Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information for Post-Transition State Bifurcations Induce Dynamical Detours in Pummerer-Like Reactions

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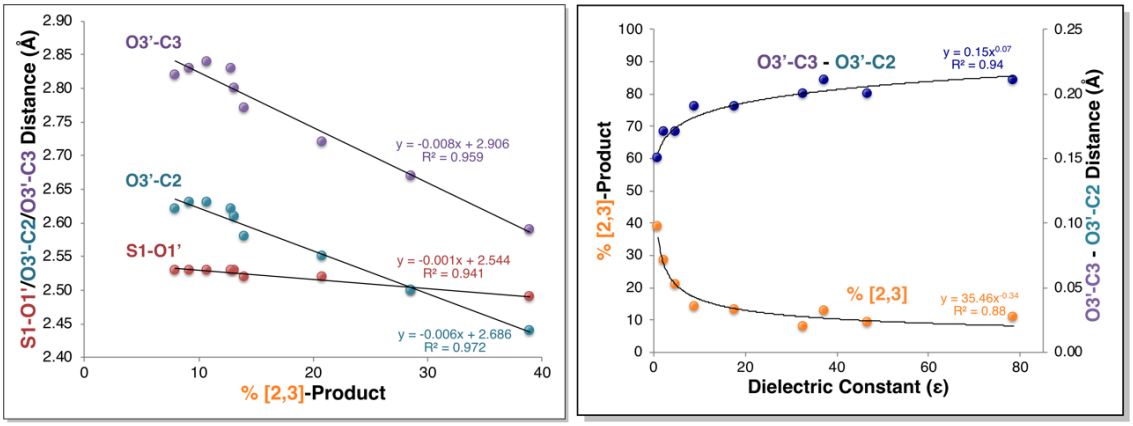
Molecular Dynamics Numerical Data

			MD Results			*TS1 Distances (Å)*		
		ε	[2,3]	[3,3]	# of trajectories	S1-O1'	O3'-C2	O3'-C3
increasing dielectric constant ↓	**gas phase**	1	39%	61%	252	2.49	2.44	2.59
	toluene	2.4	29%	71%	123	2.50	2.50	2.67
	$CHCl_3$	4.8	21%	79%	226	2.52	2.55	2.72
	DCM	9.1	14%	86%	164	2.52	2.58	2.77
	butanol	17.8	13%	87%	199	2.53	2.61	2.80
	methanol	32.6	8%	92%	178	2.53	2.62	2.82
	DMF	37.2	13%	87%	235	2.53	2.62	2.83
	DMSO	46.8	9%	91%	196	2.53	2.63	2.83
	H_2O	78.5	11%	89%	169	2.53	2.63	2.84

Figure S1. Numerical data from molecular dynamics simulations used to make Figure 4.

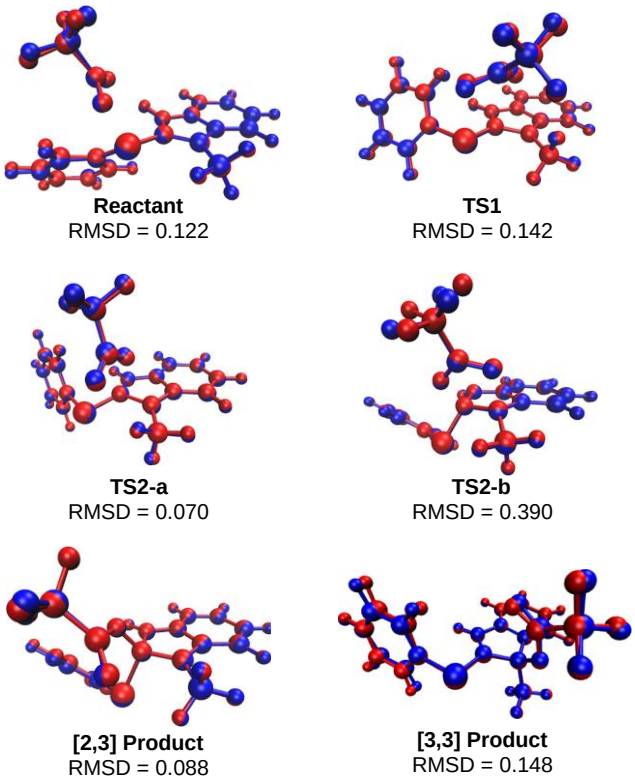
Additional Correlation Plots

Outcomes of molecular dynamics trajectories initiated from **TS1** (**R** = CH_3) in the gas phase and in various implicit solvents (PCM). Three bond distances were correlated with the percentage of trajectories forming the [2,3] product: S-O, O-C1', and O-C2' (red, cyan, and purple dots, respectively). The plot in the left shows a simple linear, inverse relationship between each distance and percentage of [2,3] product formed. The plot on the right shows the correlation between dielectric constant and [2,3] product paired with the correlation between dielectric constant and the difference between the O3'-C2 and O3'-C3 distances.



Stationary points overlaid

Overlay of stationary points from Figure 3 in the main text optimized in the gas phase (red) and in water (blue). Root mean square deviations (RMSDs) between the gas phase and water structures are reported in Å.



Full breakdown of trajectory results

The trajectory results detailed below show the results of all trajectories calculated for a given system. The column heading represents the direction a certain percentage of trajectories went; e.g., the **Reactant → Reactant** column in the first row of data indicates that 1% of trajectories in the gas phase were recrossing trajectories that generated the reactant when propagated both forward and backward in time. The trajectories discussed in the main text were specifically productive trajectories, i.e., those that progressed toward the reactant structure on one side and either the [2,3] or [3,3] product on the other. These tables illustrate the total number of various types of recrossing trajectories in addition to the productive trajectories.

Original Systems

R-group	Solvent	**Reactant → [2,3]**	**Reactant → [3,3]**	**Reactant → Reactant**	**[2,3] → [2,3]**	**[3,3] → [3,3]**	**[2,3] → [3,3]**	Total Number of Trajectories
CH_3	***Gas Phase***	**37%**	**58%**	1%	0%	0.4%	3%	264
	Toluene	**27%**	**65%**	2%	0%	4%	2%	128
	Chloroform	**20%**	**75%**	2%	0%	3%	1%	232
	Dichloromethane	**14%**	**83%**	1%	0%	1%	1%	167
	1-Butanol	**13%**	**84%**	1%	0%	2%	1%	202
	Methanol	**7%**	**87%**	3%	1%	3%	0%	183
	Dimethylformamide	**12%**	**81%**	0.4%	0%	4%	2%	241
	Dimethylsulfoxide	**9%**	**88%**	0%	0%	3%	0%	196

	Water	**10%**	**85%**	2%	1%	2%	1%	174
H	***Gas Phase***	**2%**	**92%**	5%	0%	1%	1%	145
	Water	**0%**	**92%**	5%	0%	3%	0%	113
t-butyl	***Gas Phase***	**46%**	**53%**	1%	0%	0%	1%	136
	Water	**7%**	**58%**	34%	0%	1%	0%	158
CF_3	***Gas Phase***	**2%**	**93%**	2%	0%	1%	2%	153
	Water	**3%**	**89%**	5%	0%	2%	1%	123

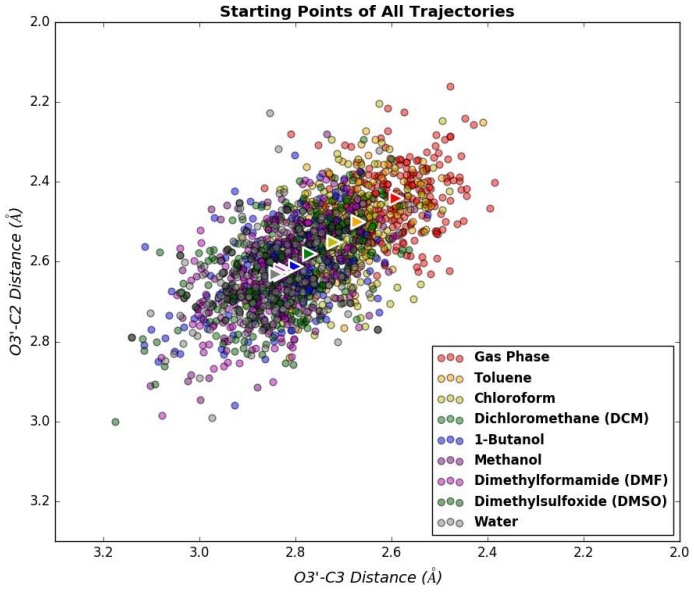
Benzothiophene System

Solvent	**Reactant → [2,3]**	**Reactant → [3,3]**	**Reactant → Reactant**	**[2,3] → [2,3]**	**[3,3] → [3,3]**	**[2,3] → [3,3]**	Total Number of Trajectories
Gas Phase	**23%**	**39%**	7%	5%	1%	24s%	82

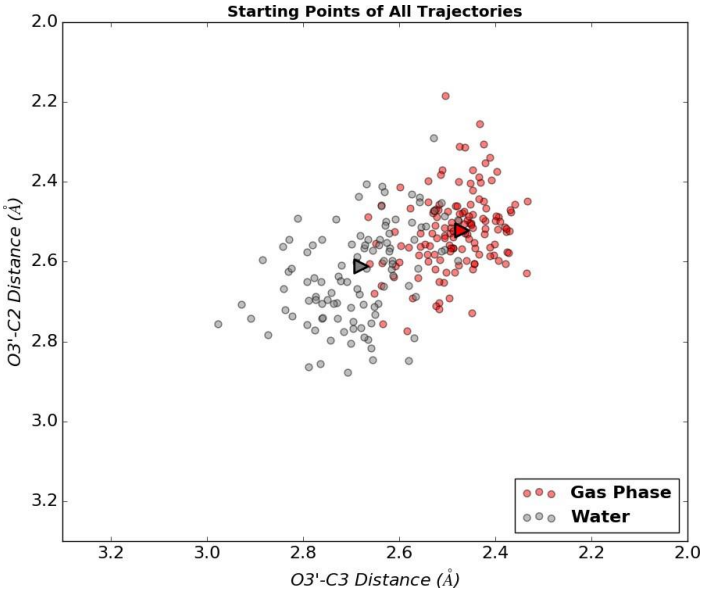
Starting points of trajectories

The plots below show the starting points for all trajectories, colored by the implicit solvent in which the TSSs were optimized and the trajectories were run. The triangles correspond to the locations of the optimized TSSs, whose vibrational modes were populated with a random amount of kinetic and potential energy to generate the scattered points in each specific solvent.

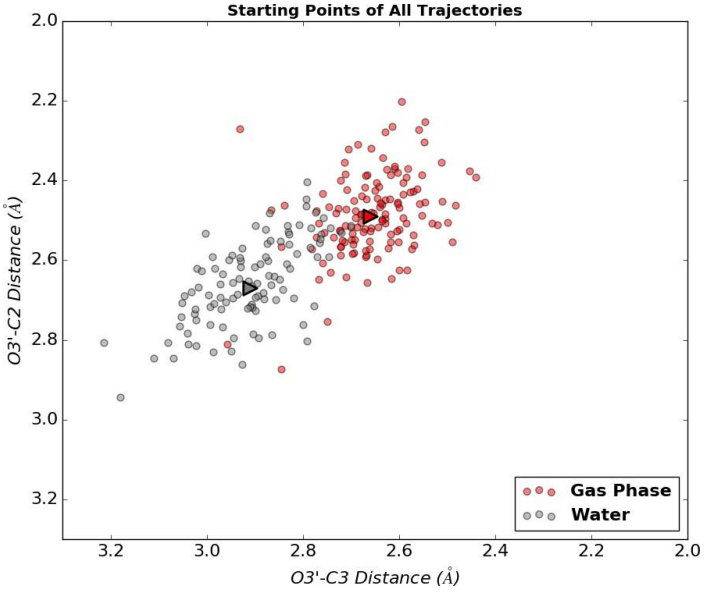
R = CH_3



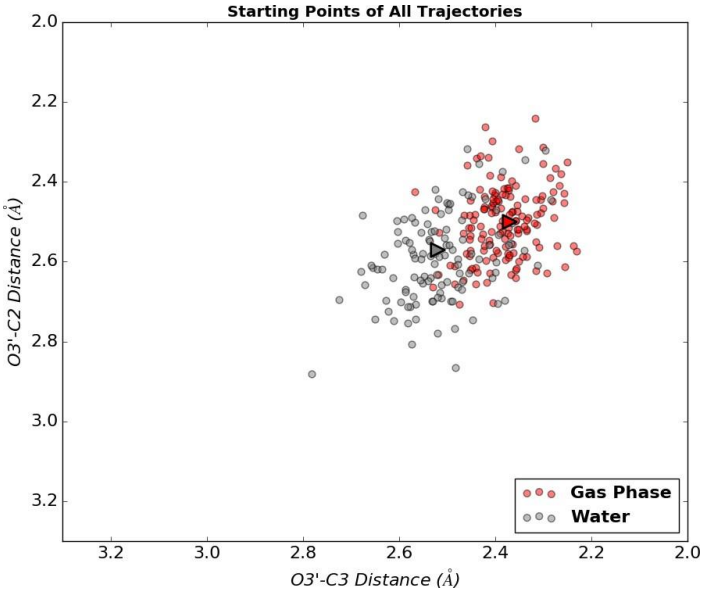
R = *H*


Starting Points of All Trajectories
O3'-C2 Distance (Å)
O3'-C3 Distance (Å)
Gas Phase
Water
2.0
2.2
2.4
2.6
2.8
3.0
3.2

R = *t-Bu*


Starting Points of All Trajectories
O3'-C2 Distance (Å)
O3'-C3 Distance (Å)
Gas Phase
Water
2.0
2.2
2.4
2.6
2.8
3.0
3.2

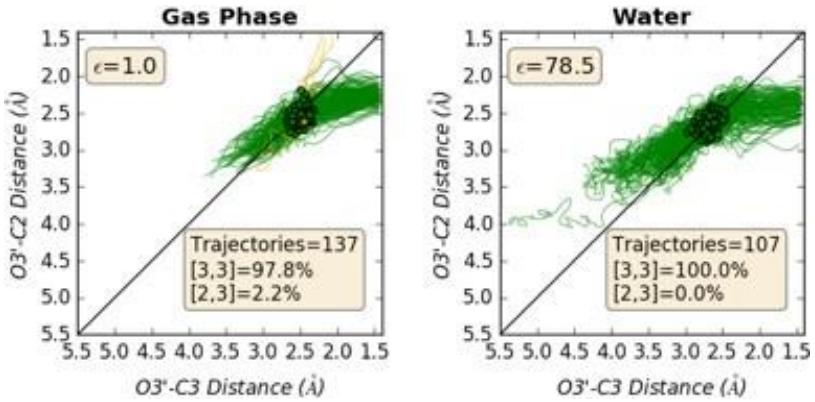
R = CF_3



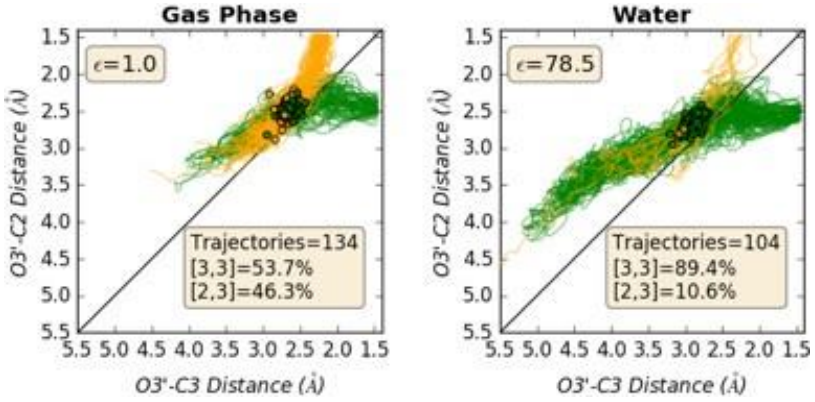
Paths of trajectories in R-group substituted systems

Paths of trajectories, with respect to O3'-C2 and O3'-C3 distances (see Figure 7 of the main text to see these results for the **R** = CH_3 system). The plots show the starting points (clustered points) of all trajectories for each system and their geometric changes along the trajectories colored by the product made: yellow-orange for [2,3] product (top region of the graphs, where the O3'-C2 distance is small) and green for [3,3] product (top right region of the graphs, where the O3'-C3 distance is small). The bottom left region of the graphs corresponds to the reactant side of the trajectories.

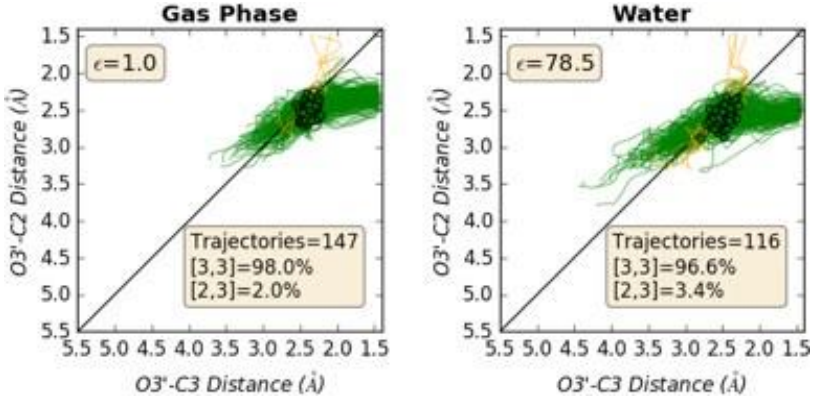
***R** = H*



***R** = t-Bu*

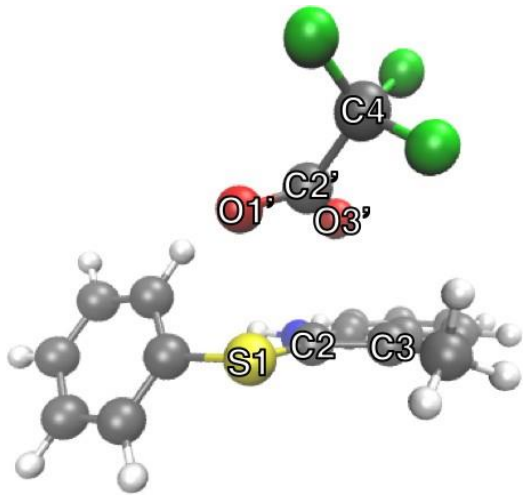


R = CF_3

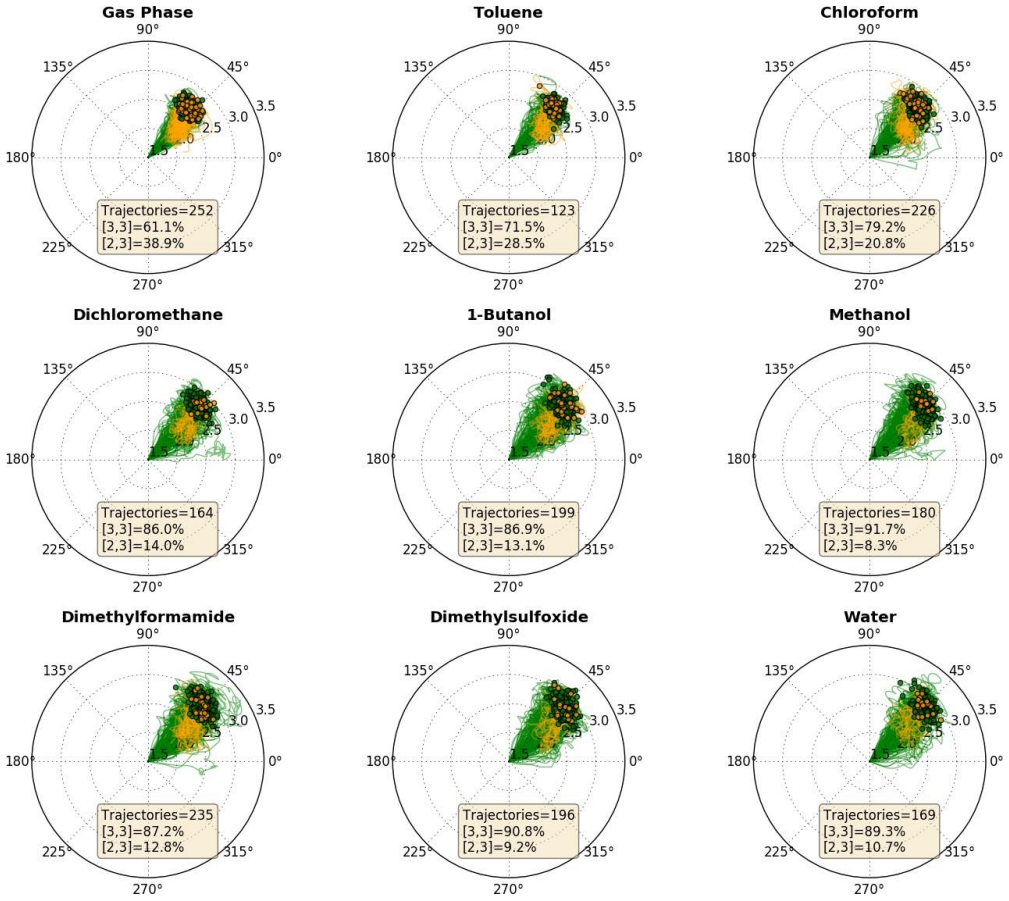


Pericyclic vs. Pseudopericyclic Discussion and Polar Plots

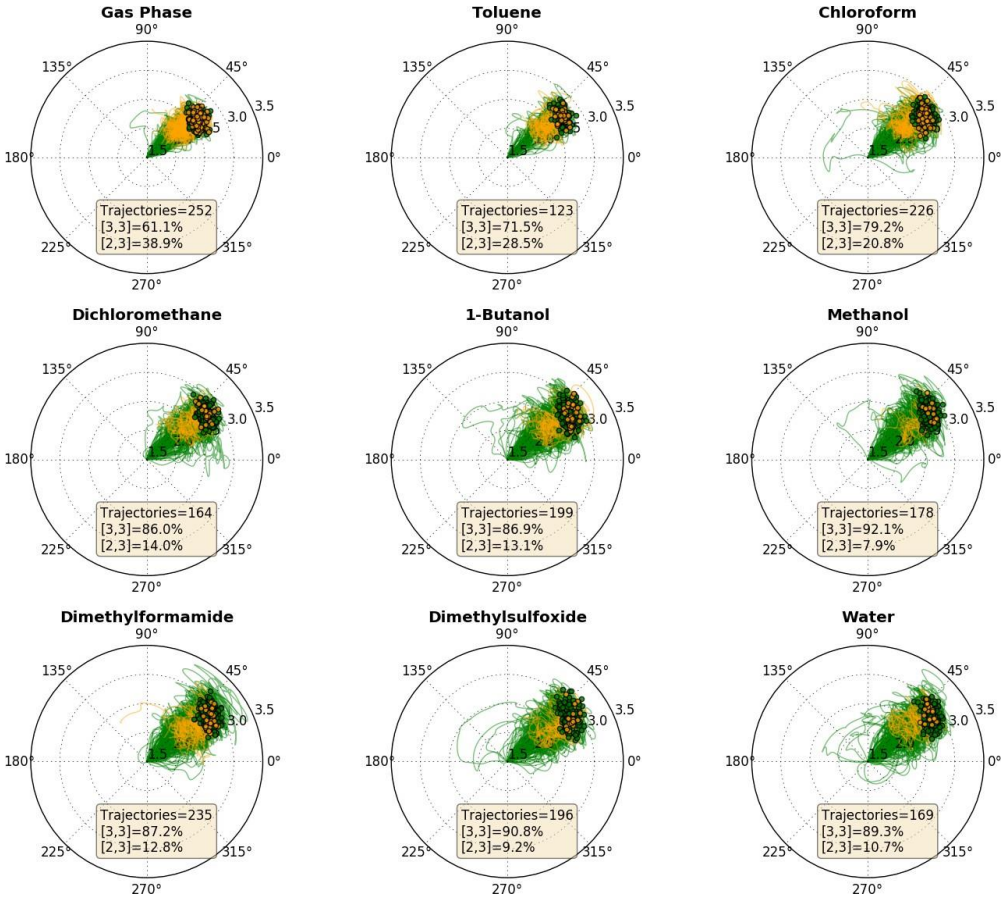
The picture below shows a ball-and-stick image of **TS1** showing atom numbering. Below the ball-and-stick picture is a plot of the dihedral angle S1-O1'-C2'-C4 vs. O3'-C3 distance (θ and r, respectively) and below that is a plot of the angle between π planes defined by O1'-C2'-O3' and S1-C2-C3 vs. O3'-C3 (θ and r, respectively). Both of the sets of plots only show the halves of the trajectories that are going in the product direction. The angle between planes is consistently somewhere between 0º and 90º, making it not straightforward to define pseudopericyclic vs. pericyclic. It is posited that this reaction can be viewed as pericyclic, with secondary orbital overlap causing the "tilt" of the migrating trifluoroacetyl group.



S1-O1'-C2'-C4 Dihedral Angle vs. O3'-C3 Distance Plots



Angle Between the Plane Containing O1'-C2'-O3' and the Plane Containing S1-C2-C3 vs. O3'-C3 Distance Plots



Electrostatic Potential Maps

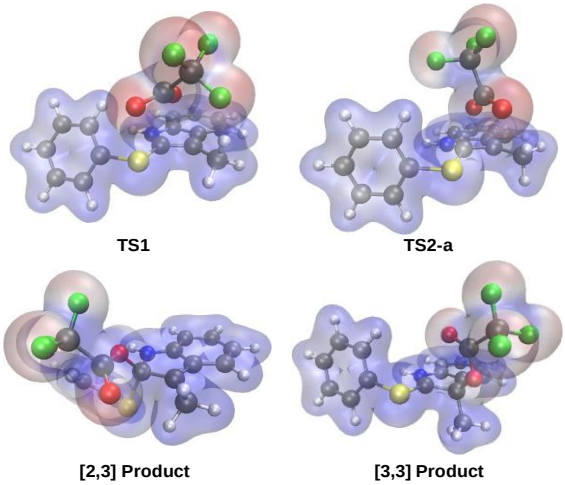


Figure **S2**. Electrostatic potential (ESP) maps of TS1, TS2-a, and [2,3] and [3,3] products in the gas phase using an isovalue of 0.02 and a charge range of 0.06 to 0.2.

Conservation of Energy Along Trajectories

To check whether the total energy of the system was conserved over the length of the trajectories, the total energy was plotted over time for a large (top graph, below) and small (bottom graph, below) subset of trajectories in the gas phase for the parent (R=CH_3) system. The oscillations seen are likely due to the fact that velocities were calculated using a linear path between points, which Progdyn's Verlet algorithm does not assume when calculating velocities on the fly. As can best be seen in the smaller subset of trajectories in the bottom plot, there is some amount of drift in the total energy of the system (on the order of 2-3 kcal/mol), which could potentially be eradicated by using a smaller time step. A related case: *J. Am. Chem. Soc.* **2006**, *128*, 7594-7607 (see Supporting Information)

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Average total energy over all trajectories in this set = 181.52 kcal/mol
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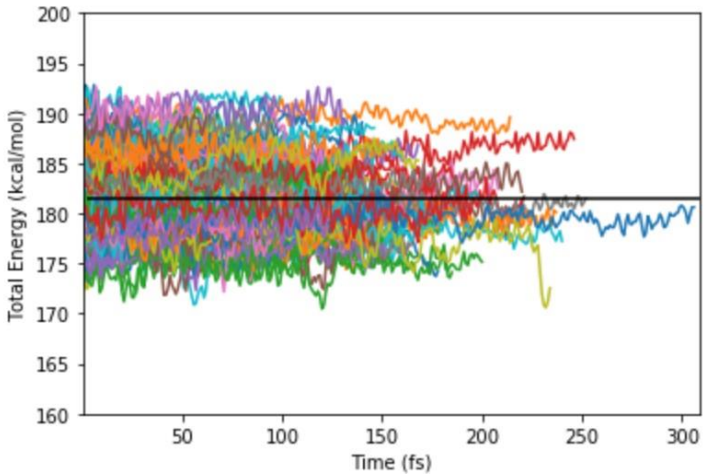
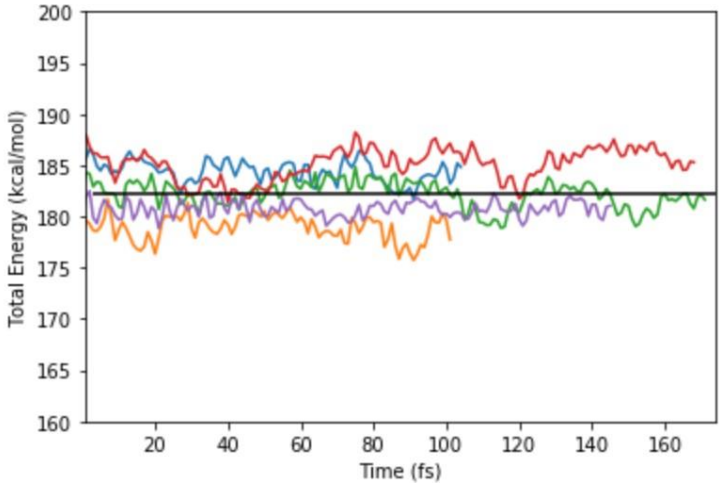


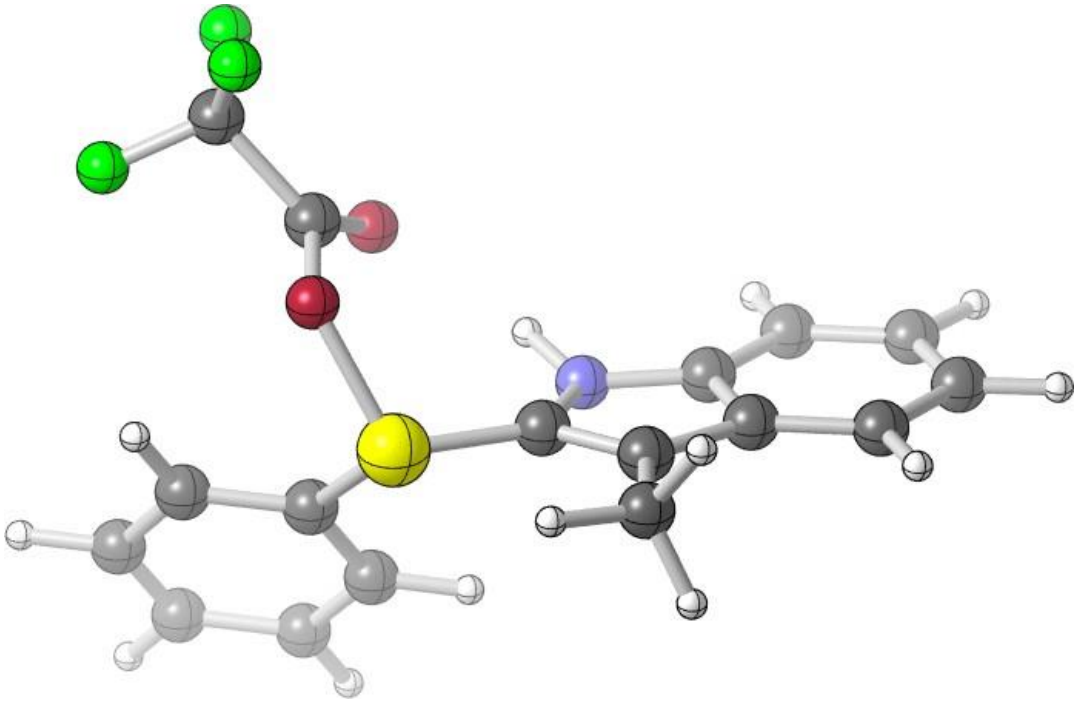
Average total energy over all trajectories in this set = 182.27 kcal/mol



Cartesian Coordinates, Electronic, and Free Energies of Optimized Structures

R = CH_3

Reactant, Gas Phase

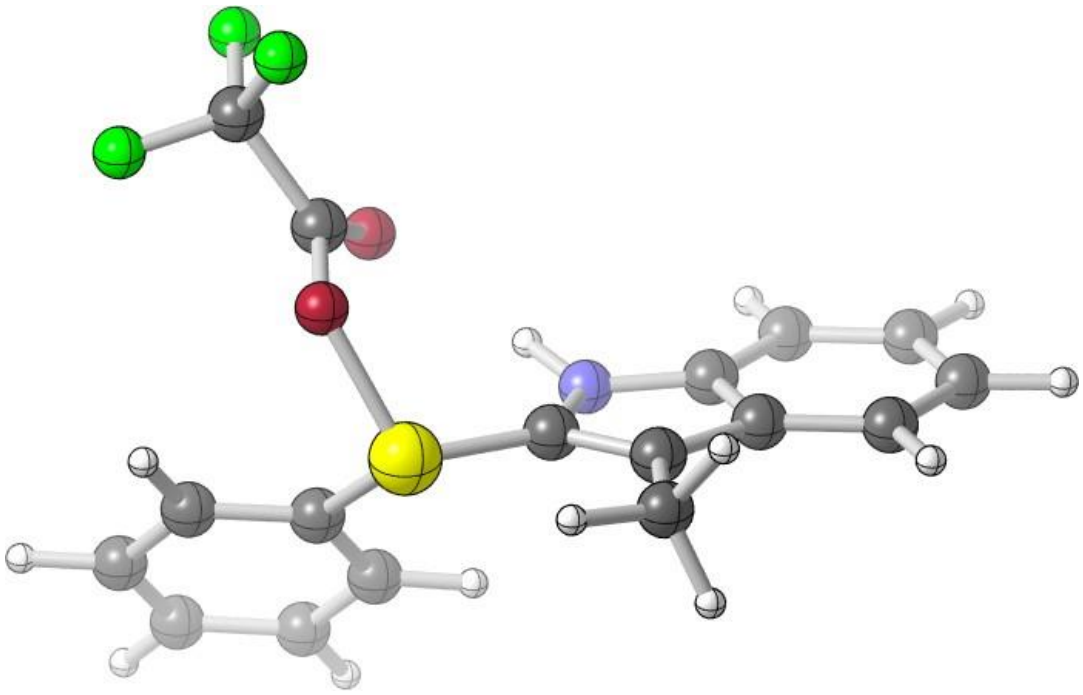


HF = -1558.2742808 hartrees (-977832.693944808 kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.057735 hartrees (-977696.80928985 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-2.772578	0.094480	0.859705
2	6	-3.342258	0.189804	-0.448464
3	6	-4.731312	0.435175	-0.591943
4	6	-5.486468	0.601638	0.548231
5	6	-4.892917	0.523087	1.837368
6	6	-3.542682	0.269056	2.016840
7	6	-1.133103	-0.206320	-0.626028
8	6	-2.301377	0.026676	-1.394514
9	1	-5.183488	0.496621	-1.576789
10	1	-6.550926	0.796913	0.470678
11	1	-5.522117	0.663644	2.711162
12	1	-3.104119	0.205123	3.007279
13	1	-0.721716	-0.006815	1.432957
14	7	-1.434325	-0.185983	0.732429
15	16	0.386997	-0.449217	-1.317671
16	8	1.491988	0.953800	-0.990363
17	6	1.250653	-1.706658	-0.361264
18	6	2.648133	-1.743736	-0.453171
19	6	0.519894	-2.711843	0.281448
20	6	3.323905	-2.799825	0.154204
21	1	3.201261	-0.960681	-0.960615
22	6	1.219962	-3.763325	0.873683
23	1	-0.562469	-2.682936	0.324679
24	6	2.613933	-3.806771	0.814328
25	1	4.407590	-2.834884	0.106114
26	1	0.668617	-4.547967	1.382070
27	1	3.149221	-4.628740	1.279241
28	6	-2.439904	0.046937	-2.882719
29	1	-2.920492	0.977909	-3.203697
30	1	-1.480415	-0.032065	-3.399333
31	1	-3.075428	-0.779185	-3.223618
32	6	1.703763	1.358941	0.279355
33	8	1.120733	0.992847	1.265997
34	6	2.889703	2.363933	0.300595
35	9	3.017514	2.881842	1.515626
36	9	4.009191	1.691942	-0.020816
37	9	2.692957	3.339744	-0.588743

Reactant, PCM H_2O

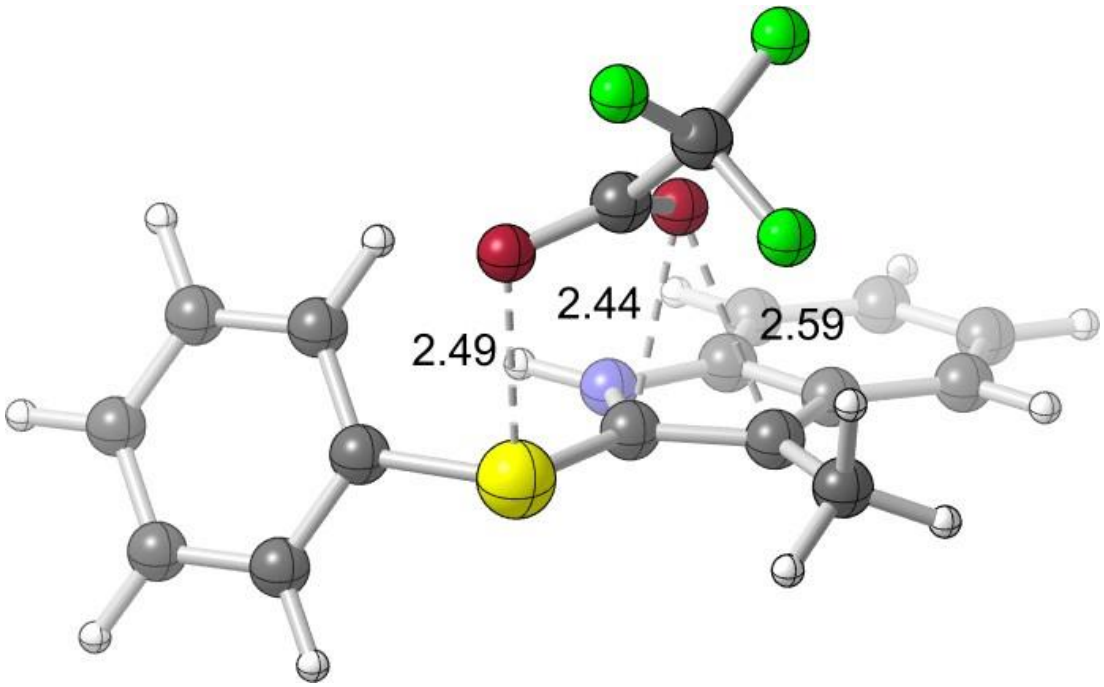


HF=-1558.3374266 hartrees (-977872.318565766 kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.123024 hartrees (-977737.77879024 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.744152	-0.047192	-0.847213
2	6	-3.302691	-0.180780	0.462612
3	6	-4.687666	-0.444839	0.611224
4	6	-5.450881	-0.588986	-0.527042
5	6	-4.868494	-0.470603	-1.819132
6	6	-3.522657	-0.199903	-2.003272
7	6	-1.098957	0.241458	0.629873
8	6	-2.257895	-0.026006	1.403918
9	1	-5.128426	-0.535638	1.598689
10	1	-6.512901	-0.796299	-0.446164
11	1	-5.503762	-0.593473	-2.691145
12	1	-3.089839	-0.105255	-2.993140
13	1	-0.711356	0.137351	-1.450049
14	7	-1.411288	0.239892	-0.723415
15	16	0.412706	0.500169	1.325430
16	8	1.541838	-0.931070	0.968242
17	6	1.268235	1.757617	0.371644
18	6	2.656633	1.842931	0.541327
19	6	0.547414	2.712539	-0.354123
20	6	3.337074	2.891009	-0.073030
21	1	3.198473	1.104232	1.121335

22	6	1.251214	3.757744	-0.952370
23	1	-0.529427	2.654799	-0.452083
24	6	2.638035	3.845117	-0.818610
25	1	4.414185	2.962037	0.036609
26	1	0.706872	4.502606	-1.523513
27	1	3.175836	4.661353	-1.290372
28	6	-2.381480	-0.078489	2.890736
29	1	-2.872986	-1.009401	3.193052
30	1	-1.414853	-0.022001	3.395485
31	1	-3.002265	0.749980	3.251578
32	6	1.717530	-1.336041	-0.292053
33	8	1.180614	-0.923793	-1.289977
34	6	2.777327	-2.472811	-0.319082
35	9	2.953139	-2.900897	-1.569946
36	9	3.947400	-2.017150	0.154848
37	9	2.376683	-3.500833	0.442675

TS1, Gas Phase

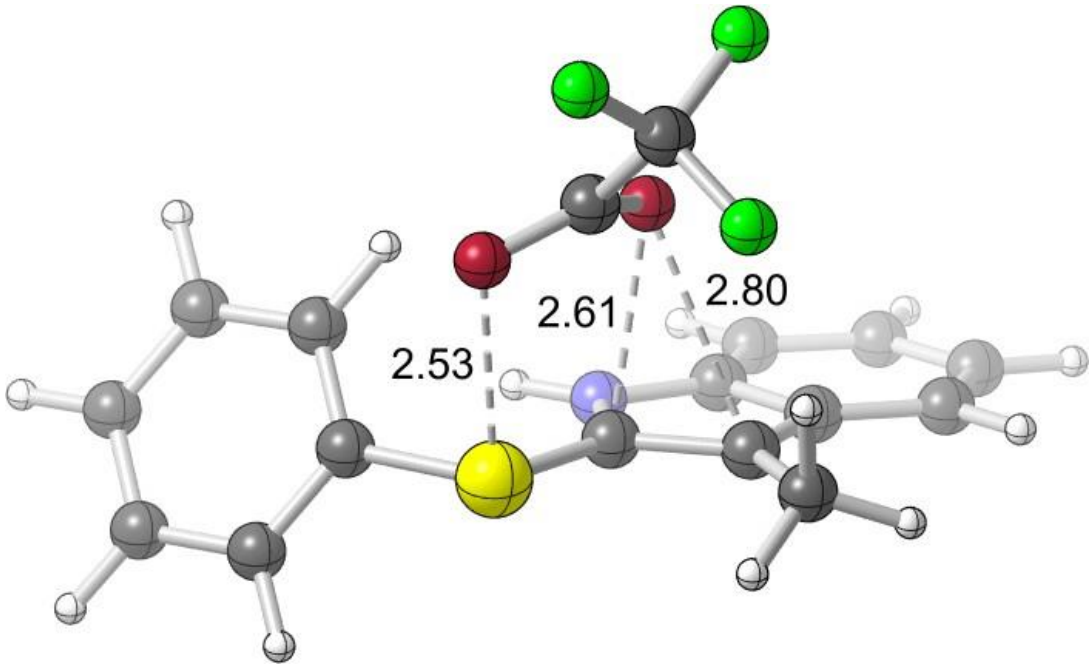


HF=-1558.2564482 hartrees (-977821.503809982 kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.040304 hartrees (-977685.87116304 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.102595	-2.307583	-0.387049

2	6	2.033580	-1.687439	0.508945
3	6	3.384695	-2.129929	0.541587
4	6	3.757184	-3.152889	-0.302856
5	6	2.811737	-3.744296	-1.178776
6	6	1.475709	-3.339660	-1.235616
7	6	-0.022610	-0.715057	0.710903
8	6	1.361382	-0.679815	1.206045
9	1	4.101306	-1.664472	1.210328
10	1	4.780102	-3.512956	-0.308435
11	1	3.139307	-4.546736	-1.833335
12	1	0.774726	-3.811597	-1.915682
13	1	-0.961051	-1.875902	-0.766933
14	7	-0.133712	-1.712570	-0.206851
15	16	-1.238474	0.274020	1.315998
16	8	-0.762862	2.110486	-0.297852
17	6	-2.714104	-0.223981	0.439225
18	6	-2.820186	-0.066588	-0.950923
19	6	-3.778523	-0.701417	1.216077
20	6	-4.012953	-0.438982	-1.569526
21	1	-2.009218	0.385819	-1.510410
22	6	-4.962576	-1.063684	0.575144
23	1	-3.685441	-0.793555	2.293909
24	6	-5.077439	-0.937589	-0.811696
25	1	-4.117864	-0.316188	-2.643105
26	1	-5.794847	-1.439651	1.161674
27	1	-6.005416	-1.214254	-1.302664
28	6	1.889578	0.235177	2.249080
29	1	2.789571	-0.176332	2.711856
30	1	2.151678	1.201267	1.798706
31	1	1.151767	0.431782	3.034295
32	6	0.455448	1.948626	-0.590005
33	8	1.005121	0.848333	-0.858000
34	6	1.372893	3.193217	-0.496687
35	9	2.369567	3.123872	-1.385381
36	9	0.698750	4.328763	-0.679206
37	9	1.927284	3.229279	0.749629

TS1, PCM 1-Butanol

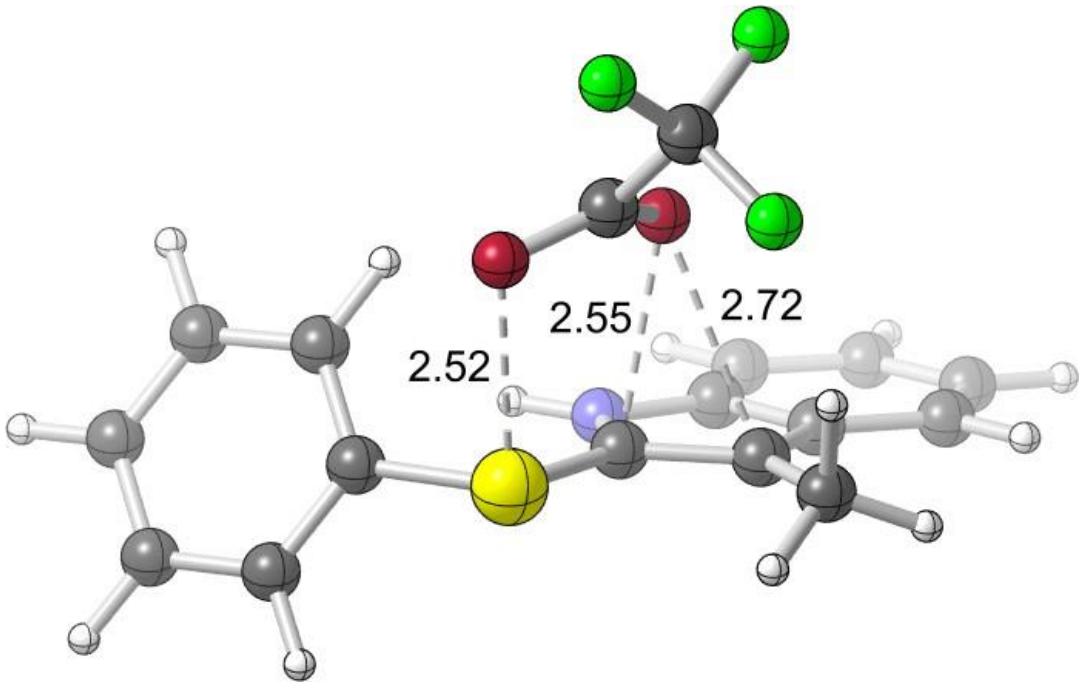


HF=-1558.3266519hartrees(-977865.557333769kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.110898 hartrees (-977730.16960398 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.335529	-2.267118	-0.395592
2	6	2.208045	-1.555035	0.495902
3	6	3.598967	-1.866452	0.526613
4	6	4.060337	-2.856462	-0.309873
5	6	3.168832	-3.543205	-1.175517
6	6	1.799526	-3.267365	-1.233962
7	6	0.060971	-0.811879	0.720613
8	6	1.445283	-0.633206	1.205014
9	1	4.267537	-1.331519	1.191945
10	1	5.111195	-3.122170	-0.317079
11	1	3.567324	-4.318761	-1.822187
12	1	1.142729	-3.809799	-1.903776
13	1	-0.771953	-2.112036	-0.713990
14	7	0.051256	-1.785048	-0.222082
15	16	-1.219989	0.063834	1.346729
16	8	-0.973836	2.110087	-0.114043
17	6	-2.652750	-0.488043	0.445329
18	6	-2.712854	-0.397685	-0.953736
19	6	-3.740115	-0.935425	1.208363
20	6	-3.880097	-0.807337	-1.594008
21	1	-1.880293	0.011940	-1.514298

22	6	-4.898458	-1.337720	0.545372
23	1	-3.680576	-0.978542	2.290858
24	6	-4.966757	-1.277909	-0.848889
25	1	-3.945299	-0.744012	-2.675396
26	1	-5.746118	-1.695376	1.120668
27	1	-5.874014	-1.588417	-1.357597
28	6	1.881466	0.333658	2.240667
29	1	2.854370	0.054002	2.648966
30	1	1.973164	1.335077	1.801456
31	1	1.158900	0.402757	3.060429
32	6	0.208158	2.044393	-0.556843
33	8	0.817077	1.031038	-0.961405
34	6	1.018276	3.368581	-0.491573
35	9	1.959862	3.424261	-1.448572
36	9	0.235494	4.454032	-0.612443
37	9	1.652641	3.458497	0.709149

TS1, PCM $CHCl_3$

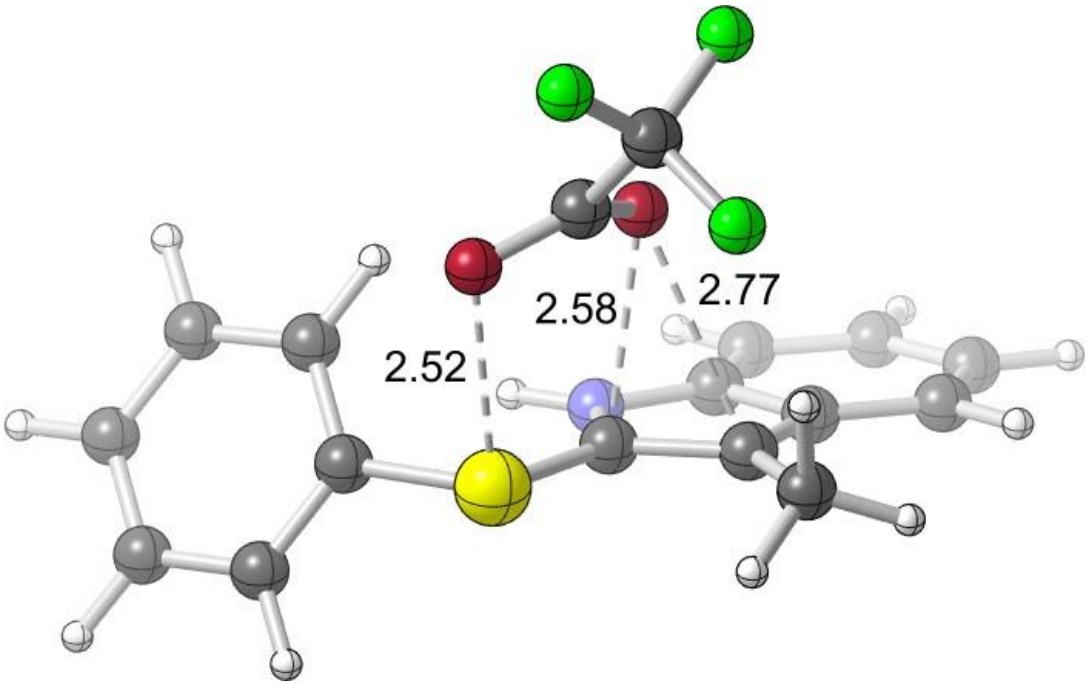


HF=-1558.3131783hartrees(-977857.102515033kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.096850 hartrees (-977721.3543435 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.257425	-2.284338	-0.397805

2	6	2.148330	-1.609999	0.503048
3	6	3.525648	-1.972409	0.540680
4	6	3.958200	-2.971800	-0.300997
5	6	3.050193	-3.617613	-1.179623
6	6	1.692451	-3.292057	-1.243306
7	6	0.030505	-0.781883	0.711370
8	6	1.415741	-0.656067	1.205219
9	1	4.209689	-1.466777	1.213113
10	1	4.999301	-3.273837	-0.302947
11	1	3.425393	-4.400087	-1.832007
12	1	1.021941	-3.803226	-1.923949
13	1	-0.836808	-2.027263	-0.749708
14	7	-0.011259	-1.760647	-0.226354
15	16	-1.229159	0.130052	1.334146
16	8	-0.899845	2.109812	-0.184872
17	6	-2.678309	-0.400417	0.442499
18	6	-2.756744	-0.287654	-0.953806
19	6	-3.758440	-0.852547	1.212901
20	6	-3.935706	-0.679508	-1.584498
21	1	-1.932101	0.134219	-1.516611
22	6	-4.928595	-1.236319	0.559713
23	1	-3.686078	-0.910529	2.294036
24	6	-5.015358	-1.154288	-0.832398
25	1	-4.016412	-0.595438	-2.663490
26	1	-5.771694	-1.595385	1.140849
27	1	-5.932351	-1.448654	-1.333221
28	6	1.883325	0.296610	2.241318
29	1	2.821872	-0.039074	2.686843
30	1	2.057900	1.280160	1.787080
31	1	1.142458	0.432650	3.035635
32	6	0.300874	2.014386	-0.566208
33	8	0.901681	0.973183	-0.917064
34	6	1.142567	3.316358	-0.490083
35	9	2.105011	3.336679	-1.425550
36	9	0.391407	4.418041	-0.632097
37	9	1.751907	3.390864	0.725407

TS1, PCM DCM

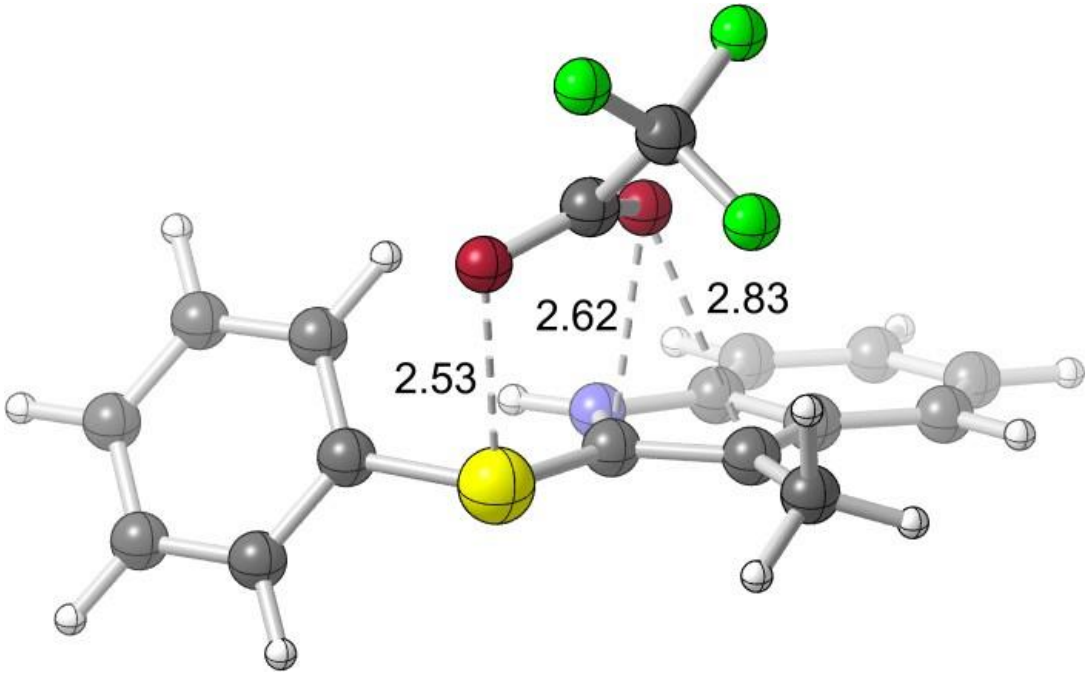


HF=-1558.3217477hartrees(-977862.479899227kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.105664 hartrees (-977726.88521664 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.302463	-2.275414	-0.397435
2	6	2.182392	-1.580500	0.499553
3	6	3.567610	-1.914340	0.534422
4	6	4.017195	-2.907790	-0.304794
5	6	3.119077	-3.575893	-1.177597
6	6	1.754662	-3.278226	-1.239405
7	6	0.047572	-0.800126	0.715518
8	6	1.432088	-0.644916	1.205442
9	1	4.242465	-1.392846	1.204044
10	1	5.063949	-3.189405	-0.308950
11	1	3.507960	-4.353986	-1.827110
12	1	1.092393	-3.806491	-1.915120
13	1	-0.799775	-2.075764	-0.732117
14	7	0.024698	-1.775066	-0.225756
15	16	-1.223616	0.093503	1.338004
16	8	-0.940963	2.107394	-0.149980
17	6	-2.664582	-0.449731	0.442900
18	6	-2.734928	-0.350940	-0.954966
19	6	-3.747508	-0.898582	1.211339
20	6	-3.908216	-0.753781	-1.588860
21	1	-1.907061	0.063822	-1.518444
22	6	-4.911940	-1.293824	0.554810

23	1	-3.680641	-0.946964	2.293223
24	6	-4.990503	-1.225757	-0.838530
25	1	-3.981909	-0.682495	-2.669227
26	1	-5.756609	-1.651687	1.134373
27	1	-5.902735	-1.529973	-1.342123
28	6	1.881166	0.315258	2.242226
29	1	2.838525	0.009537	2.668454
30	1	2.011068	1.309578	1.796564
31	1	1.148510	0.414172	3.049712
32	6	0.251261	2.031468	-0.562672
33	8	0.860873	1.007877	-0.942352
34	6	1.071595	3.348197	-0.489708
35	9	2.024289	3.392117	-1.435553
36	9	0.300020	4.439192	-0.620401
37	9	1.692703	3.431930	0.718638

TS1, PCM DMF

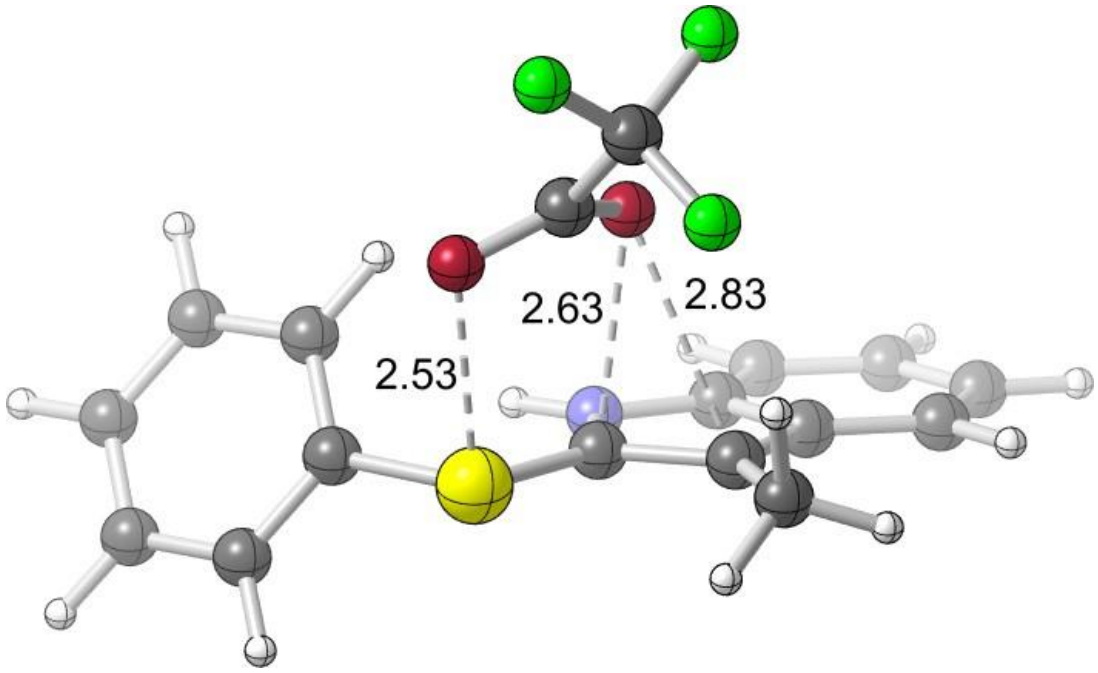


HF=-1558.3295444hartrees(-977867.372406444kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.113954 hartrees (-977732.08727454 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.359604	-2.260227	-0.394888
2	6	2.226585	-1.536210	0.492929
3	6	3.621381	-1.831366	0.520244

4	6	4.091310	-2.818172	-0.314994
5	6	3.204862	-3.517698	-1.175951
6	6	1.832231	-3.257752	-1.231535
7	6	0.071190	-0.819913	0.724192
8	6	1.455049	-0.624338	1.204491
9	1	4.285336	-1.287197	1.182698
10	1	5.144999	-3.072263	-0.324643
11	1	3.610347	-4.290719	-1.821283
12	1	1.179621	-3.809771	-1.897564
13	1	-0.750917	-2.136048	-0.702216
14	7	0.070715	-1.791781	-0.219510
15	16	-1.216928	0.041974	1.353603
16	8	-0.997663	2.111333	-0.086209
17	6	-2.643582	-0.516130	0.447271
18	6	-2.697323	-0.428472	-0.952341
19	6	-3.732998	-0.965806	1.206030
20	6	-3.860108	-0.843054	-1.597319
21	1	-1.862433	-0.019618	-1.510222
22	6	-4.886843	-1.373110	0.538277
23	1	-3.677938	-1.007646	2.288787
24	6	-4.948749	-1.315929	-0.856395
25	1	-3.920070	-0.782799	-2.679176
26	1	-5.735780	-1.733134	1.110198
27	1	-5.852334	-1.630904	-1.368875
28	6	1.881774	0.347973	2.238730
29	1	2.865158	0.087950	2.634533
30	1	1.945931	1.353281	1.803544
31	1	1.167179	0.396704	3.067020
32	6	0.176166	2.053153	-0.551233
33	8	0.783698	1.046951	-0.973684
34	6	0.978969	3.382584	-0.492421
35	9	1.910988	3.446508	-1.458648
36	9	0.188070	4.463875	-0.604912
37	9	1.624425	3.476681	0.701866

TS1, PCM DMSO

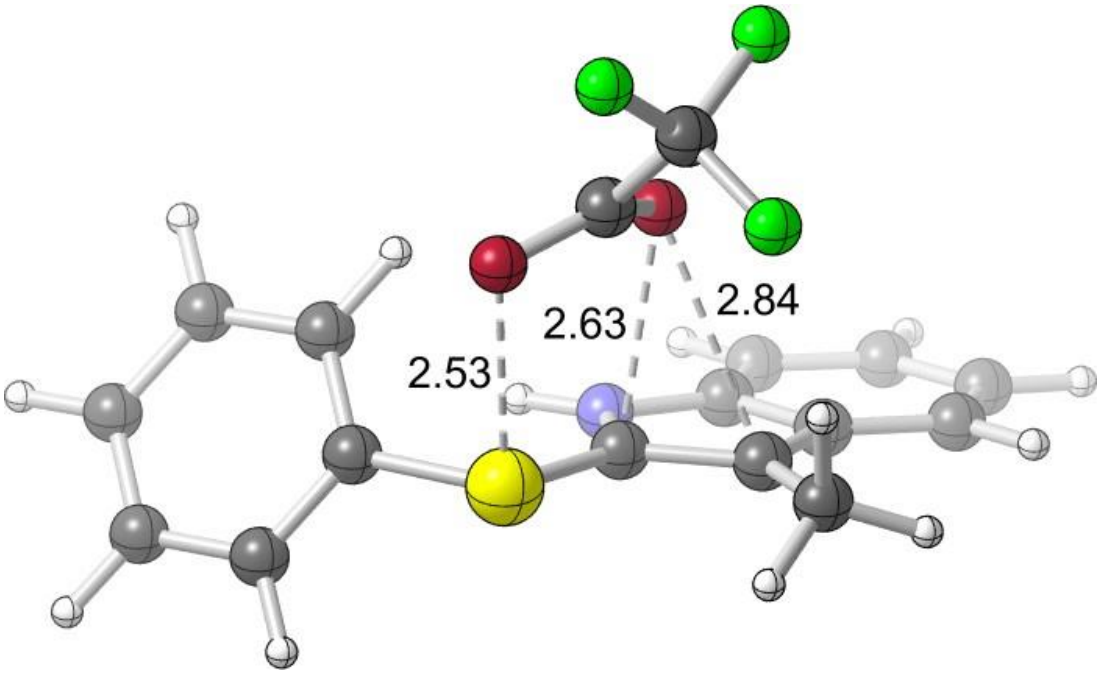


HF = -1558.3300707 hartrees (-977867.702664957 kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.114520 hartrees (-977732.4424452 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.364801	-2.258686	-0.394657
2	6	2.230483	-1.532359	0.492654
3	6	3.626015	-1.824302	0.519565
4	6	4.097829	-2.810370	-0.315423
5	6	3.212598	-3.512328	-1.175731
6	6	1.839351	-3.255552	-1.230991
7	6	0.073478	-0.821342	0.724765
8	6	1.457097	-0.622406	1.204504
9	1	4.288896	-1.278393	1.181661
10	1	5.152067	-3.062151	-0.325349
11	1	3.619615	-4.284747	-1.820814
12	1	1.187749	-3.809381	-1.896491
13	1	-0.746192	-2.140501	-0.700301
14	7	0.074984	-1.792970	-0.219145
15	16	-1.216113	0.038026	1.354319
16	8	-1.002621	2.110938	-0.081417
17	6	-2.641588	-0.521908	0.447392
18	6	-2.694563	-0.434787	-0.952298
19	6	-3.730935	-0.972574	1.205660
20	6	-3.856471	-0.850918	-1.597827
21	1	-1.859644	-0.025572	-1.509910
22	6	-4.883899	-1.381447	0.537341

23	1	-3.676394	-1.014122	2.288449
24	6	-4.945018	-1.324808	-0.857386
25	1	-3.915784	-0.791267	-2.679751
26	1	-5.732722	-1.742357	1.108870
27	1	-5.847885	-1.641106	-1.370319
28	6	1.881800	0.351148	2.238379
29	1	2.867197	0.095207	2.631795
30	1	1.940427	1.357093	1.803884
31	1	1.168820	0.395932	3.068305
32	6	0.169740	2.054845	-0.550535
33	8	0.777517	1.050398	-0.976371
34	6	0.970370	3.385716	-0.492610
35	9	1.900762	3.451800	-1.460327
36	9	0.177370	4.465777	-0.603593
37	9	1.617543	3.480813	0.700627

TS1, PCM H_2O

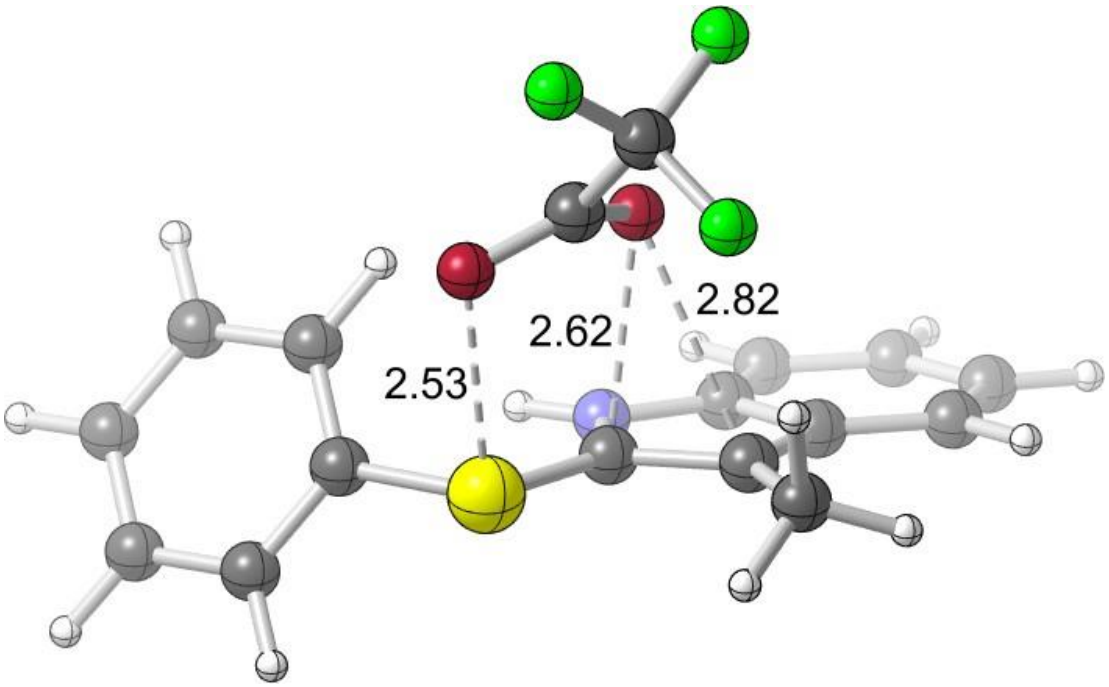


HF=-1558.330897hartrees(-977868.22117647kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.115402 hartrees (-977732.99590902 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.373473	-2.256062	-0.394229
2	6	2.236930	-1.525919	0.492323
3	6	3.633670	-1.812481	0.518606
4	6	4.108684	-2.797247	-0.316005

5	6	3.225555	-3.503213	-1.175319
6	6	1.851291	-3.251754	-1.230081
7	6	0.077264	-0.823680	0.725710
8	6	1.460428	-0.619180	1.204627
9	1	4.294726	-1.263687	1.180136
10	1	5.163833	-3.045143	-0.326369
11	1	3.635186	-4.274554	-1.820032
12	1	1.201443	-3.808564	-1.894789
13	1	-0.738263	-2.147768	-0.697211
14	7	0.082103	-1.794917	-0.218527
15	16	-1.214779	0.031473	1.355527
16	8	-1.010787	2.110177	-0.073660
17	6	-2.638317	-0.531474	0.447630
18	6	-2.690089	-0.445171	-0.952178
19	6	-3.727515	-0.983826	1.205107
20	6	-3.850572	-0.863841	-1.598581
21	1	-1.855165	-0.035317	-1.509366
22	6	-4.879045	-1.395267	0.535891
23	1	-3.673790	-1.024948	2.287944
24	6	-4.938926	-1.339454	-0.858921
25	1	-3.908862	-0.805126	-2.680610
26	1	-5.727650	-1.757677	1.106795
27	1	-5.840622	-1.657915	-1.372574
28	6	1.881590	0.356348	2.238051
29	1	2.870582	0.107716	2.627034
30	1	1.930173	1.363497	1.805124
31	1	1.171656	0.393796	3.070994
32	6	0.159135	2.057539	-0.549448
33	8	0.767357	1.055926	-0.980680
34	6	0.956149	3.390797	-0.493144
35	9	1.883313	3.460609	-1.463814
36	9	0.159619	4.468816	-0.601007
37	9	1.606813	3.487353	0.698006

TS1, PCM Methanol

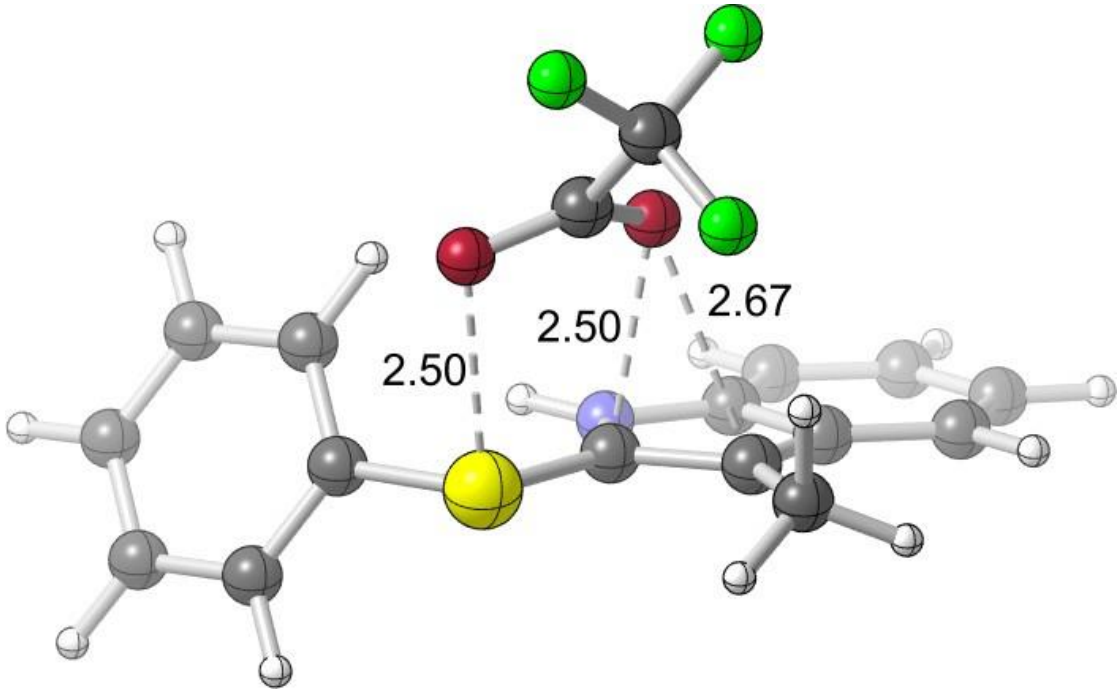


HF=-1558.3291836hartrees(-977867.146000836kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.113569 hartrees (-977731.84568319 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.356027	-2.261366	-0.394541
2	6	2.223818	-1.538904	0.493677
3	6	3.618073	-1.836395	0.521535
4	6	4.086760	-2.823835	-0.313690
5	6	3.199561	-3.521695	-1.175173
6	6	1.827392	-3.259463	-1.231228
7	6	0.069568	-0.818751	0.723907
8	6	1.453533	-0.625528	1.204777
9	1	4.282698	-1.293423	1.184302
10	1	5.140047	-3.079611	-0.322942
11	1	3.604031	-4.295227	-1.820533
12	1	1.174157	-3.810245	-1.897675
13	1	-0.754097	-2.132909	-0.703392
14	7	0.067792	-1.790919	-0.219515
15	16	-1.217568	0.045084	1.352846
16	8	-0.994232	2.111567	-0.090110
17	6	-2.644973	-0.512015	0.446962
18	6	-2.699231	-0.424156	-0.952603
19	6	-3.734380	-0.961077	1.206094
20	6	-3.862546	-0.837920	-1.597177
21	1	-1.864427	-0.015460	-1.510694
22	6	-4.888760	-1.367549	0.538757

23	1	-3.678977	-1.002982	2.288835
24	6	-4.951192	-1.310172	-0.855883
25	1	-3.922943	-0.777380	-2.678994
26	1	-5.737732	-1.727018	1.110977
27	1	-5.855216	-1.624430	-1.368031
28	6	1.881602	0.346080	2.239146
29	1	2.863576	0.083324	2.636666
30	1	1.949569	1.350873	1.803349
31	1	1.165882	0.397641	3.066277
32	6	0.180691	2.051969	-0.552117
33	8	0.788197	1.044548	-0.971986
34	6	0.984886	3.380472	-0.492748
35	9	1.917736	3.443080	-1.458217
36	9	0.195340	4.462572	-0.605912
37	9	1.629511	3.473774	0.702075

TS1, PCM Toluene

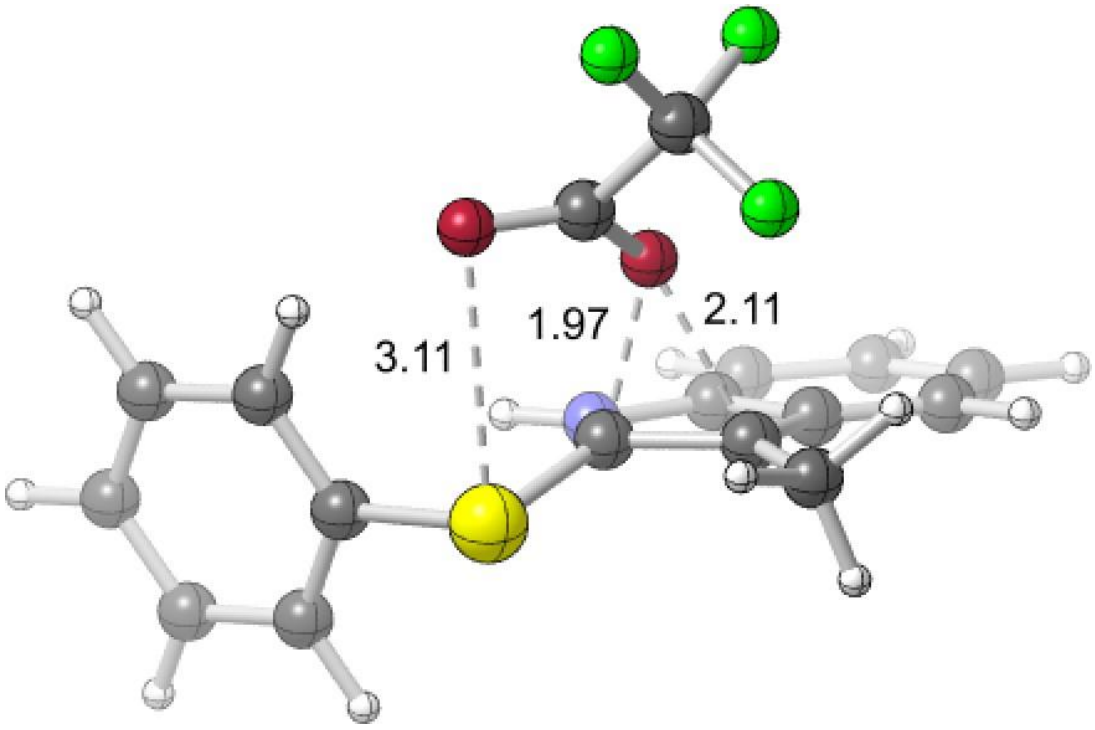


HF=-1558.2967614hartrees(-977846.800746114kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.080315 hartrees (-977710.97846565 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.184155	-2.299409	-0.396747
2	6	2.097947	-1.652845	0.500555
3	6	3.460518	-2.063772	0.539685

4	6	3.857748	-3.082092	-0.297352
5	6	2.927512	-3.700878	-1.171893
6	6	1.582295	-3.328309	-1.236129
7	6	0.012736	-0.745466	0.703774
8	6	1.399251	-0.667507	1.197307
9	1	4.162569	-1.578693	1.208899
10	1	4.887957	-3.419791	-0.298142
11	1	3.274934	-4.500147	-1.819518
12	1	0.893252	-3.821684	-1.912063
13	1	-0.891636	-1.943099	-0.771558
14	7	-0.065067	-1.731931	-0.225929
15	16	-1.226958	0.196402	1.327106
16	8	-0.842817	2.120662	-0.226739
17	6	-2.688561	-0.322351	0.444742
18	6	-2.781274	-0.191574	-0.949044
19	6	-3.759155	-0.788940	1.219555
20	6	-3.965345	-0.579600	-1.573223
21	1	-1.964462	0.245482	-1.511699
22	6	-4.934592	-1.168321	0.572999
23	1	-3.676433	-0.860376	2.299289
24	6	-5.035594	-1.068472	-0.816974
25	1	-4.058029	-0.479656	-2.650005
26	1	-5.770920	-1.537658	1.157575
27	1	-5.956757	-1.359074	-1.312400
28	6	1.902122	0.272652	2.229167
29	1	2.819800	-0.101674	2.687869
30	1	2.127243	1.241809	1.766122
31	1	1.161794	0.452969	3.015129
32	6	0.365412	1.997411	-0.575074
33	8	0.945359	0.932284	-0.896153
34	6	1.239062	3.276174	-0.491987
35	9	2.210501	3.265181	-1.415725
36	9	0.517807	4.393339	-0.641317
37	9	1.835218	3.330248	0.732073

TS2-a conf 1, Gas Phase

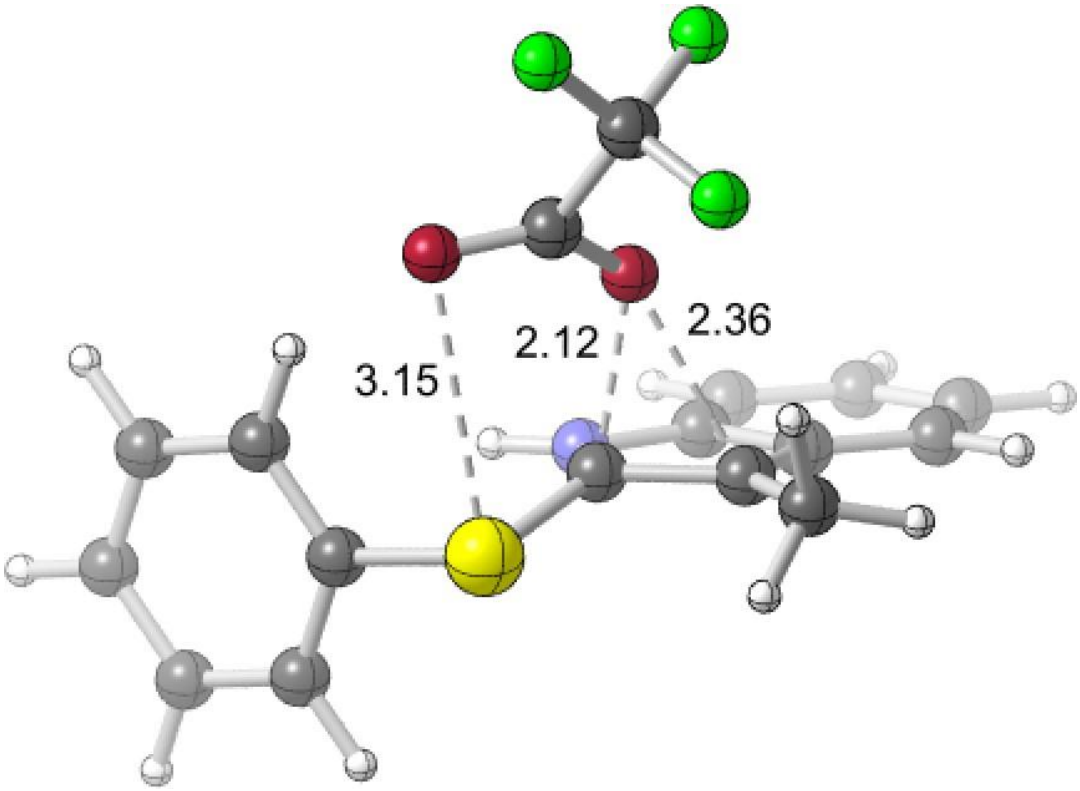


HF=-1558.2602927hartrees(-977823.916272177kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.045100 hartrees (-977688.880701 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.558746	2.318213	-0.478066
2	6	-1.607754	1.925753	0.409790
3	6	-2.815090	2.664099	0.457669
4	6	-2.936975	3.769970	-0.361576
5	6	-1.882004	4.135977	-1.228819
6	6	-0.680554	3.423247	-1.306090
7	6	0.183138	0.463571	0.568376
8	6	-1.190324	0.769434	1.089671
9	1	-3.621300	2.363770	1.119248
10	1	-3.845855	4.361337	-0.351256
11	1	-2.009340	5.006581	-1.865744
12	1	0.109176	3.727093	-1.984683
13	1	1.386467	1.468427	-0.821633
14	7	0.510962	1.447777	-0.313389
15	16	1.336885	-0.438092	1.483786
16	8	0.151291	-2.546480	-0.465070
17	6	2.841791	-0.239369	0.511374
18	6	3.069358	-1.080882	-0.585519
19	6	3.798662	0.691088	0.938776
20	6	4.277694	-0.964268	-1.274905

21	1	2.319751	-1.808778	-0.877529
22	6	5.002132	0.786665	0.239402
23	1	3.612195	1.317516	1.805745
24	6	5.239063	-0.037334	-0.864081
25	1	4.470172	-1.609700	-2.126490
26	1	5.754952	1.499288	0.562112
27	1	6.180224	0.038076	-1.400440
28	6	-1.862728	0.065041	2.205518
29	1	-1.821328	0.699901	3.101895
30	1	-2.916688	-0.107819	1.969438
31	1	-1.397943	-0.893577	2.438983
32	6	-0.898774	-1.940368	-0.475122
33	8	-1.063451	-0.628080	-0.490679
34	6	-2.260123	-2.686993	-0.464703
35	9	-3.087821	-2.198171	-1.397638
36	9	-2.097213	-3.990409	-0.658625
37	9	-2.837488	-2.497384	0.749521

TS2-a conf 1, PCM H_2O

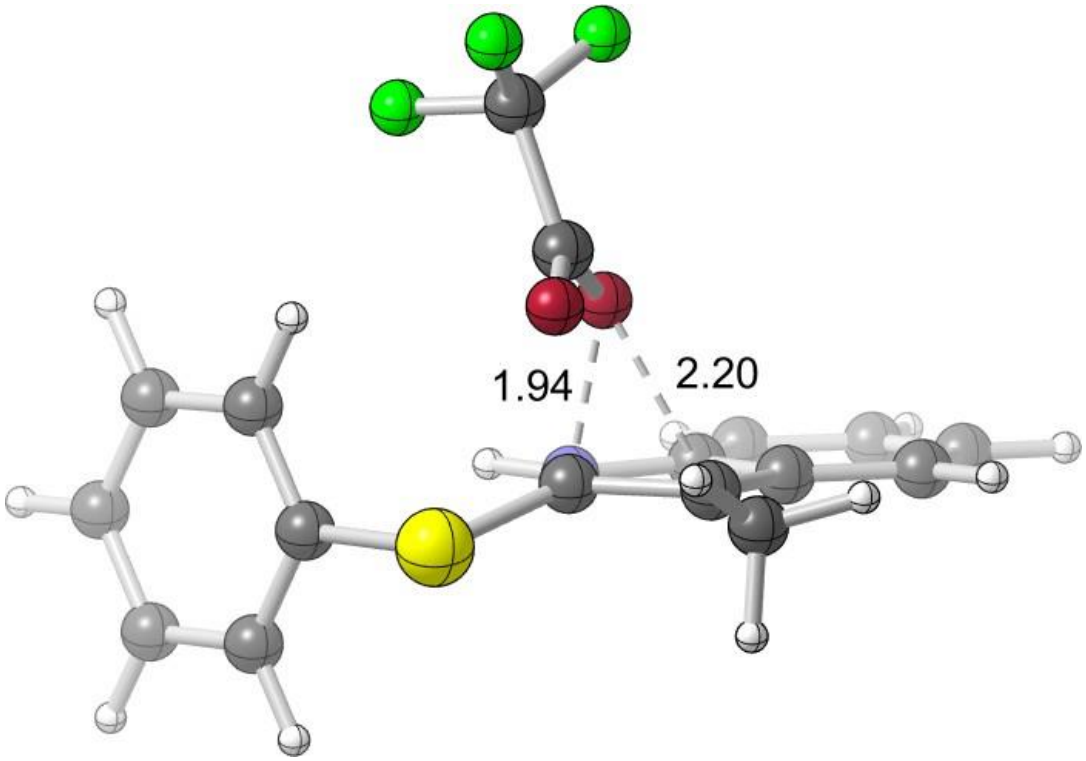


HF=-1558.3333769hartrees(-977869.777338519kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.118963 hartrees (-977735.23047213 kcal/mol)

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z

1	6	0.476032	-2.333754	-0.568167
2	6	1.486834	-2.119713	0.431854
3	6	2.615432	-2.987973	0.503029
4	6	2.694619	-4.021543	-0.401734
5	6	1.678265	-4.203195	-1.375328
6	6	0.557823	-3.371163	-1.479600
7	6	-0.171453	-0.524051	0.587368
8	6	1.132045	-1.006368	1.177181
9	1	3.384488	-2.830154	1.250890
10	1	3.534645	-4.705957	-0.381234
11	1	1.773486	-5.027930	-2.074837
12	1	-0.201074	-3.536429	-2.235013
13	1	-1.360694	-1.309127	-0.954447
14	7	-0.510183	-1.377791	-0.407899
15	16	-1.279310	0.414001	1.497495
16	8	-0.077254	2.568171	-0.463767
17	6	-2.790792	0.309248	0.523837
18	6	-2.926941	1.062820	-0.648702
19	6	-3.836192	-0.478823	1.020644
20	6	-4.135149	0.998896	-1.345381
21	1	-2.105124	1.682269	-0.991931
22	6	-5.038711	-0.520234	0.314535
23	1	-3.712500	-1.048320	1.935853
24	6	-5.186101	0.213028	-0.865881
25	1	-4.254569	1.571926	-2.259786
26	1	-5.856729	-1.129035	0.686823
27	1	-6.124083	0.173820	-1.411559
28	6	1.824228	-0.388286	2.325740
29	1	2.635114	-1.022323	2.686395
30	1	2.243491	0.577500	2.018076
31	1	1.127843	-0.192367	3.149181
32	6	0.988533	1.960516	-0.463415
33	8	1.211400	0.692659	-0.455840
34	6	2.315213	2.775157	-0.433988
35	9	3.193495	2.331779	-1.352289
36	9	2.106272	4.080873	-0.652016
37	9	2.898082	2.647641	0.784512

TS2-a conf 2, Gas Phase

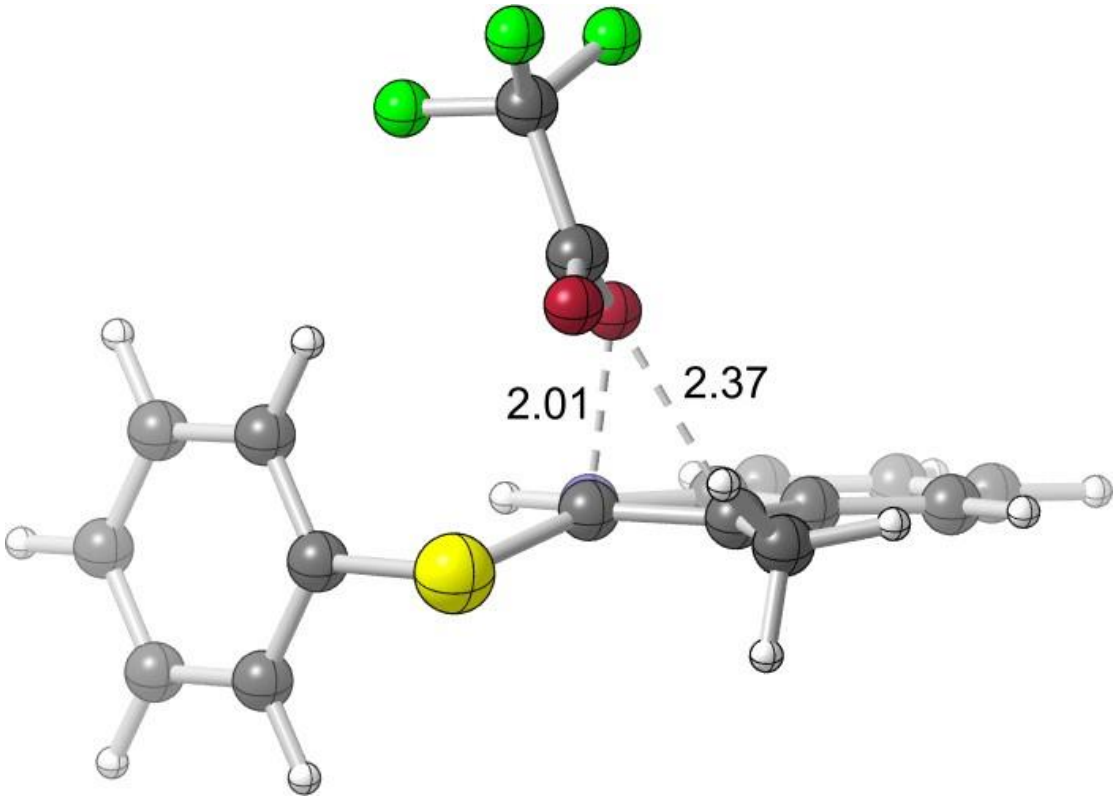


HF=-1558.2658473hartrees(-977827.401839223kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.049861 hartrees (-977691.86827611 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.588713	-1.748121	-0.642151
2	6	2.439283	-1.171765	0.349406
3	6	3.839444	-1.374092	0.292197
4	6	4.345735	-2.144450	-0.737540
5	6	3.479623	-2.700515	-1.706289
6	6	2.092662	-2.515323	-1.680179
7	6	0.230078	-0.585503	0.738327
8	6	1.635207	-0.450014	1.248531
9	1	4.494206	-0.931529	1.035862
10	1	5.412696	-2.322273	-0.814089
11	1	3.907426	-3.296452	-2.507333
12	1	1.453627	-2.954646	-2.438534
13	1	-0.542044	-1.640688	-0.894222
14	7	0.273566	-1.423422	-0.334348
15	16	-1.192598	-0.352580	1.704500
16	8	0.273343	2.511842	1.565949
17	6	-2.480991	-0.923590	0.581495
18	6	-2.857291	-0.127676	-0.511088
19	6	-3.151141	-2.116789	0.879208
20	6	-3.906655	-0.556123	-1.325363

21	1	-2.349145	0.809279	-0.716987
22	6	-4.208785	-2.520373	0.062908
23	1	-2.857909	-2.714165	1.736910
24	6	-4.582419	-1.744916	-1.037147
25	1	-4.206069	0.051100	-2.174130
26	1	-4.739208	-3.440210	0.289143
27	1	-5.407493	-2.063262	-1.667072
28	6	2.024465	0.157538	2.539217
29	1	3.091064	0.391347	2.563345
30	1	1.441410	1.057073	2.749101
31	1	1.822292	-0.574889	3.336831
32	6	0.435410	2.218650	0.402427
33	8	0.798883	1.059208	-0.113128
34	6	0.136388	3.235410	-0.741515
35	9	1.105623	3.232859	-1.664777
36	9	-1.022241	2.869548	-1.341774
37	9	-0.004538	4.461156	-0.252074

TS2-a conf 2, PCM H_2O

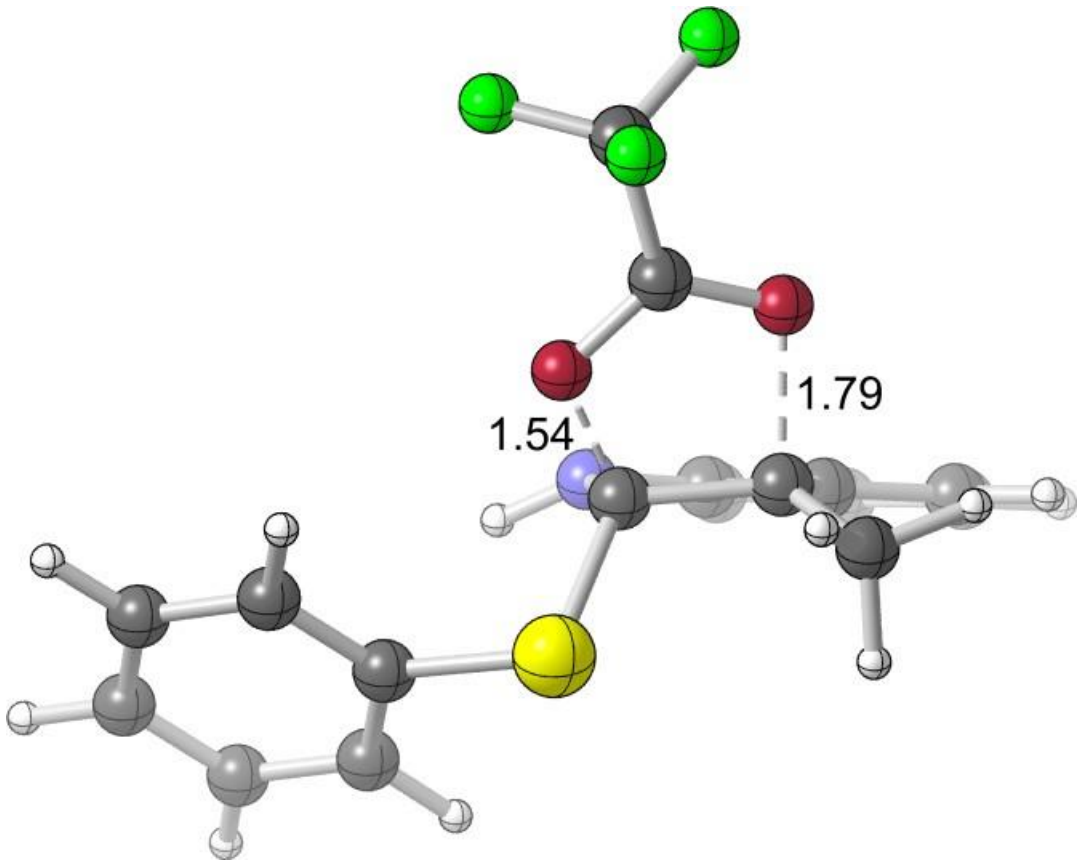


HF=-1558.3375664hartrees(-977872.406291664kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.122831 hartrees (-977737.65768081 kcal/mol)

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	1.693558	-1.669562	-0.685693
2	6	2.513773	-1.102261	0.345314
3	6	3.927152	-1.259612	0.301408
4	6	4.466784	-1.972474	-0.746869
5	6	3.627411	-2.520646	-1.748387
6	6	2.234389	-2.382201	-1.740733
7	6	0.281927	-0.623412	0.717656
8	6	1.683143	-0.460660	1.257930
9	1	4.554367	-0.827475	1.073059
10	1	5.538527	-2.117264	-0.817226
11	1	4.085242	-3.073883	-2.562628
12	1	1.619663	-2.814711	-2.521255
13	1	-0.428166	-1.672062	-0.955291
14	7	0.367597	-1.397158	-0.391689
15	16	-1.132882	-0.501623	1.702334
16	8	0.149003	2.537916	1.577332
17	6	-2.415041	-1.082214	0.580864
18	6	-2.820447	-0.281654	-0.496484
19	6	-3.044891	-2.300290	0.862228
20	6	-3.859114	-0.729281	-1.313718
21	1	-2.335775	0.668547	-0.695448
22	6	-4.092238	-2.724236	0.043129
23	1	-2.721606	-2.904924	1.703121
24	6	-4.495194	-1.943640	-1.042958
25	1	-4.175548	-0.121389	-2.155579
26	1	-4.587223	-3.667303	0.252885
27	1	-5.308367	-2.280764	-1.678523
28	6	2.020094	0.163044	2.550672
29	1	3.088338	0.370931	2.627987
30	1	1.442774	1.079424	2.700133
31	1	1.749652	-0.537140	3.355927
32	6	0.289425	2.258161	0.396930
33	8	0.654256	1.144550	-0.156196
34	6	-0.063201	3.317555	-0.690654
35	9	0.867276	3.373859	-1.658435
36	9	-1.243217	2.991353	-1.269227
37	9	-0.188524	4.537526	-0.154069

TS2-b, Gas Phase

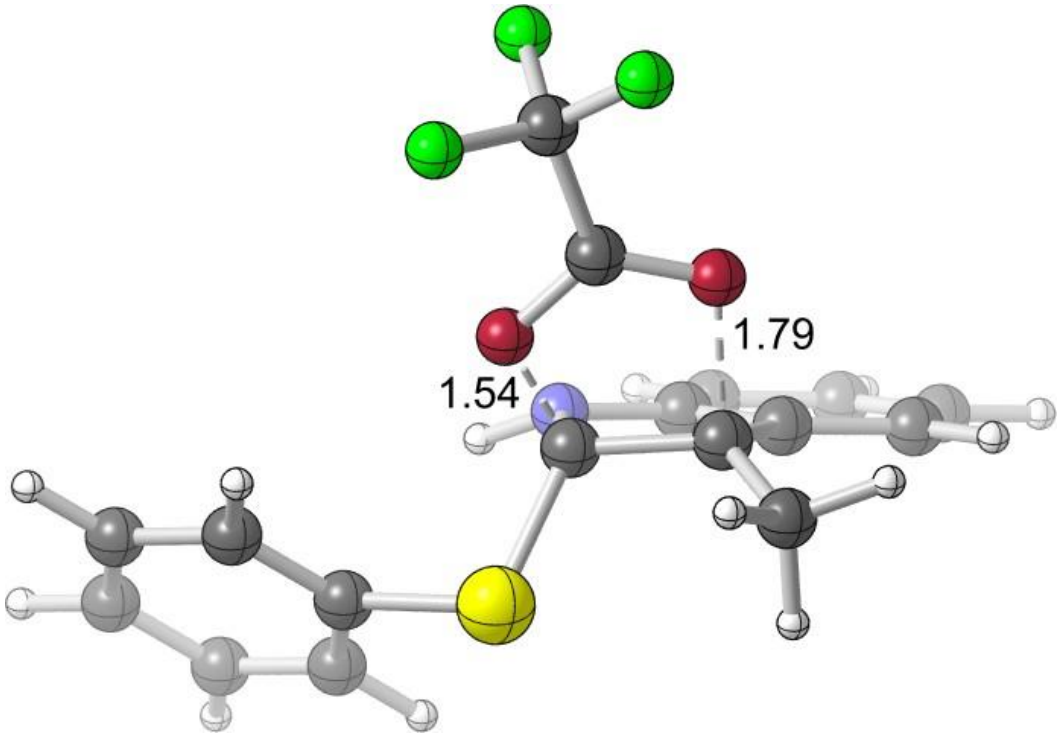


HF=-1558.284237hartrees(-977838.94155987kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.065456 hartrees (-977701.65429456 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.468952	-2.006702	-0.736996
2	6	1.441526	-1.950748	0.283954
3	6	2.359686	-2.997030	0.459484
4	6	2.275753	-4.095923	-0.385306
5	6	1.291196	-4.142753	-1.389432
6	6	0.374127	-3.107199	-1.582731
7	6	-0.028792	-0.083163	0.423148
8	6	1.277951	-0.708114	1.006742
9	1	3.117341	-2.949889	1.235581
10	1	2.969097	-4.922404	-0.273938
11	1	1.240934	-5.012103	-2.038424
12	1	-0.375902	-3.160886	-2.365022
13	1	-1.279169	-0.873504	-1.052993
14	7	-0.316981	-0.848454	-0.730942
15	16	-1.341612	0.106793	1.671182
16	8	2.383444	0.489291	0.276056
17	6	-2.794042	0.265733	0.624582

18	6	-3.161015	1.521987	0.120511
19	6	-3.591977	-0.863329	0.383922
20	6	-4.323203	1.639488	-0.641119
21	1	-2.549347	2.393442	0.330175
22	6	-4.754521	-0.730890	-0.377868
23	1	-3.315523	-1.825119	0.805611
24	6	-5.117242	0.516638	-0.890208
25	1	-4.613062	2.610010	-1.032186
26	1	-5.379611	-1.599743	-0.560517
27	1	-6.025247	0.616608	-1.477257
28	6	1.654217	-0.548382	2.451239
29	1	2.697733	-0.837780	2.600740
30	1	1.515643	0.475045	2.807816
31	1	1.027259	-1.214643	3.053929
32	6	1.647477	1.419967	-0.109184
33	8	0.365679	1.329599	-0.050192
34	6	2.244439	2.758024	-0.604788
35	9	2.359096	3.562799	0.455968
36	9	3.439108	2.536814	-1.139196
37	9	1.432278	3.306465	-1.503265

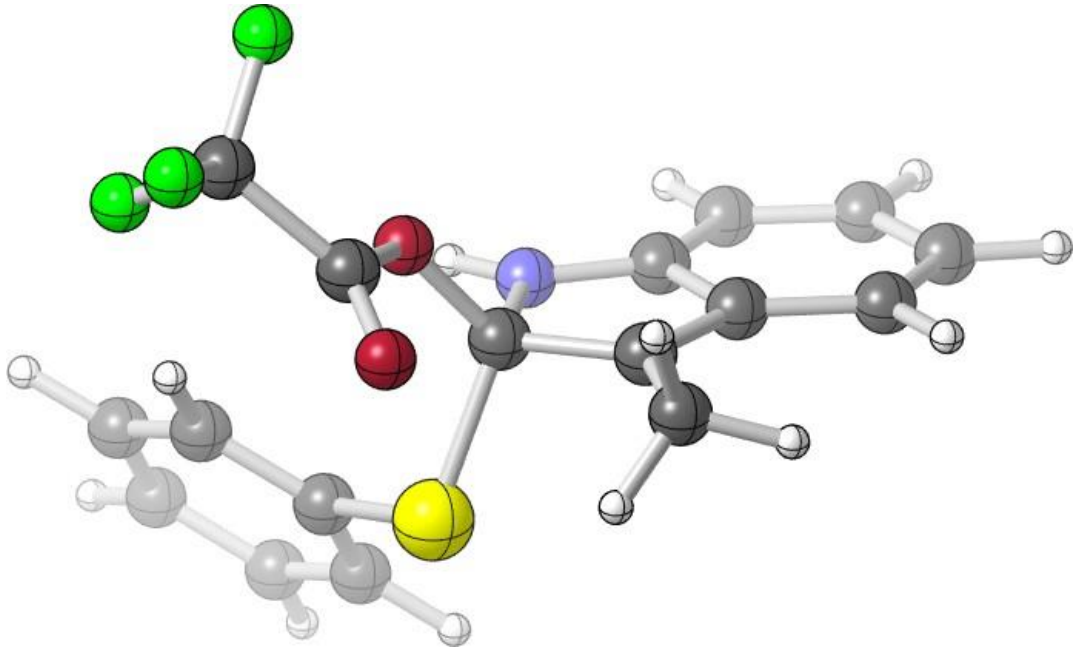
TS2-b, PCM H_2O



HF=-1558.3465998hartrees(-977878.074840498kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.128587 hartrees (-977741.26962837 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.712942	-1.950748	-0.744764
2	6	1.667912	-1.797685	0.282553
3	6	2.704731	-2.727330	0.446308
4	6	2.759603	-3.810847	-0.421434
5	6	1.792095	-3.957175	-1.432996
6	6	0.756055	-3.038750	-1.612411
7	6	-0.022801	-0.127330	0.446634
8	6	1.345526	-0.604481	1.036129
9	1	3.443896	-2.603154	1.231172
10	1	3.547312	-4.549367	-0.319897
11	1	1.849496	-4.814014	-2.097693
12	1	0.016838	-3.168109	-2.395185
13	1	-1.141919	-1.013740	-1.095266
14	7	-0.207018	-0.902363	-0.718895
15	16	-1.358859	-0.113585	1.688413
16	8	2.301643	0.739677	0.348767
17	6	-2.807823	-0.012962	0.630054
18	6	-3.264335	1.236266	0.185444
19	6	-3.510311	-1.184496	0.313462
20	6	-4.420374	1.305320	-0.591747
21	1	-2.721788	2.138835	0.446735
22	6	-4.668353	-1.101766	-0.462694
23	1	-3.157293	-2.144533	0.676300
24	6	-5.120714	0.139484	-0.915305
25	1	-4.775887	2.270241	-0.940434
26	1	-5.214972	-2.006890	-0.709333
27	1	-6.022347	0.200026	-1.517618
28	6	1.683722	-0.444932	2.487581
29	1	2.749564	-0.628841	2.642121
30	1	1.431973	0.546472	2.868950
31	1	1.126185	-1.195545	3.058227
32	6	1.459135	1.574517	-0.031854
33	8	0.198025	1.326555	0.004393
34	6	1.889665	2.944652	-0.597520
35	9	3.070705	3.287376	-0.090345
36	9	1.986148	2.837120	-1.926335
37	9	0.978970	3.866863	-0.290026

[2,3] Product, Gas Phase

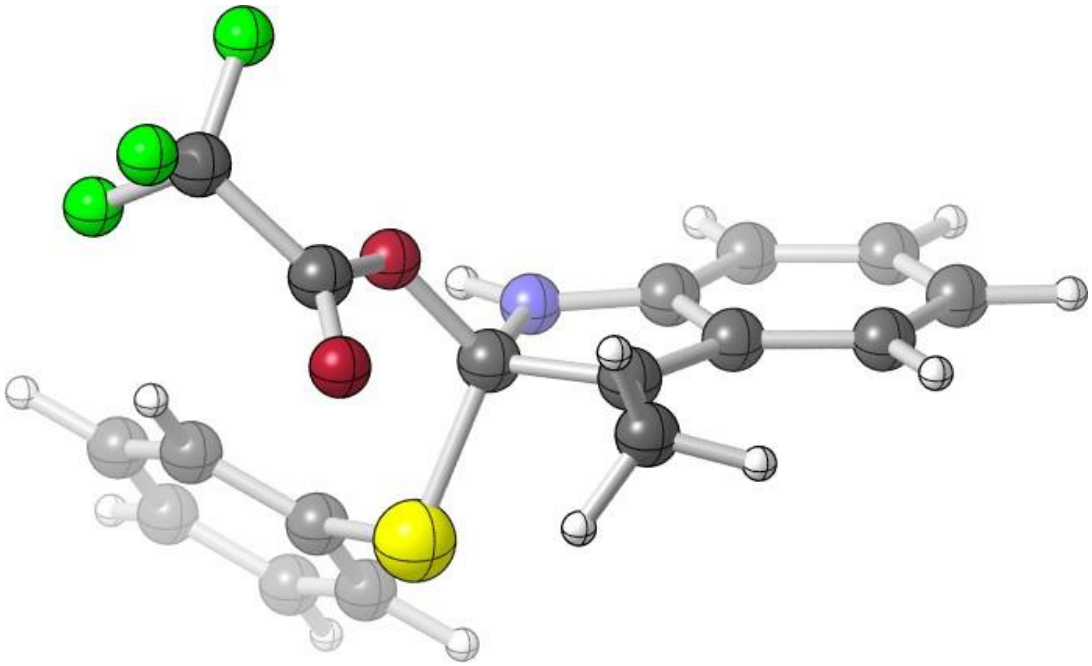


HF=-1558.2940137hartrees(-977845.076536887kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.076869 hartrees (-977708.81606619 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.348161	0.025417	-0.837132
2	6	2.610704	1.033948	0.169757
3	6	3.940261	1.542595	0.331710
4	6	4.925964	1.054579	-0.480237
5	6	4.637707	0.048976	-1.461268
6	6	3.377764	-0.481656	-1.650541
7	6	0.348222	0.413198	0.239739
8	6	1.433575	1.315092	0.832336
9	1	4.148943	2.301245	1.078386
10	1	5.943220	1.419852	-0.390767
11	1	5.453415	-0.310123	-2.082431
12	1	3.186821	-1.242940	-2.399034
13	1	0.590110	-1.010320	-1.357271
14	7	1.046911	-0.293878	-0.806431
15	16	-0.145036	-0.739279	1.626357
16	8	-1.615232	2.145263	1.381153
17	6	-0.628827	-2.218819	0.741723
18	6	-1.792808	-2.240886	-0.045035
19	6	0.132742	-3.383258	0.922685
20	6	-2.175261	-3.430965	-0.663728
21	1	-2.395471	-1.347075	-0.165646
22	6	-0.274914	-4.571387	0.316229

23	1	1.024923	-3.357758	1.540695
24	6	-1.422463	-4.594341	-0.480078
25	1	-3.073744	-3.452862	-1.273050
26	1	0.304710	-5.477380	0.465206
27	1	-1.735880	-5.520977	-0.951446
28	6	1.243621	2.268232	1.952652
29	1	2.204534	2.567434	2.376649
30	1	0.716445	3.167299	1.609536
31	1	0.612679	1.841981	2.739432
32	6	-1.686006	1.762900	0.249888
33	8	-0.760311	1.030157	-0.426042
34	6	-2.894688	2.006459	-0.685856
35	9	-2.488757	2.506620	-1.858877
36	9	-3.511530	0.827871	-0.909622
37	9	-3.747121	2.843662	-0.112044

[2,3] Product, PCM H_2O

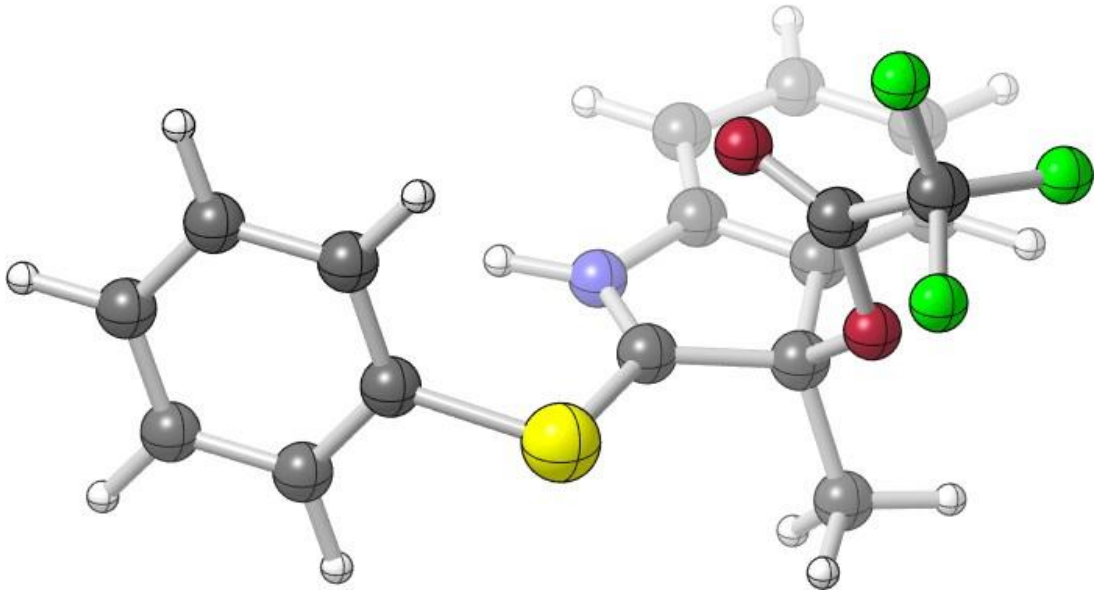


HF=-1558.3607296hartrees(-977886.941431296kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.143615 hartrees (-977750.69984865 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.358723	-0.040240	-0.824580
2	6	2.645721	0.968102	0.178839
3	6	3.987268	1.450014	0.336674

4	6	4.956623	0.936595	-0.476245
5	6	4.642668	-0.066604	-1.455203
6	6	3.373230	-0.570735	-1.641695
7	6	0.376899	0.387660	0.254631
8	6	1.480228	1.277448	0.839072
9	1	4.212783	2.204301	1.081958
10	1	5.982459	1.276983	-0.391476
11	1	5.449349	-0.445014	-2.075674
12	1	3.160134	-1.330572	-2.384228
13	1	0.587558	-1.028992	-1.362105
14	7	1.053889	-0.334886	-0.790627
15	16	-0.160037	-0.743600	1.638058
16	8	-1.597814	2.153896	1.386547
17	6	-0.707928	-2.202791	0.752827
18	6	-1.924370	-2.204070	0.052368
19	6	0.065679	-3.369411	0.838994
20	6	-2.351569	-3.374819	-0.574562
21	1	-2.527262	-1.304571	-0.006938
22	6	-0.381812	-4.538324	0.222707
23	1	1.004442	-3.358044	1.383182
24	6	-1.585612	-4.540477	-0.486272
25	1	-3.288738	-3.377084	-1.122872
26	1	0.213587	-5.443652	0.292129
27	1	-1.928501	-5.451005	-0.968650
28	6	1.302913	2.245678	1.947289
29	1	2.269632	2.555783	2.347348
30	1	0.767810	3.135401	1.594535
31	1	0.694117	1.823447	2.753320
32	6	-1.627221	1.788440	0.244614
33	8	-0.719495	1.041643	-0.413263
34	6	-2.810942	2.078777	-0.708898
35	9	-2.390651	2.418276	-1.933206
36	9	-3.570534	0.968966	-0.809903
37	9	-3.558650	3.064876	-0.212969

[3,3] Product, Gas Phase

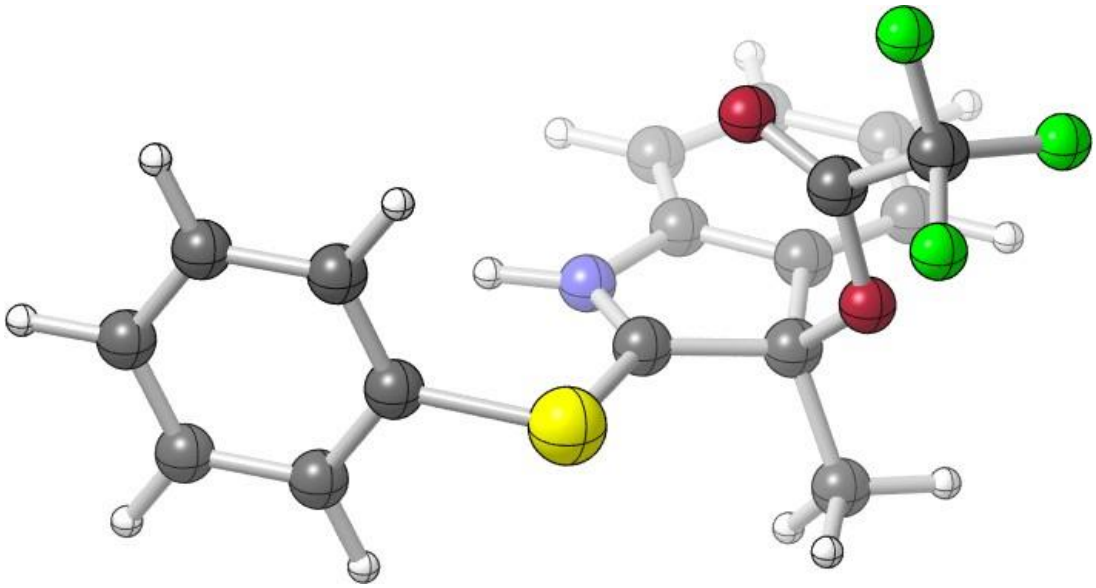


HF=-1558.3223165hartrees(-977862.836826915kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.103157 hartrees (-977725.31204907 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.250650	2.229477	-0.290447
2	6	-1.382864	1.731992	0.356367
3	6	-2.593102	2.398491	0.240749
4	6	-2.631525	3.562531	-0.541229
5	6	-1.482602	4.046564	-1.174277
6	6	-0.254382	3.382854	-1.057367
7	6	0.479478	0.319074	0.716282
8	6	-0.991340	0.501521	1.156295
9	1	-3.490306	2.028353	0.727637
10	1	-3.569356	4.096335	-0.655624
11	1	-1.539158	4.952094	-1.769613
12	1	0.638725	3.755991	-1.548452
13	1	1.770739	1.448611	-0.407555
14	7	0.837056	1.351333	-0.014976
15	16	1.453910	-0.996196	1.217888
16	8	-0.984200	-0.828218	-1.225976
17	6	2.990612	-0.682873	0.328972
18	6	3.084437	-1.042737	-1.023342
19	6	4.088705	-0.165816	1.027773
20	6	4.299416	-0.859160	-1.684196
21	1	2.228823	-1.464186	-1.542726
22	6	5.298159	0.002611	0.351616
23	1	4.004298	0.088422	2.079842

24	6	5.401688	-0.341141	-0.998339
25	1	4.386618	-1.135242	-2.730515
26	1	6.158517	0.397074	0.883260
27	1	6.347129	-0.212661	-1.516489
28	6	-1.088316	0.711800	2.673339
29	1	-0.484852	1.569669	2.981593
30	1	-2.131777	0.905840	2.934837
31	1	-0.750661	-0.181410	3.206420
32	6	-1.738781	-1.184990	-0.359388
33	8	-1.797957	-0.666305	0.884463
34	6	-2.776496	-2.322637	-0.505057
35	9	-4.009150	-1.824009	-0.336283
36	9	-2.678169	-2.866562	-1.713099
37	9	-2.551356	-3.258126	0.427340

[3,3] Product, PCM H_2O



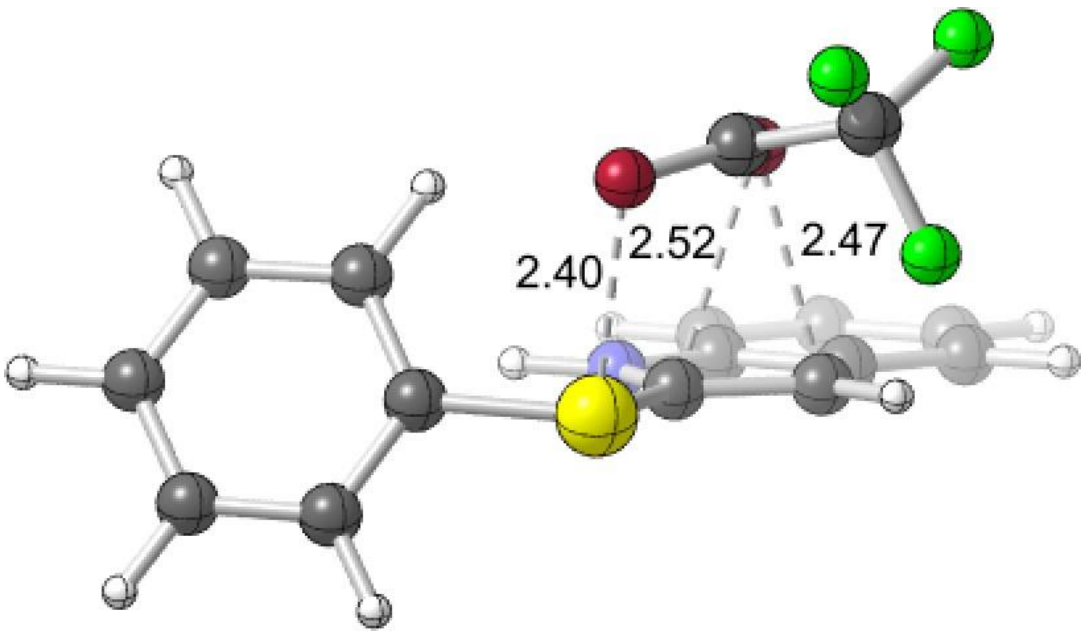
HF=-1558.3890583 hartrees (-977904.717973833 kcal/mol)
Sum of electronic and thermal Free Energies =
-1558.170271 hartrees (-977767.42675521 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.191183	2.225333	-0.315101
2	6	-1.330234	1.754566	0.339900
3	6	-2.520770	2.459187	0.252735
4	6	-2.533569	3.633930	-0.514187
5	6	-1.378582	4.090568	-1.156981

6	6	-0.169280	3.388778	-1.066024
7	6	0.500156	0.290993	0.663339
8	6	-0.958143	0.510776	1.125723
9	1	-3.419901	2.112129	0.751526
10	1	-3.455777	4.198273	-0.606699
11	1	-1.414530	5.005823	-1.738860
12	1	0.731236	3.737303	-1.559540
13	1	1.810683	1.416530	-0.451184
14	7	0.872753	1.313797	-0.068749
15	16	1.435787	-1.057960	1.147059
16	8	-1.181396	-0.751415	-1.320371
17	6	3.004950	-0.754105	0.314860
18	6	3.202932	-1.265162	-0.974222
19	6	4.024213	-0.080836	0.999696
20	6	4.441669	-1.080239	-1.589009
21	1	2.405564	-1.795492	-1.484224
22	6	5.257182	0.094150	0.369717
23	1	3.857402	0.296534	2.003207
24	6	5.464396	-0.403778	-0.919026
25	1	4.605915	-1.469136	-2.589038
26	1	6.054116	0.616519	0.889617
27	1	6.427210	-0.266830	-1.401915
28	6	-1.027388	0.715976	2.643461
29	1	-0.392315	1.552808	2.943307
30	1	-2.061110	0.940799	2.917790
31	1	-0.704273	-0.188583	3.165339
32	6	-1.840741	-1.124907	-0.385763
33	8	-1.798109	-0.643029	0.864856
34	6	-2.878168	-2.268305	-0.462283
35	9	-4.105432	-1.795045	-0.193634
36	9	-2.876639	-2.801029	-1.685225
37	9	-2.584005	-3.225246	0.431313

R = *H*

TS1, Gas Phase

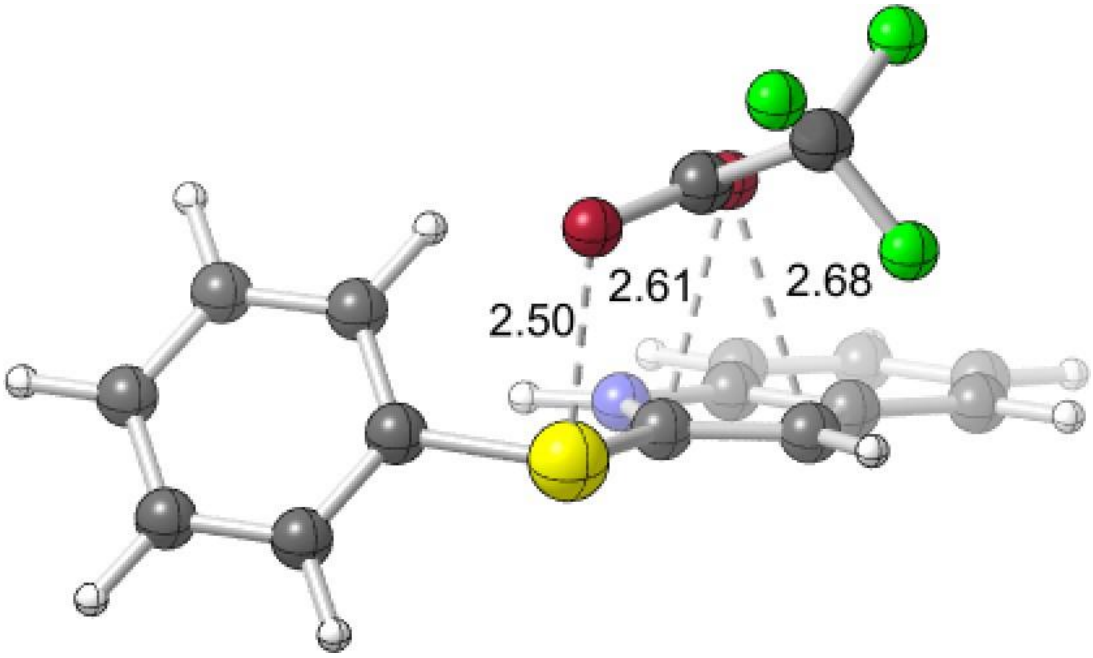


HF=-1518.9284931 hartrees (-953142.818705181 kcal/mol)
Sum of electronic and thermal Free Energies =
-1518.737812 hartrees (-953023.16440812 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.254785	-2.312471	-0.097646
2	6	2.182287	-1.446697	0.572961
3	6	3.563480	-1.780155	0.613816
4	6	3.966404	-2.949639	0.006401
5	6	3.025232	-3.787555	-0.643989
6	6	1.660962	-3.490590	-0.707285
7	6	0.068726	-0.589760	0.710144
8	6	1.459193	-0.359931	1.055284
9	1	4.271311	-1.123401	1.108918
10	1	5.011659	-3.238594	0.015899
11	1	3.379460	-4.699385	-1.115829
12	1	0.965963	-4.150926	-1.214811
13	1	-0.862444	-2.121660	-0.395499
14	7	-0.010859	-1.755963	0.011446
15	16	-1.164808	0.466779	1.150355
16	8	-0.733682	2.074575	-0.581981
17	6	-2.632007	-0.206929	0.395492
18	6	-2.725921	-0.327630	-1.000298
19	6	-3.704605	-0.514377	1.244318
20	6	-3.915799	-0.809611	-1.542086
21	1	-1.908282	0.001717	-1.632695
22	6	-4.884416	-0.994695	0.677988

23	1	-3.620465	-0.387721	2.319420
24	6	-4.987677	-1.145343	-0.707496
25	1	-4.014041	-0.899798	-2.619456
26	1	-5.723231	-1.244068	1.319943
27	1	-5.913626	-1.510141	-1.141363
28	6	0.520661	1.953246	-0.724640
29	8	1.112123	0.892172	-1.041407
30	6	1.391249	3.136750	-0.245605
31	9	2.564148	3.186082	-0.879923
32	9	0.774522	4.310445	-0.359277
33	9	1.642031	2.916695	1.083843
34	1	1.817476	0.496578	1.610813

TS1, PCM H2O



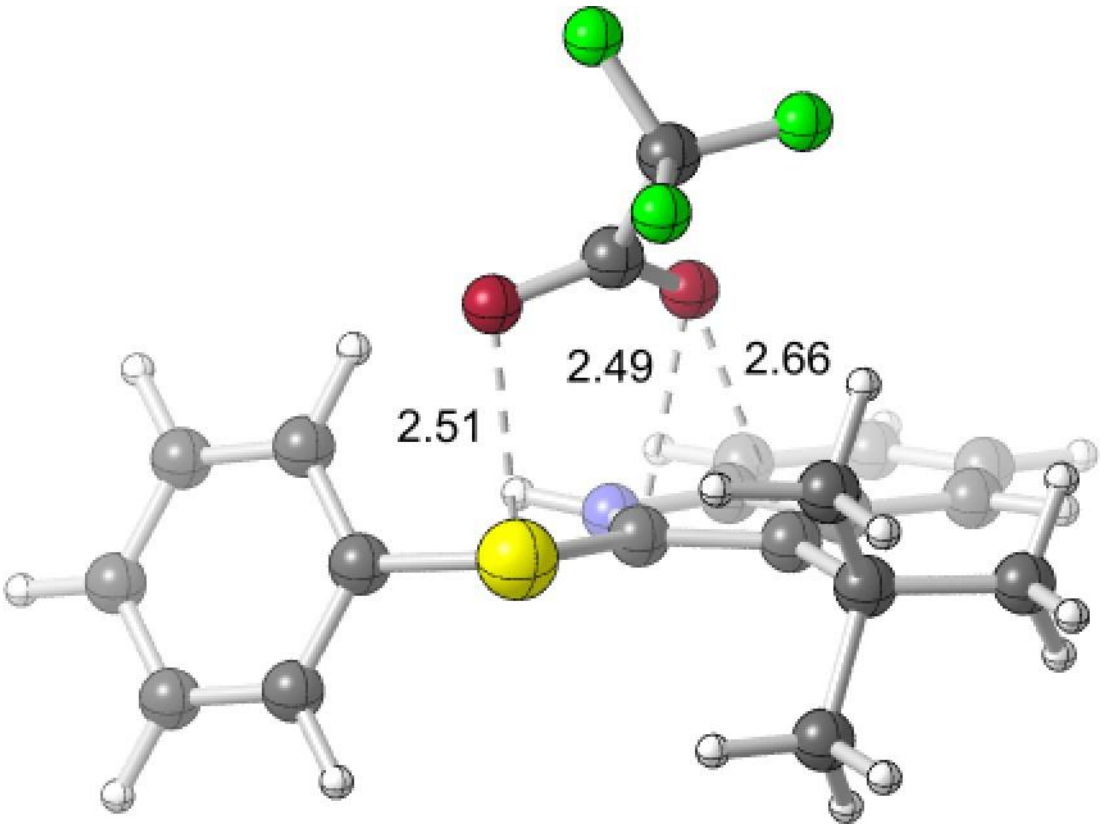
HF=-1519.0039549hartrees(-953190.171739299kcal/mol)
Sum of electronic and thermal Free Energies =
-1518.815422 hartrees (-953071.86545922 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.305653	-2.323924	-0.160454
2	6	2.199861	-1.500538	0.615568
3	6	3.589882	-1.818973	0.679293
4	6	4.027950	-2.925988	-0.006300
5	6	3.117729	-3.720867	-0.757329
6	6	1.751965	-3.441531	-0.848126

7	6	0.066596	-0.707019	0.755766
8	6	1.445330	-0.488870	1.175757
9	1	4.264450	-1.196571	1.256714
10	1	5.074719	-3.206731	0.015529
11	1	3.503147	-4.586173	-1.287605
12	1	1.084812	-4.066662	-1.429751
13	1	-0.804510	-2.198598	-0.461477
14	7	0.032732	-1.798041	-0.054131
15	16	-1.188080	0.268516	1.287186
16	8	-0.800452	2.178472	-0.271843
17	6	-2.628974	-0.313361	0.427473
18	6	-2.651389	-0.385178	-0.974797
19	6	-3.757979	-0.606976	1.205872
20	6	-3.824593	-0.802667	-1.597157
21	1	-1.785110	-0.086399	-1.554558
22	6	-4.920483	-1.023158	0.559913
23	1	-3.725622	-0.524812	2.287267
24	6	-4.952385	-1.124765	-0.833604
25	1	-3.862199	-0.862045	-2.679995
26	1	-5.800229	-1.265657	1.146854
27	1	-5.863603	-1.444593	-1.329216
28	6	0.416643	2.038283	-0.582376
29	8	0.975095	1.000904	-1.002344
30	6	1.342809	3.242099	-0.270660
31	9	2.344589	3.344069	-1.162416
32	9	0.682114	4.411933	-0.251086
33	9	1.901578	3.065483	0.954120
34	1	1.770932	0.320479	1.815074

R = *t-Bu*

TS1, Gas Phase

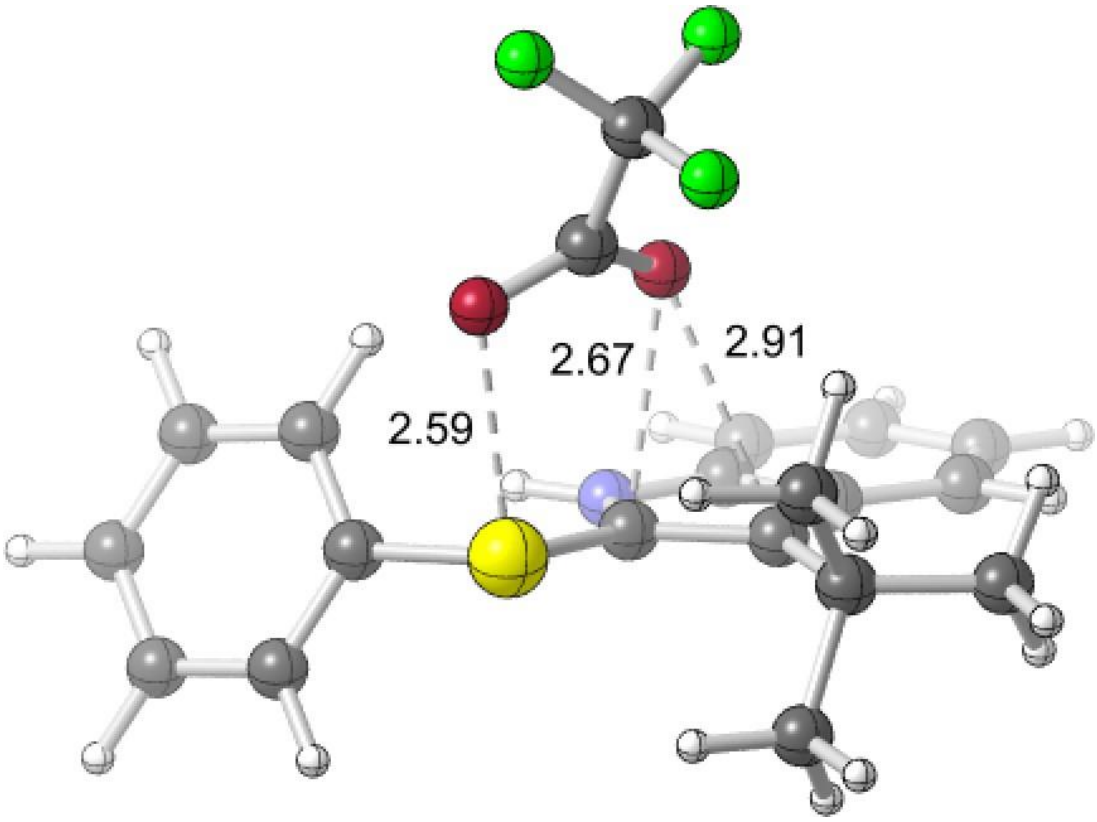


HF = -1676.1866406 hartrees (-1051823.87884291 kcal/mol)
Sum of electronic and thermal Free Energies =
-1675.888008 hartrees (-1051636.48390008 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.650845	-2.252724	-0.966522
2	6	1.759369	-1.825125	-0.158623
3	6	3.042621	-2.390166	-0.442993
4	6	3.161915	-3.310506	-1.461326
5	6	2.037682	-3.702510	-2.225810
6	6	0.765848	-3.182439	-1.988750
7	6	-0.160885	-0.729188	0.452793
8	6	1.291546	-0.867719	0.765492
9	1	3.918219	-2.096472	0.114745
10	1	4.132164	-3.738123	-1.689296
11	1	2.168870	-4.428482	-3.022845
12	1	-0.089113	-3.488479	-2.582275
13	1	-1.385029	-1.618808	-0.991033
14	7	-0.483690	-1.606952	-0.528469
15	16	-1.273549	0.292190	1.199680
16	8	-1.012926	2.058681	-0.557544
17	6	-2.867752	-0.203929	0.535861

18	6	-3.244681	0.095146	-0.780903
19	6	-3.743895	-0.829899	1.433192
20	6	-4.519339	-0.281891	-1.206411
21	1	-2.572545	0.653535	-1.422084
22	6	-5.013908	-1.192798	0.986060
23	1	-3.444163	-1.031331	2.457160
24	6	-5.398312	-0.923928	-0.330010
25	1	-4.831247	-0.051104	-2.220440
26	1	-5.702044	-1.680576	1.669282
27	1	-6.391384	-1.202491	-0.669187
28	6	1.993189	-0.207719	1.936697
29	6	0.197468	1.956824	-0.917007
30	8	0.799270	0.885942	-1.174827
31	6	0.985487	3.292013	-0.975612
32	9	2.288693	3.079796	-1.223008
33	9	0.490451	4.087208	-1.934908
34	9	0.885599	3.936490	0.205348
35	6	1.881575	1.340158	1.874640
36	1	0.852886	1.707017	1.867767
37	1	2.367000	1.755389	2.763116
38	1	2.393219	1.725940	0.990877
39	6	1.333217	-0.734539	3.251695
40	1	0.290813	-0.424141	3.352461
41	1	1.380372	-1.826864	3.313419
42	1	1.888682	-0.324154	4.100666
43	6	3.494755	-0.548301	2.009546
44	1	3.672156	-1.616986	2.164633
45	1	4.035049	-0.209768	1.120233
46	1	3.924818	-0.023468	2.867218

TS1, PCM H2O



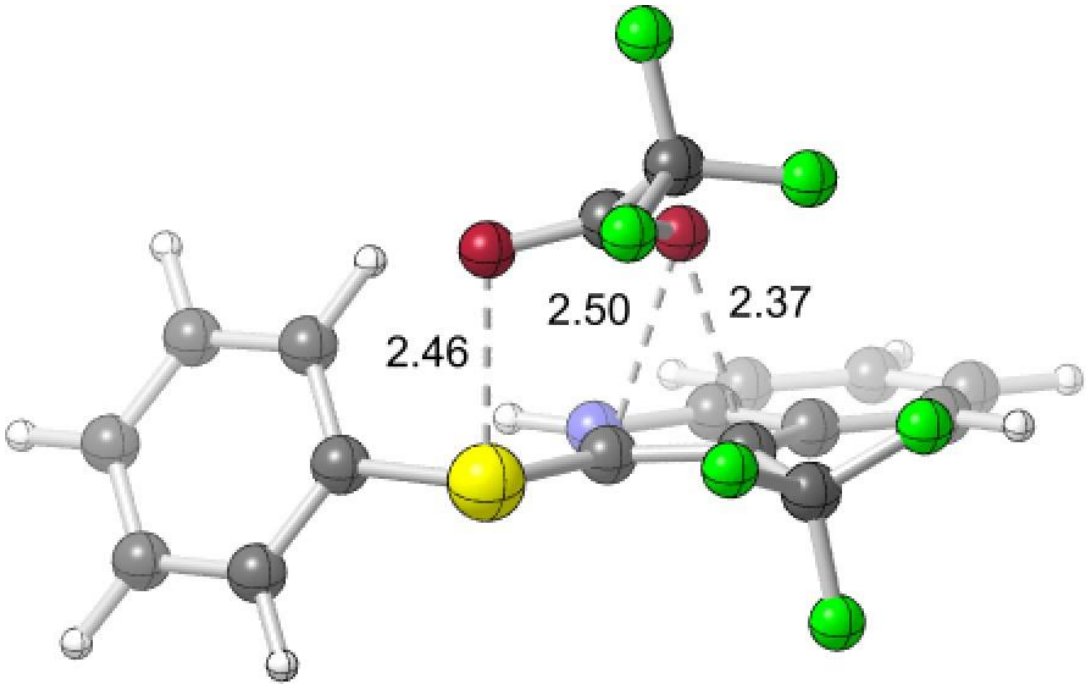
HF=-1676.2583582 hartrees (-1051868.88235408 kcal/mol)
Sum of electronic and thermal Free Energies =
-1675.961101 hartrees (-1051682.35048851 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.963879	-2.104019	-1.128520
2	6	2.010035	-1.625629	-0.260307
3	6	3.361207	-1.984128	-0.586546
4	6	3.597322	-2.761360	-1.696226
5	6	2.530246	-3.212126	-2.511885
6	6	1.198349	-2.893426	-2.239981
7	6	-0.045479	-0.890840	0.447370
8	6	1.423201	-0.868620	0.762079
9	1	4.190198	-1.645060	0.014014
10	1	4.613543	-3.033800	-1.957038
11	1	2.754365	-3.824944	-3.379325
12	1	0.391266	-3.244954	-2.871848
13	1	-1.144436	-1.815751	-1.082770
14	7	-0.244208	-1.656236	-0.644367
15	16	-1.249877	-0.094379	1.300204
16	8	-1.241718	2.075783	-0.107392
17	6	-2.785114	-0.614444	0.541493

18	6	-3.116996	-0.268506	-0.775893
19	6	-3.668816	-1.323944	1.366235
20	6	-4.349197	-0.682872	-1.280199
21	1	-2.442444	0.335064	-1.370765
22	6	-4.897082	-1.723766	0.841347
23	1	-3.401662	-1.566564	2.389476
24	6	-5.234076	-1.408531	-0.477309
25	1	-4.620811	-0.424905	-2.298820
26	1	-5.587939	-2.280964	1.465763
27	1	-6.193396	-1.720808	-0.878185
28	6	2.029931	-0.245846	2.001506
29	6	-0.129325	2.123669	-0.706219
30	8	0.566704	1.175016	-1.122041
31	6	0.454379	3.556318	-0.876713
32	9	1.312390	3.624827	-1.910671
33	9	-0.510965	4.473737	-1.079577
34	9	1.131685	3.924752	0.239620
35	6	1.730360	1.277258	2.072766
36	1	0.664774	1.510384	2.120360
37	1	2.193611	1.671046	2.982568
38	1	2.158245	1.796557	1.213121
39	6	1.431720	-0.964425	3.253284
40	1	0.360180	-0.790335	3.368313
41	1	1.608144	-2.043449	3.209294
42	1	1.934968	-0.569851	4.141334
43	6	3.560599	-0.410168	2.070007
44	1	3.862613	-1.460907	2.105500
45	1	4.065317	0.088593	1.237228
46	1	3.912217	0.060564	2.992462

R = CF_3

TS1, Gas Phase

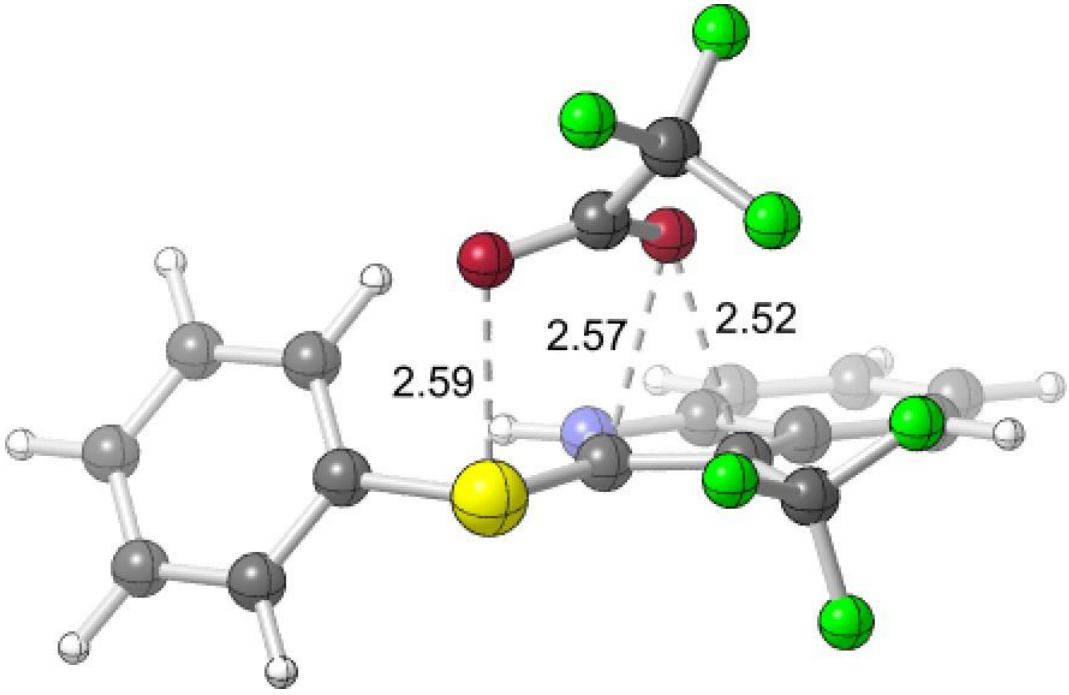


HF=-1855.9506043 hartrees (-1164627.56370429 kcal/mol)
Sum of electronic and thermal Free Energies =
-1855.760833 hartrees (-1164508.48031583 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.487743	2.544372	-0.550904
2	6	-1.614743	1.900118	0.054487
3	6	-2.914895	2.459009	-0.090203
4	6	-3.038062	3.629530	-0.806732
5	6	-1.902958	4.246676	-1.390148
6	6	-0.613222	3.720693	-1.274050
7	6	0.306997	0.717957	0.490366
8	6	-1.140595	0.742847	0.674595
9	1	-3.774762	1.967701	0.349217
10	1	-4.012824	4.086474	-0.937760
11	1	-2.040310	5.165260	-1.952957
12	1	0.237856	4.212598	-1.732605
13	1	1.581990	1.981453	-0.594967
14	7	0.644412	1.800384	-0.256478
15	16	1.335182	-0.483190	1.078110
16	8	0.834247	-1.970535	-0.815259
17	6	2.945383	-0.028193	0.461014
18	6	3.211208	-0.002253	-0.918035
19	6	3.948632	0.193310	1.415982
20	6	4.506986	0.296028	-1.335659
21	1	2.435399	-0.269587	-1.627218

22	6	5.236393	0.490446	0.972911
23	1	3.729748	0.140754	2.478214
24	6	5.513068	0.545674	-0.395985
25	1	4.736001	0.308827	-2.396757
26	1	6.023124	0.671760	1.698240
27	1	6.521169	0.767250	-0.732648
28	6	-0.394558	-1.760212	-1.026406
29	8	-0.896129	-0.621498	-1.248813
30	6	-1.342495	-2.984544	-0.962961
31	9	-1.274485	-3.664171	-2.118725
32	9	-0.987369	-3.801584	0.039369
33	9	-2.611489	-2.595135	-0.766801
34	6	-1.934386	-0.167311	1.582735
35	9	-1.350737	-1.376120	1.699753
36	9	-1.990093	0.384376	2.807584
37	9	-3.177626	-0.328783	1.127861

TS1, PCM H2O



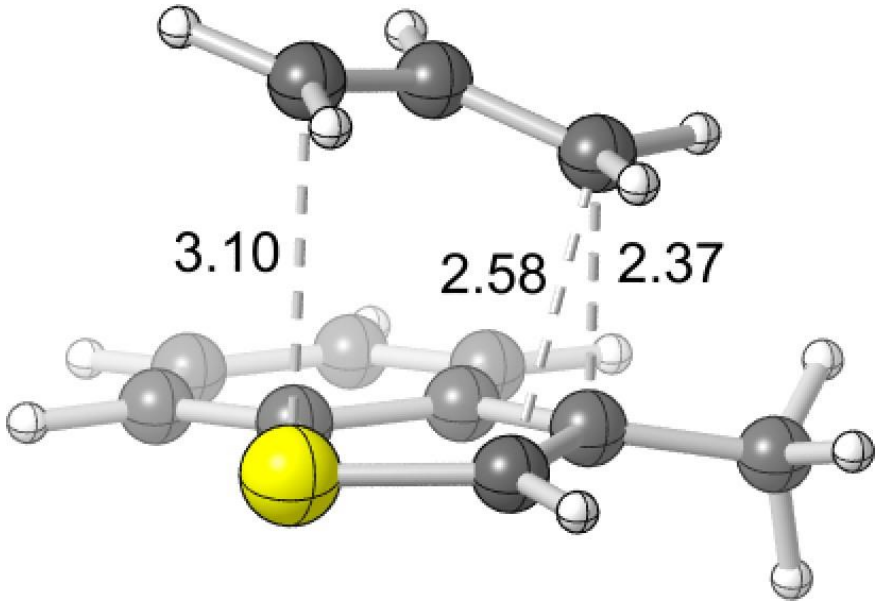
HF=-1856.0262525hartrees(-1164675.03370628kcal/mol)
Sum of electronic and thermal Free Energies =
-1855.836900 hartrees (-1164556.213119 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-0.511783	2.512402	-0.670724
2	6	-1.624610	1.915483	0.023954
3	6	-2.935130	2.468999	-0.122325
4	6	-3.075353	3.578745	-0.917132
5	6	-1.951658	4.149552	-1.579916
6	6	-0.658644	3.632806	-1.471202
7	6	0.317947	0.783135	0.485160
8	6	-1.129001	0.831307	0.724826
9	1	-3.780382	2.018268	0.382716
10	1	-4.049890	4.033163	-1.052949
11	1	-2.107732	5.026130	-2.200633
12	1	0.179389	4.086609	-1.986782
13	1	1.557445	2.001051	-0.700384
14	7	0.623435	1.791558	-0.365002
15	16	1.368942	-0.321523	1.194387
16	8	0.839336	-2.130264	-0.586623
17	6	2.957229	0.043171	0.487609
18	6	3.165382	0.012310	-0.901573
19	6	4.007193	0.267512	1.391442
20	6	4.448236	0.257033	-1.384106
21	1	2.353404	-0.238512	-1.574297
22	6	5.281367	0.510648	0.883953
23	1	3.829055	0.266722	2.461603
24	6	5.500150	0.510368	-0.496806
25	1	4.628432	0.234744	-2.453871
26	1	6.101798	0.699718	1.568248
27	1	6.497007	0.696203	-0.883967
28	6	-0.346879	-1.895298	-0.927562
29	8	-0.849922	-0.772414	-1.199543
30	6	-1.331102	-3.094349	-0.978827
31	9	-0.710676	-4.274819	-0.821870
32	9	-2.263592	-2.982808	-0.006518
33	9	-1.980258	-3.118655	-2.161126
34	6	-1.905301	-0.038949	1.681097
35	9	-1.280298	-1.210940	1.907367
36	9	-2.041303	0.588233	2.861637
37	9	-3.128230	-0.297505	1.199096

Benzothiophene System

TS1, Gas Phase



HF = -863.0101291 hartrees (-541547.486111541 kcal/mol)
Sum of electronic and thermal Free Energies =
-862.833213 hartrees (-541436.46948963 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.240740	-0.475785	-0.640460
2	6	-1.217681	0.260613	0.055519
3	6	-2.338995	-0.416987	0.538005
4	6	-2.450973	-1.794017	0.322456
5	6	-1.467463	-2.497530	-0.378617
6	6	-0.340693	-1.837542	-0.884481
7	6	0.254425	2.023134	-0.453205
8	6	-0.909909	1.696441	0.146900
9	1	-3.119830	0.119244	1.068022
10	1	-3.321699	-2.322752	0.697089
11	1	-1.578234	-3.564171	-0.545045
12	1	0.411511	-2.378269	-1.449613
13	6	-1.816566	2.680419	0.820908
14	1	-1.978976	2.399305	1.868181
15	1	-1.405492	3.691765	0.794068
16	1	-2.797537	2.694500	0.330962
17	16	1.041957	0.622230	-1.225937
18	6	2.627072	0.322134	-0.118557
19	1	3.413961	0.338324	-0.875989
20	1	2.671145	1.221760	0.497143
21	6	2.589500	-0.929354	0.674880

```
  22      1        2.741019  -1.862284   0.136881
  23      6        2.444009  -0.933836   2.004067
  24      1        2.310280  -0.017371   2.574086
  25      1        2.480531  -1.858737   2.571592
  26      1        0.710090   2.996876  -0.576880
 ---------------------------------------------------------------
```

Example Configuration File for Molecular Dynamics Simulations (in implicit water solvent)

```
#*** method --The following word is copied exactly to the gaussian input
file.
method b3lyp/6-31g(d)
#Rotationmode controls whether molecular rotations are turned on. They should be
turned on with rotationmode 1 but this can be set #at 0 to reproduce older
calculations.
rotationmode 1
#*** method2 --The options here are restricted, unrestricted, and read.
restricted is the default
#If the method is U..., put unrestricted here and the .com files will have in
them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which
sometimes makes things faster, sometimes not.
#The use of read requires a specifically defined checkpoint file name using
the keyword checkpoint.
method2 restricted charge
1
multiplicity 1
processors 16
#*** memory --The following "word" is copied exactly to the gaussian input
file after %mem=.
memory 16GB
#*** killcheck and checkpoint -- You can use a specifically defined checkpoint
file name by putting
#the name after the keyword checkpoint.          This is necessary if you use
the read option with method2.
#Defined checkpoint names are an unnecessary modest hastle and if you do not
want to bother, use killcheck 1
killcheck 1 #checkpoint
g09.chk
#*** diagnostics -- 0 prints out nothing extra, 1 (default) prints out extra
stuff to a
#file "diagnostics", 2 adds more stuff, 3 adds velocities to a file "vellist"
#4 adds the apparent temperature to vellist, but this is
meaningless with quasiclassical calculations diagnostics 3
#*** title -- the title keyword must be followed by exactly four words
title Pummerer 33shift Molecular Dynamics
```

```
#*** initialdis -- 0 (default) turns off displacement of the normal modes, so
that all trajectories start from the same place # and only the energies and
signs of the motion in the modes are randomized
# 1 gives a flat distribution of displacements where all of the possible
values are equally likely
# 2 (recommended) gives a QM-like gaussian distribution of displacements, so
that displacements in the middle are more likely that
# those at the end by 1/e initialdis 2
#*** timestep -- this is the time between points in the trajectory.   Typical
values would be 1E-15 or 0.5E-15 or 0.25E-15 timestep 1E-15
#*** scaling -- this lets you scale the gaussian frequencies by a constant
scaling 1.0
temperature 298.15
#*** method3, method4, method5, and method6 -- These keywords let you add extra
lines to the gaussian input file.
#method3 and method4 add lines at the top of the input after the lines
defining the method, and
#this is useful to implement things like the iop for mPW1k #method5 and
method6 add lines after the geometry, after a blank line of course
#only a single term with no spaces can be added, one per method line.  Here
are some examples to uncomment if needed
#method3 IOp(3/76=0572004280)
method3 scrf=(pcm,solvent=water)
#add the line below with big structures to get it to put out the distance
matrix and the input orientation
#method3 iop(2/9=2000)
#method4 scrf=(pcm,solvent=dmso,read) #method4
IOp(3/76=1000001970)IOp(3/77=0800008000)IOp(3/78=0700010000)
#method5 radii=bondi
#method6
#*** methodfile -- This keyword lets you add more complicated endings to
gaussian input files
#such as a gen basis set.        Put after the keyword the number of lines
in a file you create called
#methodfile that contains the test you want to add to the end of the gaussian
input
#methodfile 10
#*** numimag --This tells the program the number of imaginary frequencies in
the starting structure.
#if 0, treats as ground state and direction of all modes is random
#if 1, motion along the reaction coordinate will start out in the direction
defined by searchdir
```

```
#if 2, only lowest freq will go direction of searchdir and other imag mode
will go in random direction
numimag 1
#*** searchdir -- This keyword says what direction to follow the mode
associated with the imaginary frequency.
#The choices are "negative" and "positive".           Positive moves in
the direction defined in the gaussian frequency calculation #for the
imaginary frequency, while negative moves in the opposite direction.  The
correct choice can be made either #by a careful inspection of the normal
modes and standard orientation geometry, or by trial and error.
searchdir negative
#*** classical --      for quassiclassical dynamics, the default, use
0.   for classical dynamics, use 1
#if there are no normal modes and the velocities are to be generated from
scratch, use classical 2
classical 0
#*** keepevery --This tells the program how often to write the gaussian
output file to file dyn, after the first two points. #Use 1 for most dynamics
to start with, but use a higher number to save on disk space or molden loading
time.
keepevery 1
#*** highlevel --For ONIOM jobs, the following line states the number of
highlevel atoms,
#which must come before the medium level atoms.            Use some high
value such as 999 if not using ONIOM
highlevel 999
#*** boxon and boxsize - With boxon 1, a cubic box is set such that atoms that
reach the edge
#are reflected back toward the middle.          Useful for dynamics with
solvent molecules.       This is a crude
#implementation that is ok for a few thousand femtoseconds but will not
conserve energy long term.
#Set the box size so as to fit the entire initial molecule but not have too
much extra room.
#The dimensions of the box are two times the boxsize, e.g. boxsize 7.5
leads to a box that is 15 x 15 x 15 angstroms boxon 0
boxsize 7.5
#*** etolerance --This sets the allowable difference between the desired
energy in a trajectory and the actual
#energy, known after point 1 from the potential energy + the kinetic energy in
the initial velocities.
#The unit is kcal/mol and 1 is a normal value for mid-sized organic
systems.              For very large and floppy molecules, a larger value
#may be needed, but the value must stay way below the average thermal energy
in the molecule (not counting zpe).
#If initialdis is not 0 and few trajectories are being rejected, decrease the
value.
```

etolerance 1.0
#*** damping -- The damping keyword lets you add or subtract energy from the system at each point, by multiplying the velocities
#by the damping factor. A damping of 1 has no effect, and since you mostly want to change the energy slowly, normal values range #from 0.95 to 1.05.
The use of damping lets one do simulated annealing - you add energy until the structure is moving enough #to sample the kinds of possibilities you are interested in, then you take away the energy slowly.
damping 1
#*** reversetraj --This keyword sets the trajectories so that both directions from a transition state are explored. reversetraj true