Free Energy Barrier	kcal/mol	9.9325399310		
Delta G	kcal/mol	13.9492494469		

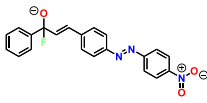
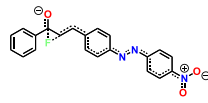
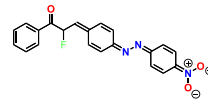
**Table S38:** Thermodynamics data of **18**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1164.47365803	-1164.45344667	-1164.45985700
ZPE (M05-2X/SMD)	a.u.	-1164.57857158	-1164.55327344	-1164.55600868
Solvation delta G	kJ/mol	-275.45052552	-262.09518464	-252.44623584
ZPE (M06-2X/IEFPCM)	a.u.	-1163.35015983	-1163.32566887	-1163.33054839
ZPE (double hybrid)	a.u.	-1162.91361254	-1162.90319436	-1162.89943623
ZPE_corr	a.u.	0.400408	0.399714	0.400258
U_corr	a.u.	0.424463	0.423651	0.424424
H_corr	a.u.	0.425407	0.424595	0.425369
G_corr	a.u.	0.344234	0.344505	0.343922
U(T)	a.u.	-1162.4891495374	-1162.4795433553	-1162.4750122276
H(T)	a.u.	-1162.4882055374	-1162.4785993553	-1162.4740672276
G(T)	a.u.	-1162.5693785374	-1162.5586893553	-1162.5555142276
Electron energy barrier	kJ/mol	64.3010154796		
Delta electron energy	kJ/mol	51.4898357196		
Gibbs Free Energy Barrier	kJ/mol	41.4197884934		
Delta G	kJ/mol	59.4050350649		
Electron energy barrier	kcal/mol	15.3683115391		
Delta electron energy	kcal/mol	12.3063660898		
Gibbs Free Energy Barrier	kcal/mol	9.8995670395		
Delta G	kcal/mol	14.1981441360		


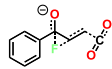
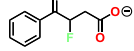
**Table S39:** Thermodynamics data of **19**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1557.81953800	-1557.80090489	-1557.80781555
ZPE (M05-2X/SMD)	a.u.	-1557.92900877	-1557.90366315	-1557.90612128
Solvation delta G	kJ/mol	-287.41550664	-269.79181163	-258.10169411
ZPE (M06-2X/IEFPCM)	a.u.	-1556.54072160	-1556.51612949	-1556.52035702
ZPE (double hybrid)	a.u.	-1555.84483822	-1555.83569553	-1555.83281780
ZPE_corr	a.u.	0.402682	0.402069	0.402520
U_corr	a.u.	0.428253	0.427459	0.428255
H_corr	a.u.	0.429197	0.428403	0.429199
G_corr	a.u.	0.341843	0.342266	0.341233
U(T)	a.u.	-1555.4165852171	-1555.4082365322	-1555.4045627951
H(T)	a.u.	-1555.4156412171	-1555.4072925322	-1555.4036187951
G(T)	a.u.	-1555.5029952171	-1555.4934295322	-1555.4915847951
Electron energy barrier	kJ/mol	64.5665848055		
Delta electron energy	kJ/mol	53.4672047905		
Gibbs Free Energy Barrier	kJ/mol	42.7384007111		
Delta G	kJ/mol	59.2718754818		
Electron energy barrier	kcal/mol	15.4317841313		
Delta electron energy	kcal/mol	12.7789686402		
Gibbs Free Energy Barrier	kcal/mol	10.2147229233		
Delta G	kcal/mol	14.1663182318		


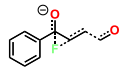
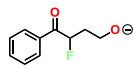
**Table S40:** Thermodynamics data of **20**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1298.78802112	-1298.77426131	-1298.80400300
ZPE (M05-2X/SMD)	a.u.	-1298.88477562	-1298.86410544	-1298.88544668
Solvation delta G	kJ/mol	-254.02893975	-235.88576332	-213.83038184
ZPE (M06-2X/IEFPCM)	a.u.	-1297.53108004	-1297.51124202	-1297.53443425
ZPE (double hybrid)	a.u.	-1297.09227697	-1297.09193053	-1297.10712965
ZPE_corr	a.u.	0.322474	0.321925	0.323491
U_corr	a.u.	0.345668	0.344979	0.346415
H_corr	a.u.	0.346613	0.345923	0.347359
G_corr	a.u.	0.264019	0.264752	0.267044
U(T)	a.u.	-1296.7466089662	-1296.7469515311	-1296.7607146533
H(T)	a.u.	-1296.7456639662	-1296.7460075311	-1296.7597706533
G(T)	a.u.	-1296.8282579662	-1296.8271785311	-1296.8400856533
Electron energy barrier	kJ/mol	52.0847215099		
Delta electron energy	kJ/mol	-8.8064783550		
Gibbs Free Energy Barrier	kJ/mol	20.9772332904		
Delta G	kJ/mol	9.1449654286		
Electron energy barrier	kcal/mol	12.4485472060		
Delta electron energy	kcal/mol	-2.1047988420		
Gibbs Free Energy Barrier	kcal/mol	5.0136790847		
Delta G	kcal/mol	2.1856991942		




**Table S41:** Thermodynamics data of the reaction of **21** and **22**.

Structure			CO <sub>2</sub>		
ZPE (M05-2X/Gas)	a.u.	-522.77478819	-188.55290226	-711.30502637	-711.36104732
ZPE (M05-2X/SMD)	a.u.	-522.87027155	-188.55322108	-711.39147931	-711.46012928
Solvation delta G	kJ/mol	-250.69157481	-0.83707766	-226.98219397	-260.13966235
ZPE (M06-2X/IEFPCM)	a.u.	-522.32728049	-188.37322033	-710.66692025	-710.73464067
ZPE (double hybrid)	a.u.	-522.11771680	-188.36815455	-710.46486579	-710.50588455
ZPE_corr	a.u.	0.145773	0.012012	0.157416	0.163534
U_corr	a.u.	0.155191	0.014629	0.170725	0.175524
H_corr	a.u.	0.156135	0.015574	0.171669	0.176468
G_corr	a.u.	0.110742	-0.008673	0.114985	0.123406
U(T)	a.u.	-521.9625257958	-188.3535255507	-710.2941407903	-710.3303605501
H(T)	a.u.	-521.9615817958	-188.3525805507	-710.2931967903	-710.3294165501
G(T)	a.u.	-522.0069747958	-188.3768275507	-710.3498807903	-710.3824785501
Electron energy barrier	kJ/mol	88.1657707822			
Delta electron energy	kJ/mol	-89.6341761749			
Gibbs Free Energy Barrier	kJ/mol	113.6075043829			
Delta G	kJ/mol	-5.1353823791			
Electron energy barrier	kcal/mol	21.0721249480			
Delta electron energy	kcal/mol	-21.4230822598			
Gibbs Free Energy Barrier	kcal/mol	27.1528452158			
Delta G	kcal/mol	-1.2273858459			




**Table S42:** Thermodynamics data of the reaction of **21** and **23**.

Structure			HCHO		
ZPE (M05-2X/Gas)	a.u.	-522.77478819	-114.47527365	-637.23214750	-637.25447175
ZPE (M05-2X/SMD)	a.u.	-522.87027155	-114.47944252	-637.31948565	-637.35880398
Solvation delta G	kJ/mol	-250.69157481	-10.94537344	-229.30632333	-273.92428824
ZPE (M06-2X/IEFPCM)	a.u.	-522.32728049	-114.36510008	-636.70078348	-636.70191680
ZPE (double hybrid)	a.u.	-522.11771680	-114.35682972	-636.45939476	-636.47540989
ZPE_corr	a.u.	0.145773	0.027211	0.174630	0.179245
U_corr	a.u.	0.155191	0.030077	0.187371	0.190928
H_corr	a.u.	0.156135	0.031021	0.188315	0.191872
G_corr	a.u.	0.110742	0.005552	0.134290	0.139924
U(T)	a.u.	-521.9625257958	-114.3267527239	-636.2720237587	-636.2844818890
H(T)	a.u.	-521.9615817958	-114.3258087239	-636.2710797587	-636.2835378890
G(T)	a.u.	-522.0069747958	-114.3512777239	-636.3251047587	-636.3354858890
Electron energy barrier	kJ/mol	-22.0618507068			
Delta electron energy	kJ/mol	-25.0373718647			
Gibbs Free Energy Barrier	kJ/mol	119.3600714484			
Delta G	kJ/mol	47.4864488766			
Electron energy barrier	kcal/mol	-5.2729088687			
Delta electron energy	kcal/mol	-5.9840754935			
Gibbs Free Energy Barrier	kcal/mol	28.5277417420			
Delta G	kcal/mol	11.3495336703			

**Table S43:** Thermodynamics data of the reaction of **21** and **24**.




Structure			HCHO		
ZPE (M05-2X/Gas)	a.u.	-522.77478819	-114.47526324	-637.22887941	-637.30015905
ZPE (M05-2X/SMD)	a.u.	-522.87027155	-114.47942688	-637.31934410	-637.39327715
Solvation delta G	kJ/mol	-250.69157481	-10.93164470	-237.51503834	-244.48157943
ZPE (M06-2X/IEFPCM)	a.u.	-522.32728049	-114.36510050	-636.69901866	-636.73442086
ZPE (double hybrid)	a.u.	-522.11771680	-114.35681901	-636.45716380	-636.51096522
ZPE_corr	a.u.	0.145773	0.027200	0.174599	0.182237
U_corr	a.u.	0.155191	0.030065	0.187449	0.192917
H_corr	a.u.	0.156135	0.031009	0.188393	0.193862
G_corr	a.u.	0.110742	0.005541	0.133365	0.144816
U(T)	a.u.	-521.9625257958	-114.3267540060	-636.2697148042	-636.3180482221
H(T)	a.u.	-521.9615817958	-114.3258100060	-636.2687708042	-636.3171032221
G(T)	a.u.	-522.0069747958	-114.3512780060	-636.3237988042	-636.3661492221
Electron energy barrier	kJ/mol	-17.4272130870			
Delta electron energy	kJ/mol	-110.3756813106			
Gibbs Free Energy Barrier	kJ/mol	114.5671518854			
Delta G	kJ/mol	-3.5904115248			
Electron energy barrier	kcal/mol	-4.1652038927			
Delta electron energy	kcal/mol	-26.3804209633			
Gibbs Free Energy Barrier	kcal/mol	27.3822064736			
Delta G	kcal/mol	-0.8581289495			

**Table S44:** Thermodynamics data of the reaction of **21** and **25**.


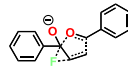
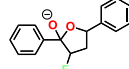
Structure			CH <sub>3</sub> CHO		
ZPE (M05-2X/Gas)	a.u.	-522.77478819	-153.79662761	-676.54589144	-676.62025408
ZPE (M05-2X/SMD)	a.u.	-522.87027155	-153.80381438	-676.63675195	-676.71117263
Solvation delta G	kJ/mol	-250.69157481	-18.86887514	-238.55427951	-238.70666615
ZPE (M06-2X/IEFPCM)	a.u.	-522.32728049	-153.64262547	-675.97337370	-676.00800088
ZPE (double hybrid)	a.u.	-522.11771680	-153.61928002	-675.71347098	-675.77060093
ZPE_corr	a.u.	0.145773	0.055901	0.202886	0.210056
U_corr	a.u.	0.155191	0.059789	0.216813	0.221979
H_corr	a.u.	0.156135	0.060733	0.217758	0.222923
G_corr	a.u.	0.110742	0.030972	0.161592	0.171338
U(T)	a.u.	-521.9625257958	-153.5594910155	-675.4966579797	-675.5486219350
H(T)	a.u.	-521.9615817958	-153.5585470155	-675.4957129797	-675.5476779350
G(T)	a.u.	-522.0069747958	-153.5883080155	-675.5518789797	-675.5992629350
Electron energy barrier	kJ/mol	-9.1045644974			
Delta electron energy	kJ/mol	-100.0182098344			
Gibbs Free Energy Barrier	kJ/mol	144.9629301987			
Delta G	kJ/mol	20.4039691232			
Electron energy barrier	kcal/mol	-2.1760431399			
Delta electron energy	kcal/mol	-23.9049258686			
Gibbs Free Energy Barrier	kcal/mol	34.6469718448			
Delta G	kcal/mol	4.8766656604			




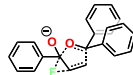
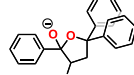
**Table S45:** Thermodynamics data of the reaction of **21** and **26**.

Structure			CH <sub>3</sub> COCH <sub>3</sub>		
ZPE (M05-2X/Gas)	a.u.	-522.77478819	-193.11546085	-715.86415875	-715.93463565
ZPE (M05-2X/SMD)	a.u.	-522.87027155	-193.12426270	-715.95304498	-716.02464296
Solvation delta G	kJ/mol	-250.69157481	-23.10925717	-233.37079424	-236.31419241
ZPE (M06-2X/IEFPCM)	a.u.	-522.32728049	-192.91762108	-715.25274604	-715.27755718
ZPE (double hybrid)	a.u.	-522.11771680	-192.87904601	-714.97064375	-715.02678689
ZPE_corr	a.u.	0.145773	0.083901	0.230686	0.237754
U_corr	a.u.	0.155191	0.089234	0.245979	0.250876
H_corr	a.u.	0.156135	0.090178	0.246924	0.251820
G_corr	a.u.	0.110742	0.055908	0.187404	0.198610
U(T)	a.u.	-521.9625257958	-192.7898120056	-714.7246647503	-714.7759108863
H(T)	a.u.	-521.9615817958	-192.7888680056	-714.7237197503	-714.7749668863
G(T)	a.u.	-522.0069747958	-192.8231380056	-714.7832397503	-714.8281768863
Electron energy barrier	kJ/mol	-20.5956533596			
Delta electron energy	kJ/mol	-85.7372883019			
Gibbs Free Energy Barrier	kJ/mol	163.4952334587			
Delta G	kJ/mol	42.5693846990			
Electron energy barrier	kcal/mol	-4.9224792924			
Delta electron energy	kcal/mol	-20.4917037050			
Gibbs Free Energy Barrier	kcal/mol	39.0762986278			
Delta G	kcal/mol	10.1743271269			



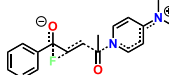
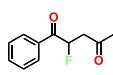

**Table S46:** Thermodynamics data of the reaction of **21** and **27**.

Structure			C <sub>6</sub> H <sub>5</sub> CHO		
ZPE (M05-2X/Gas)	a.u.	-522.77478819	-345.52810710	-868.27998367	-868.35504290
ZPE (M05-2X/SMD)	a.u.	-522.87027155	-345.54089581	-868.37558405	-868.44802155
Solvation delta G	kJ/mol	-250.69157481	-33.57675811	-250.99880032	-244.11545608
ZPE (M06-2X/IEFPCM)	a.u.	-522.32728049	-345.17365197	-867.50618829	-867.53977854
ZPE (double hybrid)	a.u.	-522.11771680	-345.05268763	-867.15228545	-867.20790248
ZPE_corr	a.u.	0.145773	0.111093	0.257102	0.263947
U_corr	a.u.	0.155191	0.117354	0.274068	0.278953
H_corr	a.u.	0.156135	0.118298	0.275012	0.279898
G_corr	a.u.	0.110742	0.080578	0.210475	0.220462
U(T)	a.u.	-521.9625257958	-344.9353336255	-866.8782174544	-866.9289494788
H(T)	a.u.	-521.9615817958	-344.9343896255	-866.8772734544	-866.9280044788
G(T)	a.u.	-522.0069747958	-344.9721096255	-866.9418104544	-866.9874404788
Electron energy barrier	kJ/mol	-13.7992052946			
Delta electron energy	kJ/mol	-101.9903935421			
Gibbs Free Energy Barrier	kJ/mol	131.1323325880			
Delta G	kJ/mol	18.2140477909			
Electron energy barrier	kcal/mol	-3.2980892195			
Delta electron energy	kcal/mol	-24.3762890875			
Gibbs Free Energy Barrier	kcal/mol	31.3413796816			
Delta G	kcal/mol	4.3532619003			


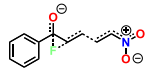
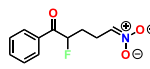
**Table S47:** Thermodynamics data of the reaction of **21** and **28**.

Structure			$C_6H_5COC_6H_5$		
ZPE (M05-2X/Gas)	a.u.	-522.77478819	-576.57055597	-1099.32338466	-1099.39431656
ZPE (M05-2X/SMD)	a.u.	-522.87027155	-576.58971426	-1099.42001454	-1099.48998652
Solvation delta G	kJ/mol	-250.69157481	-50.30007202	-253.70174994	-251.18147998
ZPE (M06-2X/IEFPCM)	a.u.	-522.32728049	-575.97250424	-1098.26756456	-1098.33536421
ZPE (double hybrid)	a.u.	-522.11771680	-575.73991917	-1097.84007911	-1097.89380577
ZPE_corr	a.u.	0.145773	0.193475	0.339074	0.345498
U_corr	a.u.	0.155191	0.204108	0.360448	0.364970
H_corr	a.u.	0.156135	0.205052	0.361393	0.365914
G_corr	a.u.	0.110742	0.156013	0.286406	0.296467
U(T)	a.u.	-521.9625257958	-575.5358111672	-1097.4796311086	-1097.5288357707
H(T)	a.u.	-521.9615817958	-575.5348671672	-1097.4786861086	-1097.5278917707
G(T)	a.u.	-522.0069747958	-575.5839061672	-1097.5536731086	-1097.5973387707
Electron energy barrier	kJ/mol	84.5940642116			
Delta electron energy	kJ/mol	-93.4139168636			
Gibbs Free Energy Barrier	kJ/mol	144.9791186639			
Delta G	kJ/mol	32.8551927803			
Electron energy barrier	kcal/mol	20.2184665898			
Delta electron energy	kcal/mol	-22.3264619655			
Gibbs Free Energy Barrier	kcal/mol	34.6508409808			
Delta G	kcal/mol	7.8525795364			

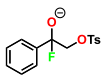
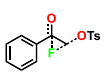
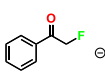
**Table S48:** Thermodynamics data of the reaction of **21** and **29**.

Structure						
ZPE (M05-2X/Gas)	a.u.	-522.77478819	-535.22560396	-1058.09769515	-675.99204777	-382.20283048
ZPE (M05-2X/SMD)	a.u.	-522.87027155	-535.31499060	-1058.15582881	-676.01269179	-382.21887469
Solvation delta G	kJ/mol	-250.69157481	-234.68462595	-152.62992433	-54.20087714	-42.12408648
ZPE (M06-2X/IEFPCM)	a.u.	-522.32728049	-534.73724526	-1057.04312189	-675.30405308	-381.80935035
ZPE (double hybrid)	a.u.	-522.11771680	-534.50319629	-1056.71848374	-675.13813399	-381.66519353
ZPE_corr	a.u.	0.145773	0.214555	0.360924	0.198628	0.163213
U_corr	a.u.	0.155191	0.226554	0.383584	0.211550	0.171700
H_corr	a.u.	0.156135	0.227498	0.384528	0.212494	0.172644
G_corr	a.u.	0.110742	0.175760	0.307564	0.157637	0.129765
U(T)	a.u.	-521.9625257958	-534.2766422895	-1056.3348997371	-674.9265839939	-381.4934935264
H(T)	a.u.	-521.9615817958	-534.2756982895	-1056.3339557371	-674.9256399939	-381.4925495264
G(T)	a.u.	-522.0069747958	-534.3274362895	-1056.4109197371	-674.9804969939	-381.5354285264
Electron energy barrier	kJ/mol	56.1958396808				
Delta electron energy	kJ/mol	-128.3283383376				
Gibbs Free Energy Barrier	kJ/mol	131.8728112531				
Delta G	kJ/mol	-87.5149118782				
Electron energy barrier	kcal/mol	13.4311280308				
Delta electron energy	kcal/mol	-30.6712089717				
Gibbs Free Energy Barrier	kcal/mol	31.5183583301				
Delta G	kcal/mol	-20.9165659365				

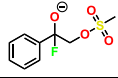
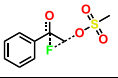


**Table S49:** Thermodynamics data of the reaction of **21** and **30**.

Structure			CH <sub>2</sub> CHNO <sub>2</sub>		
ZPE (M05-2X/Gas)	a.u.	-522.77478819	-283.03814450	-805.80161146	-805.87592820
ZPE (M05-2X/SMD)	a.u.	-522.87027155	-283.04659078	-805.88944510	-805.96888340
Solvation delta G	kJ/mol	-250.69157481	-22.17571339	-230.60721394	-244.05388548
ZPE (M06-2X/IEFPCM)	a.u.	-522.32728049	-282.75729771	-805.06116946	-805.14201849
ZPE (double hybrid)	a.u.	-522.11771680	-282.73135176	-804.84102977	-804.90025427
ZPE_corr	a.u.	0.145773	0.055971	0.202055	0.208541
U_corr	a.u.	0.155191	0.060631	0.217398	0.222712
H_corr	a.u.	0.156135	0.061575	0.218343	0.223657
G_corr	a.u.	0.110742	0.028172	0.158525	0.165728
U(T)	a.u.	-521.9625257958	-282.6707207625	-804.6236317654	-804.6775422724
H(T)	a.u.	-521.9615817958	-282.6697767625	-804.6226867654	-804.6765972724
G(T)	a.u.	-522.0069747958	-282.7031797625	-804.6825047654	-804.7345262724
Electron energy barrier	kJ/mol	61.4596337424			
Delta electron energy	kJ/mol	-150.8094945228			
Gibbs Free Energy Barrier	kJ/mol	114.8546055142			
Delta G	kJ/mol	-35.1745326476			
Electron energy barrier	kcal/mol	14.6892050054			
Delta electron energy	kcal/mol	-36.0443342550			
Gibbs Free Energy Barrier	kcal/mol	27.4509095397			
Delta G	kcal/mol	-8.4069150687			

**Table S50:** Thermodynamics data of the reaction of **31**.

Structure				
ZPE (M05-2X/Gas)	a.u.	-1378.79788270	-1378.77525980	-1378.83756710
ZPE (M05-2X/SMD)	a.u.	-1378.89622400	-1378.87323440	-1378.93155740
Solvation delta G	kJ/mol	-250.26920163	-249.30643078	-238.84565113
ZPE (M06-2X/IEFPCM)	a.u.	-1377.75464940	-1377.72437140	-1377.78963390
ZPE (double hybrid)	a.u.	-1377.35938710	-1377.34911530	-1377.40173130
ZPE_corr	a.u.	0.266249	0.264445	0.265474
U_corr	a.u.	0.285003	0.283602	0.285565
H_corr	a.u.	0.285948	0.284547	0.286510
G_corr	a.u.	0.217990	0.215609	0.214499
U(T)	a.u.	-1377.07438410	-1377.06551330	-1377.11616630
H(T)	a.u.	-1377.07343910	-1377.06456830	-1377.11522130
G(T)	a.u.	-1377.14139710	-1377.13350630	-1377.18723230
Electron energy barrier	kJ/mol	79.49488900		
Delta electron energy	kJ/mol	-91.85180475		
Gibbs Free Energy Barrier	kJ/mol	21.68006625		
Delta G	kJ/mol	-108.91676710		
Electron energy barrier	kcal/mol	18.99973446		
Delta electron energy	kcal/mol	-21.95310821		
Gibbs Free Energy Barrier	kcal/mol	5.18166019		
Delta G	kcal/mol	-26.03173210		

**Table S51:** Thermodynamics data of the reaction of **32**.

Structure					
ZPE (M05-2X/Gas)	a.u.	-1147.76714490	-1147.74067650	-484.06053320	-663.71424230
ZPE (M05-2X/SMD)	a.u.	-1147.85890140	-1147.83234830	-484.07503940	-663.80698220
Solvation delta G	kJ/mol	-232.98080923	-232.75842938	-30.16014658	-235.56272593
ZPE (M06-2X/IEFPCM)	a.u.	-1146.96315630	-1146.92914870	-483.56788820	-663.40794030
ZPE (double hybrid)	a.u.	-1146.67917830	-1146.66643730	-483.45032990	-663.24197410
ZPE_corr	a.u.	0.185253	0.183262	0.132542	0.050853
U_corr	a.u.	0.199009	0.197658	0.140919	0.055847
H_corr	a.u.	0.199953	0.198602	0.141863	0.056791
G_corr	a.u.	0.144564	0.139859	0.098306	0.022629
U(T)	a.u.	-1146.48016930	-1146.46877930	-483.30941090	-663.18612710
H(T)	a.u.	-1146.47922530	-1146.46783530	-483.30846690	-663.18518310
G(T)	a.u.	-1146.53461430	-1146.52657830	-483.35202390	-663.21934510
Electron energy barrier	kJ/mol	89.28695380			
Delta electron energy	kJ/mol	-33.27086110			
Gibbs Free Energy Barrier	kJ/mol	21.32089785			
Delta G	kJ/mol	-129.24152813			
Electron energy barrier	kcal/mol	21.34009412			
Delta electron energy	kcal/mol	-7.95192665			
Gibbs Free Energy Barrier	kcal/mol	5.09581689			
Delta G	kcal/mol	-30.88946657			

**Table S52:** Thermodynamics data of the reaction of **33**.

Structure					I <sup>-</sup>
ZPE (M05-2X/Gas)	a.u.	-781.40195350	-781.39101820	-484.06053320	-297.74503850
ZPE (M05-2X/SMD)	a.u.	-781.49091390	-781.47943800	-484.07503940	-297.84671810
Solvation delta G	kJ/mol	-225.63964868	-224.22030338	-30.16014658	-259.03390828
ZPE (M06-2X/IEFPCM)	a.u.	-781.32296510	-781.30564550	-483.56788820	-297.80569510
ZPE (double hybrid)	a.u.	-780.87181130	-780.86666390	-483.45032990	-297.44266230
ZPE_corr	a.u.	0.130749	0.129956	0.132542	0.000000
U_corr	a.u.	0.140757	0.140241	0.140919	0.001416
H_corr	a.u.	0.141701	0.141186	0.141863	0.002360
G_corr	a.u.	0.092491	0.091426	0.098306	-0.016848
U(T)	a.u.	-780.73105430	-780.72642290	-483.30941090	-297.44124630
H(T)	a.u.	-780.73011030	-780.72547790	-483.30846690	-297.44030230
G(T)	a.u.	-780.77932030	-780.77523790	-483.35202390	-297.45951030
Electron energy barrier	kJ/mol	45.47260980			
Delta electron energy	kJ/mol	-132.89808410			
Gibbs Free Energy Barrier	kJ/mol	12.1376864998			
Delta G	kJ/mol	-148.1320006295			
Electron energy barrier	kcal/mol	10.86821458			
Delta electron energy	kcal/mol	-31.76340442			
Gibbs Free Energy Barrier	kcal/mol	2.9009766969			
Delta G	kcal/mol	-35.4043978560			