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In-silico Investigation on the Separation of Disulfide Bond by N- Heterocyclic Carbene

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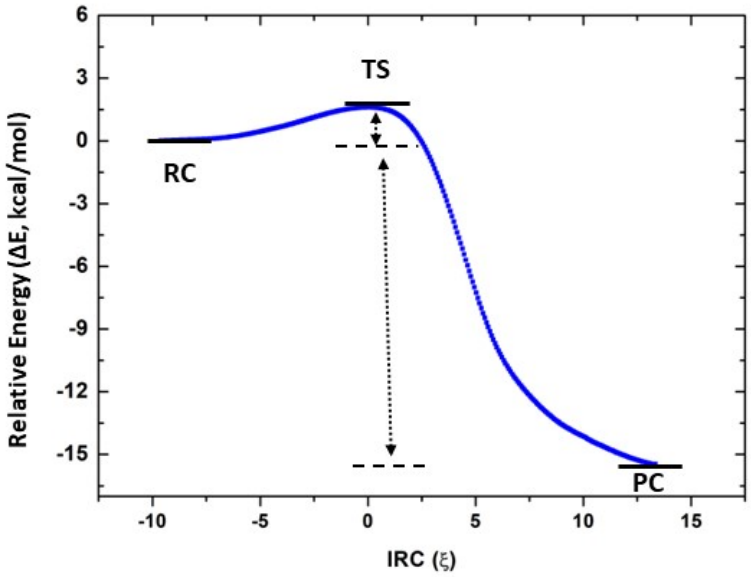

Fig. S1: The calculated IRC of the Reaction-3, the relative energy data is given with respect to reactant complex (RC) in water medium. (In kcal/mol unit)

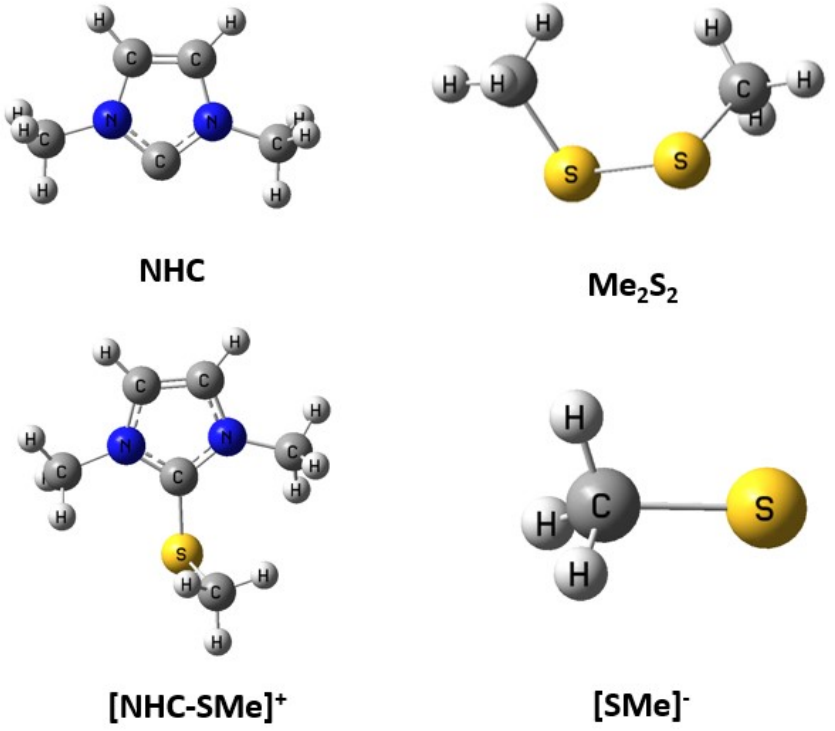

Fig. S2: The optimized geometries of individual reactants and products at M06-2X/6-311G (d, p) in water medium.

Table S1: The AIM analysis of reactant complex (RC), TS and product complex (PC) at BCPs for Reaction 3 in a.u. unit.

Systems	Bond	BCP	Electron Density	Energy Density H(r)
Reactant Complex	S-S	Yes	0.1374	-0.0673
	C-S	No	-	-
TS	S-S	Yes	0.0991	-0.0320
	C-S	Yes	0.0369	-0.0038
Product Complex	S-S	No	-	-
	C-S	Yes	0.1940	-0.1707

Table S2: Calculated thermodynamic parameter in both gas and solvent phase at M06-2X/6311G (d, p) level. (data given in kcal/mol unit)

No	Activation Energy								Reaction Energy							
	Gas		Water		DMSO		Acetone		Gas		Water		DMSO		Acetone	
	$\Delta G^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta H^{\ddagger}$	ΔG_R	ΔH_R	ΔG_R	ΔH_R	ΔG_R	ΔH_R	ΔG_R	ΔH_R
Rea1	43.5	42.1	15.7	12.5	15.7	12.6	16.1	13.0	26.1	24.6	9.3	4.9	8.8	6.1	10.6	7.8
Rea2	40.6	39.8	15.8	16.3	16.2	16.5	17.2	17.1	19.0	18.3	13.4	12.7	15.4	12.6	16.3	15.0
Rea3	22.2	21.8	6.8	8.0	7.1	8.1	7.4	8.1	3.8	4.2	-8.4	-7.9	-7.8	-7.4	-7.1	-6.0

Reaction Coordinate:

For Reaction 1

Reactant Complex (RC)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.000812	0.414526	-0.655242
2	16	0	-1.177974	0.145803	0.298208
3	6	0	-4.176883	0.128549	0.702191
4	1	0	-4.008894	0.846906	1.501735
5	1	0	-5.171556	0.275138	0.280009
6	1	0	-4.091816	-0.889144	1.078538
7	6	0	-0.991259	-1.661110	0.209155
8	1	0	-0.989463	-1.987799	-0.829320
9	1	0	-0.029392	-1.889766	0.669906
10	1	0	-1.787433	-2.155633	0.762420
11	15	0	2.359528	-0.018461	0.382261
12	6	0	2.364697	1.756047	-0.137074
13	1	0	2.680506	2.380035	0.700972
14	1	0	3.039350	1.923115	-0.980876
15	6	0	4.183325	-0.290596	0.537964
16	1	0	4.715623	0.046978	-0.355278
17	1	0	4.559984	0.254421	1.405345
18	6	0	2.081396	-0.810362	-1.267156

19	1	0	2.179082	-1.894244	-1.176762
20	1	0	1.069706	-0.585056	-1.611053
21	1	0	1.352969	2.050997	-0.421617
22	1	0	4.381976	-1.352837	0.691145
23	1	0	2.799356	-0.446630	-2.007005

Transition State (TS)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.047904	-0.352576	-0.003206
2	16	0	-0.650748	-0.156689	-0.002478
3	6	0	-3.264219	1.455866	0.004455
4	1	0	-2.807200	1.901535	-0.880106
5	1	0	-4.328686	1.687798	0.001666
6	1	0	-2.813376	1.893414	0.896153
7	6	0	-0.558843	-1.983643	0.004288
8	1	0	-1.057472	-2.364855	-0.884302
9	1	0	0.481485	-2.302597	0.000765
10	1	0	-1.049940	-2.358355	0.899782
11	15	0	1.753725	0.133195	-0.000247
12	6	0	1.877798	1.949416	-0.005299
13	1	0	1.378678	2.345593	0.880297
14	1	0	2.921828	2.266434	-0.005388
15	6	0	2.735406	-0.392043	1.447995
16	1	0	3.748175	0.013019	1.390878
17	1	0	2.249774	-0.033695	2.356322
18	6	0	2.740630	-0.400492	-1.441876
19	1	0	2.787599	-1.489741	-1.469733
20	1	0	2.259351	-0.045685	-2.353899
21	1	0	1.380016	2.340649	-0.893841
22	1	0	2.783910	-1.481078	1.481115
23	1	0	3.753792	0.003255	-1.382426

Product Complex (PC)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.598245	-0.371372	-0.037329
2	16	0	-0.248913	-0.129023	-0.003536
3	6	0	-3.236853	1.431646	0.046393
4	1	0	-2.626228	1.745595	-0.802906

5	1	0	-4.155817	2.020029	0.036813
6	1	0	-2.687703	1.677229	0.957665
7	6	0	-0.249370	-1.956265	0.036832
8	1	0	-1.309395	-2.202638	0.009475
9	1	0	0.249634	-2.370406	-0.836568
10	1	0	0.192052	-2.325098	0.960050
11	15	0	1.806886	0.201820	-0.004057
12	6	0	1.980738	1.991622	0.085170
13	1	0	1.533445	2.353665	1.010682
14	1	0	3.041633	2.242871	0.065833
15	6	0	2.612164	-0.559111	1.418149
16	1	0	3.662011	-0.260575	1.420982
17	1	0	2.123643	-0.215316	2.329706
18	6	0	2.587073	-0.398266	-1.514967
19	1	0	2.481800	-1.480843	-1.583289
20	1	0	2.108594	0.075911	-2.371594
21	1	0	1.481483	2.445129	-0.771125
22	1	0	2.546565	-1.644695	1.345908
23	1	0	3.646999	-0.139590	-1.486407

For Reaction 2

Reactant Complex (RC)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	4.886781	-1.600354	0.380015
2	16	0	2.835079	-1.586465	0.693711
3	6	0	5.132239	0.031722	-0.382156
4	1	0	4.794441	0.822510	0.286436
5	1	0	6.204709	0.135809	-0.549646
6	1	0	4.604561	0.084411	-1.332438
7	6	0	2.731736	-0.756442	2.308300
8	1	0	3.168978	0.240479	2.257876
9	1	0	1.668817	-0.676333	2.540339
10	1	0	3.234131	-1.349633	3.069187
11	15	0	-0.717049	-0.475372	0.421920
12	6	0	0.258491	0.322965	-0.940781
13	1	0	0.860338	-0.468369	-1.392569
14	1	0	-0.394535	0.718559	-1.723421
15	6	0	-1.980032	-1.357278	-0.616206
16	1	0	-2.377272	-0.699665	-1.394005
17	1	0	-1.458005	-2.171849	-1.124711
18	6	0	-1.701540	0.967377	1.065803
19	1	0	-2.365002	0.581538	1.844360
20	1	0	-0.994365	1.621537	1.583311

21	6	0	1.177939	1.414409	-0.409332
22	1	0	0.634579	2.337284	-0.185835
23	1	0	1.662823	1.116662	0.526853
24	6	0	-2.500040	1.768449	0.048977
25	1	0	-1.870791	2.150920	-0.760733
26	1	0	-3.277210	1.167262	-0.431234
27	6	0	-3.114001	-1.925442	0.225324
28	1	0	-3.691540	-1.139406	0.721668
29	1	0	-2.738083	-2.573320	1.023591
30	6	0	2.287120	1.759844	-1.368502
31	8	0	2.503403	1.219052	-2.421420
32	8	0	3.049737	2.757044	-0.896819
33	1	0	3.748726	2.934781	-1.542839
34	6	0	-3.183802	2.961010	0.669576
35	8	0	-3.105460	3.294664	1.822258
36	8	0	-3.909744	3.635422	-0.233446
37	1	0	-4.317446	4.391503	0.212675
38	6	0	-4.082308	-2.740268	-0.593636
39	8	0	-3.978183	-2.981956	-1.766981
40	8	0	-5.104366	-3.184423	0.151272
41	1	0	-5.689775	-3.701517	-0.420398

Transition State (TS)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.987418	-2.015554	-1.332809
2	16	0	-1.806040	-1.052575	-0.655128
3	6	0	-4.789795	-1.239674	0.109515
4	1	0	-4.569289	-0.170522	0.138649
5	1	0	-5.869629	-1.367405	0.040780
6	1	0	-4.442889	-1.694589	1.038173
7	6	0	-1.048433	-1.942315	-2.064483
8	1	0	-1.598000	-1.676906	-2.964506
9	1	0	-0.005856	-1.653302	-2.183288
10	1	0	-1.116271	-3.012990	-1.885399
11	15	0	0.179833	-0.092857	0.095750
12	6	0	-0.461519	1.192605	1.223296
13	1	0	-1.205144	0.704531	1.859848
14	1	0	0.341125	1.540823	1.877719
15	6	0	1.201411	-1.166538	1.167939
16	1	0	1.992611	-0.577556	1.638728
17	1	0	0.539981	-1.517127	1.964312
18	6	0	1.313821	0.751681	-1.072184
19	1	0	1.766659	-0.009171	-1.712069
20	1	0	0.692365	1.369051	-1.725886
21	6	0	-1.102093	2.353672	0.471468

22	1	0	-0.371903	2.925847	-0.107251
23	1	0	-1.856306	2.004226	-0.240280
24	6	0	2.398548	1.590234	-0.405180
25	1	0	1.983467	2.366220	0.244158
26	1	0	3.059654	0.985080	0.220559
27	6	0	1.779777	-2.355252	0.410699
28	1	0	2.456488	-2.048098	-0.391900
29	1	0	0.992167	-2.955380	-0.055216
30	6	0	-1.783040	3.312484	1.416473
31	8	0	-1.878684	3.167336	2.605642
32	8	0	-2.284919	4.365160	0.761952
33	1	0	-2.717140	4.944764	1.405839
34	6	0	3.264032	2.279900	-1.432887
35	8	0	3.136986	2.185030	-2.623978
36	8	0	4.210074	3.023545	-0.850389
37	1	0	4.737852	3.442437	-1.545772
38	6	0	2.554874	-3.267359	1.329609
39	8	0	2.689616	-3.109035	2.513254
40	8	0	3.084038	-4.297158	0.660671
41	1	0	3.565522	-4.852667	1.290739

Product Complex (PC)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-4.464713	-1.972755	-1.549762
2	16	0	-1.525164	-0.891679	-0.562221
3	6	0	-4.793307	-1.328585	0.141602
4	1	0	-4.311509	-0.358963	0.289526
5	1	0	-5.863155	-1.201643	0.314604
6	1	0	-4.407259	-2.011514	0.901054
7	6	0	-0.886265	-1.445697	-2.185833
8	1	0	-1.749157	-1.945163	-2.622220
9	1	0	-0.603666	-0.594288	-2.799749
10	1	0	-0.066350	-2.151541	-2.076400
11	15	0	0.199357	-0.027546	0.240550
12	6	0	-0.375817	1.311763	1.320311
13	1	0	-1.126153	0.879959	1.988137
14	1	0	0.466293	1.624254	1.943953
15	6	0	1.122393	-1.203232	1.268212
16	1	0	1.960488	-0.670152	1.724274
17	1	0	0.444881	-1.497534	2.073683
18	6	0	1.269965	0.647832	-1.060003
19	1	0	1.602057	-0.174788	-1.696908
20	1	0	0.654927	1.303567	-1.682173
21	6	0	-0.962189	2.484500	0.542741
22	1	0	-0.211365	3.003768	-0.058258
23	1	0	-1.749128	2.159870	-0.144124

24	6	0	2.471292	1.401957	-0.496146
25	1	0	2.176487	2.242510	0.137561
26	1	0	3.116130	0.761276	0.110677
27	6	0	1.598239	-2.428291	0.497937
28	1	0	2.270908	-2.172188	-0.325126
29	1	0	0.758989	-2.984479	0.070380
30	6	0	-1.570221	3.493220	1.488000
31	8	0	-1.636700	3.367055	2.680594
32	8	0	-2.035752	4.554164	0.826228
33	1	0	-2.424654	5.167684	1.466698
34	6	0	3.314265	1.954568	-1.622633
35	8	0	3.075378	1.815795	-2.790999
36	8	0	4.368659	2.621451	-1.151522
37	1	0	4.878706	2.958262	-1.902712
38	6	0	2.343022	-3.370065	1.414669
39	8	0	2.527290	-3.186187	2.587053
40	8	0	2.775877	-4.445138	0.753717
41	1	0	3.243933	-5.019701	1.376897

For Reaction 3

Reactant Complex (RC)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.025760	-0.851992	-0.377587
2	16	0	1.042740	-0.635288	0.199932
3	6	0	3.424235	0.844792	-0.895660
4	1	0	3.326815	1.534548	-0.058972
5	1	0	4.461343	0.831271	-1.232002
6	1	0	2.777096	1.148410	-1.715986
7	6	0	1.234020	-0.038518	1.907472
8	1	0	1.764682	0.912534	1.925861
9	1	0	0.218488	0.097636	2.281635
10	1	0	1.760724	-0.778232	2.506652
11	6	0	-2.058347	0.189622	0.842769
12	6	0	-1.831617	1.050209	-1.262757
13	6	0	-2.398588	-0.171666	-1.388834
14	7	0	-1.643320	1.247551	0.092066
15	7	0	-2.526264	-0.668697	-0.104300
16	1	0	-1.555201	1.781825	-2.003810
17	1	0	-2.719267	-0.716863	-2.261117
18	6	0	-0.963182	2.406588	0.642997
19	1	0	-1.397585	3.324539	0.246672
20	1	0	-1.080814	2.384717	1.724082
21	1	0	0.100167	2.371007	0.392173
22	6	0	-3.066944	-1.983363	0.199248
23	1	0	-2.420788	-2.762634	-0.207854
24	1	0	-3.114676	-2.080889	1.280999

25	1	0	-4.067365	-2.089365	-0.221630

Transition State (TS)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.366861	-0.108197	0.075223
2	16	0	-1.121152	-0.038268	0.160836
3	6	0	-3.486944	0.780236	-1.505201
4	1	0	-2.979070	0.227379	-2.295551
5	1	0	-4.541808	0.874460	-1.759707
6	1	0	-3.052517	1.776364	-1.419177
7	6	0	-1.138766	-0.962896	1.731891
8	1	0	-1.606069	-1.935942	1.583188
9	1	0	-0.105730	-1.087294	2.042914
10	1	0	-1.688336	-0.400423	2.485611
11	6	0	1.284453	-0.011029	0.204076
12	6	0	3.327852	-0.473306	-0.657298
13	6	0	3.301597	0.847530	-0.363936
14	7	0	2.086025	-0.972803	-0.307454
15	7	0	2.045420	1.105139	0.156027
16	1	0	4.104603	-1.089878	-1.077423
17	1	0	4.050294	1.613333	-0.477662
18	6	0	1.692221	-2.367927	-0.444096
19	1	0	2.212612	-2.983185	0.290182
20	1	0	0.618282	-2.429811	-0.281333
21	1	0	1.928509	-2.721603	-1.447141
22	6	0	1.601694	2.415032	0.611880
23	1	0	1.683696	3.139284	-0.198399
24	1	0	0.562401	2.324726	0.918217
25	1	0	2.208586	2.743838	1.455424

Product Complex (PC)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.933929	-0.265509	0.139050
2	16	0	-0.556485	-0.068268	0.101305
3	6	0	-3.524485	0.876491	-1.245639
4	1	0	-2.805117	0.419302	-1.928480
5	1	0	-4.415599	1.136296	-1.819445

6	1	0	-3.083281	1.802010	-0.870017
7	6	0	-0.630535	-0.958007	1.696965
8	1	0	-0.210914	-1.957459	1.601165
9	1	0	-0.115991	-0.388151	2.467181
10	1	0	-1.696458	-1.018390	1.909566
11	6	0	1.189058	0.037462	-0.041741
12	6	0	3.313389	-0.454757	-0.430302
13	6	0	3.237132	0.871977	-0.151136
14	7	0	2.035694	-0.953358	-0.367140
15	7	0	1.916053	1.157618	0.091469
16	1	0	4.157376	-1.078908	-0.667882
17	1	0	4.001137	1.628121	-0.102780
18	6	0	1.669229	-2.351278	-0.589103
19	1	0	1.801090	-2.915302	0.333228
20	1	0	0.631309	-2.391319	-0.911982
21	1	0	2.313340	-2.753891	-1.366419
22	6	0	1.383553	2.481894	0.417853
23	1	0	0.887573	2.903919	-0.454253
24	1	0	0.677794	2.390048	1.239754
25	1	0	2.218095	3.111637	0.712992

ETS-NOCV Study

NOCV Pair energy for TS of Reaction 1

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-76.14	1	0.88371	-113.26	258	-0.88371	-27.09
2	-4.89	2	0.18494	-55.96	257	-0.18494	-29.51
3	-5.98	3	0.16410	-65.56	256	-0.16410	-29.12
4	-1.70	4	0.09026	-91.00	255	-0.09026	-72.21
5	-1.43	5	0.08905	-15.52	254	-0.08905	0.55
6	-1.06	6	0.06773	-53.09	253	-0.06773	-37.49
7	-0.57	7	0.04384	-118.43	252	-0.04384	-105.37
8	-0.46	8	0.04246	-69.91	251	-0.04246	-58.99
9	-0.47	9	0.03616	-71.69	250	-0.03616	-58.63
10	-0.26	10	0.03187	-27.85	249	-0.03187	-19.76
11	-0.24	11	0.03138	-22.75	248	-0.03138	-15.20
12	-0.22	12	0.02698	-100.14	247	-0.02698	-91.89

13	-0.14	13	0.02448	-66.08	246	-0.02448	-60.17
14	-0.12	14	0.02265	-67.62	245	-0.02265	-62.40
15	-0.10	15	0.02087	-87.11	244	-0.02087	-82.16
16	-0.10	16	0.02016	-77.60	243	-0.02016	-72.72
17	-0.09	17	0.01856	-48.73	242	-0.01856	-43.94
18	-0.07	18	0.01703	-63.46	241	-0.01703	-59.45
19	-0.09	19	0.01619	-64.85	240	-0.01619	-59.53
20	-0.05	20	0.01474	-53.54	239	-0.01474	-49.98
21	-0.04	21	0.01086	-178.38	238	-0.01086	-174.38
22	-0.03	22	0.00906	-151.87	237	-0.00906	-148.55
23	-0.03	23	0.00893	-55.77	236	-0.00893	-52.69
24	-0.03	24	0.00834	-215.82	235	-0.00834	-212.49
25	-0.02	25	0.00693	-108.83	234	-0.00693	-106.64
26	-0.02	26	0.00594	-156.34	233	-0.00594	-153.71
27	-0.02	27	0.00293	-2137.46	232	-0.00293	-2129.37
28	-0.01	28	0.00207	-1709.39	231	-0.00207	-1703.87
29	-0.01	29	0.00194	-1975.40	230	-0.00194	-1970.32
30	-0.00	30	0.00126	-1437.32	229	-0.00126	-1434.03
31	-0.00	31	0.00120	-1244.79	228	-0.00120	-1242.46
32	-0.00	32	0.00111	-1213.01	227	-0.00111	-1210.64
33	-0.00	33	0.00104	-1049.05	226	-0.00104	-1046.12

Sum of NOCV eigenvalues: 0.00000

Sum of pair energies: -94.40 kcal/mol

NOCV Pair energy for TS of Reaction2

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-96.91	1	0.98431	-122.76	510	-0.98431	-24.30
2	-7.64	2	0.23280	-68.09	509	-0.23280	-35.25

3	-8.39	3	0.19386	-79.71	508	-0.19386	-36.42
4	-2.60	4	0.11333	-95.32	507	-0.11333	-72.35
5	-1.96	5	0.10530	-15.36	506	-0.10530	3.27
6	-1.38	6	0.07816	-48.45	505	-0.07816	-30.86
7	-0.69	7	0.05178	-104.91	504	-0.05178	-91.68
8	-0.75	8	0.04995	-98.81	503	-0.04995	-83.87
9	-0.54	9	0.04122	-81.29	502	-0.04122	-68.16
10	-0.38	10	0.03826	-35.09	501	-0.03826	-25.11
11	-0.33	11	0.03609	-32.64	500	-0.03609	-23.43
12	-0.30	12	0.03110	-79.56	499	-0.03110	-69.96
13	-0.20	13	0.02893	-73.35	498	-0.02893	-66.40
14	-0.19	14	0.02792	-81.84	497	-0.02792	-74.94
15	-0.17	15	0.02680	-74.59	496	-0.02680	-68.38
16	-0.17	16	0.02498	-74.08	495	-0.02498	-67.24
17	-0.15	17	0.02417	-68.05	494	-0.02417	-61.92
18	-0.13	18	0.02179	-55.63	493	-0.02179	-49.79
19	-0.12	19	0.02072	-36.28	492	-0.02072	-30.68
20	-0.10	20	0.01997	-64.25	491	-0.01997	-59.32
21	-0.10	21	0.01838	-43.17	490	-0.01838	-37.91
22	-0.05	22	0.01455	-57.73	489	-0.01455	-54.04
23	-0.06	23	0.01423	-55.58	488	-0.01423	-51.26
24	-0.06	24	0.01378	-32.43	487	-0.01378	-28.33
25	-0.05	25	0.01286	-116.92	486	-0.01286	-112.69
26	-0.04	26	0.01279	-66.67	485	-0.01279	-63.56
27	-0.05	27	0.01219	-80.16	484	-0.01219	-76.02
28	-0.03	28	0.01080	-109.90	483	-0.01080	-106.69
29	-0.03	29	0.01027	-73.06	482	-0.01027	-69.85
30	-0.04	30	0.00970	-132.00	481	-0.00970	-128.31
31	-0.03	31	0.00945	-46.91	480	-0.00945	-43.75

32	-0.03	32	0.00916	-72.98	479	-0.00916	-70.00
33	-0.03	33	0.00875	-65.97	478	-0.00875	-63.07
34	-0.02	34	0.00782	-25.39	477	-0.00782	-22.25
35	-0.02	35	0.00710	-58.84	476	-0.00710	-56.39
36	-0.01	36	0.00605	-64.70	475	-0.00605	-62.22
37	-0.01	37	0.00575	-61.01	474	-0.00575	-58.96
38	-0.01	38	0.00504	-72.75	473	-0.00504	-71.21
39	-0.01	39	0.00484	-120.97	472	-0.00484	-119.08
40	-0.01	40	0.00469	-160.50	471	-0.00469	-158.39
41	-0.01	41	0.00435	-71.26	470	-0.00435	-69.87
42	-0.01	42	0.00413	-338.28	469	-0.00413	-335.45
43	-0.01	43	0.00371	-281.07	468	-0.00371	-278.89
44	-0.01	44	0.00335	-158.20	467	-0.00335	-156.63
45	-0.00	45	0.00317	-56.56	466	-0.00317	-55.26
46	-0.00	46	0.00314	-97.35	465	-0.00314	-96.14
47	-0.00	47	0.00298	-161.29	464	-0.00298	-159.72
48	-0.00	48	0.00268	-129.90	463	-0.00268	-128.69
49	-0.00	49	0.00263	-103.95	462	-0.00263	-102.51
50	-0.01	50	0.00238	-507.90	461	-0.00238	-505.22
51	-0.01	51	0.00233	-734.75	460	-0.00233	-731.66
52	-0.00	52	0.00227	-73.81	459	-0.00227	-72.88
53	-0.01	53	0.00211	-783.01	458	-0.00211	-780.08
54	-0.00	54	0.00202	-489.95	457	-0.00202	-487.75
55	-0.00	55	0.00167	-271.14	456	-0.00167	-269.97
56	-0.01	56	0.00159	-1457.91	455	-0.00159	-1454.19
57	-0.00	57	0.00139	-1283.09	454	-0.00139	-1280.26
58	-0.00	58	0.00134	-1386.66	453	-0.00134	-1383.45
59	-0.00	59	0.00127	-1187.25	452	-0.00127	-1184.65
60	-0.00	60	0.00118	-865.29	451	-0.00118	-861.69

61	-0.00	61	0.00105	-1471.84	450	-0.00105	-1469.49

Sum of NOCV eigenvalues: -0.00000

Sum of pair energies: -123.89 kcal/mol

NOCV Pair energy for TS of Reaction3

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-35.56	1	0.57504	-95.83	298	-0.57504	-34.00
2	-3.08	2	0.12724	-67.74	297	-0.12724	-43.51
3	-1.71	3	0.09241	4.65	296	-0.09241	23.14
4	-0.85	4	0.06512	-46.79	295	-0.06512	-33.72
5	-0.71	5	0.05980	-10.01	294	-0.05980	1.79
6	-0.45	6	0.04296	-45.44	293	-0.04296	-35.01
7	-0.21	7	0.02911	-38.46	292	-0.02911	-31.15
8	-0.23	8	0.02847	-86.86	291	-0.02847	-78.65
9	-0.16	9	0.02327	-44.14	290	-0.02327	-37.28
10	-0.16	10	0.02051	-67.82	289	-0.02051	-60.20
11	-0.12	11	0.01885	-53.45	288	-0.01885	-47.00
12	-0.07	12	0.01711	-61.54	287	-0.01711	-57.23
13	-0.07	13	0.01651	-56.63	286	-0.01651	-52.36
14	-0.06	14	0.01528	-32.63	285	-0.01528	-28.65
15	-0.06	15	0.01507	-38.25	284	-0.01507	-34.27
16	-0.06	16	0.01415	-30.24	283	-0.01415	-26.28
17	-0.05	17	0.01323	-75.20	282	-0.01323	-71.29
18	-0.04	18	0.01232	-66.42	281	-0.01232	-63.11
19	-0.05	19	0.01158	-36.90	280	-0.01158	-32.81
20	-0.03	20	0.00989	-44.25	279	-0.00989	-41.16
21	-0.03	21	0.00874	-108.32	278	-0.00874	-104.68
22	-0.02	22	0.00816	-88.56	277	-0.00816	-85.81
23	-0.02	23	0.00758	-87.89	276	-0.00758	-85.52

24	-0.02	24	0.00699	-117.51	275	-0.00699	-115.00
25	-0.01	25	0.00681	-103.56	274	-0.00681	-101.46
26	-0.01	26	0.00658	-102.73	273	-0.00658	-100.48
27	-0.02	27	0.00625	-106.68	272	-0.00625	-104.21
28	-0.01	28	0.00532	-168.47	271	-0.00532	-165.76
29	-0.01	29	0.00427	-117.28	270	-0.00427	-115.43
30	-0.00	30	0.00304	-120.34	269	-0.00304	-119.00
31	-0.00	31	0.00289	-211.27	268	-0.00289	-209.79
32	-0.00	32	0.00233	-246.26	267	-0.00233	-245.03
33	-0.01	33	0.00183	-2194.15	266	-0.00183	-2189.01
34	-0.01	34	0.00138	-2019.37	265	-0.00138	-2015.22
35	-0.00	35	0.00133	-1588.97	264	-0.00133	-1585.72

Sum of NOCV eigenvalues: -0.00000

Sum of pair energies: -43.92 kcal/mol