Electronic Supplementary Information

Solvent Effects in Ionic Liquids: Linear Energy-Density Relationships.

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Table S1. Cross validation analysis.

Eq. 11 Acrolein-CP		Multiparameter regression constants					Statistical parameters for multiparameter fitting		
Run	Excluded	a_1	a_2	a_3	a_4	a_5	R^2	F	P
1	HbimN$(Tf)_2$	-2.97	-4.96	2.71	-0.22	0.05	0.984	59.6	< 0.0008
2	MepipTFA	-2.43	-11.34	8.97	-0.5	0.002	0.968	29.9	< 0.0031
3	Bmim BF_4	-4.16	-11.31	-214	-0.49	1.71	0.975	39.6	< 0.0018
4	Bmim PF_6	-4.55	-9.59	23.4	-0.28	-0.45	0.939	15.3	< 0.011
5	Emim N$(Tf)_2$	-4.06	-9.37	-9.44	-0.27	-0.0004	0.87	8.6	< 0.030
6	Bmim Otf	-4.05	-9.8	-10.07	-0.34	-0.04	0.897	8.7	< 0.030
7	Bmim N$(Tf)_2$	-4	-9.44	-11.66	-0.29	0.02	0.894	8.4	< 0.031
8	Omim N$(Tf)_2$	-4.03	-9.37	-10.41	-0.28	0.009	0.89	8.1	< 0.033
9	Bmpy N$(Tf)_2$	-5.43	-9.44	-2.14	0.041	0.011	0.919	11.3	< 0.019
10	Bm_2im N$(Tf)_2$	-4.16	-10.04	-17.28	-0.3	0.06	0.91	10.2	< 0.022

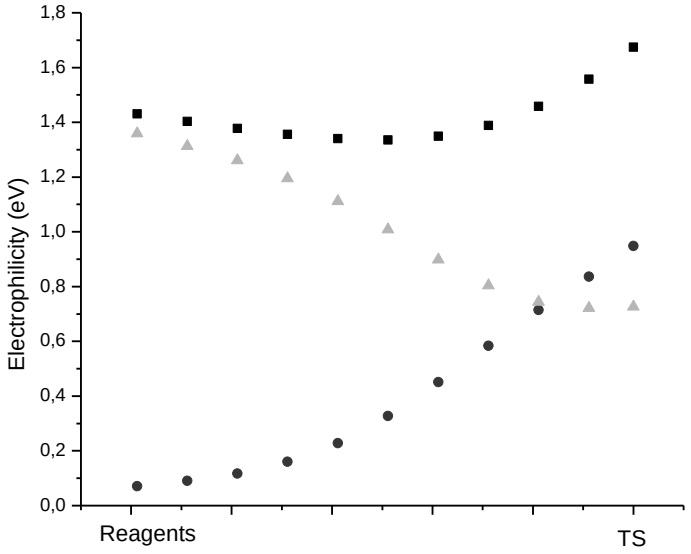

Fig F1. The IRC- electrophilicity profile for the isolated TS for the reaction acrolein + CP. Global electrophilicity (filled squares); Dienophile moiety electrophilicity (filled triangles); Diene moiety electrophilicity (filled circles).

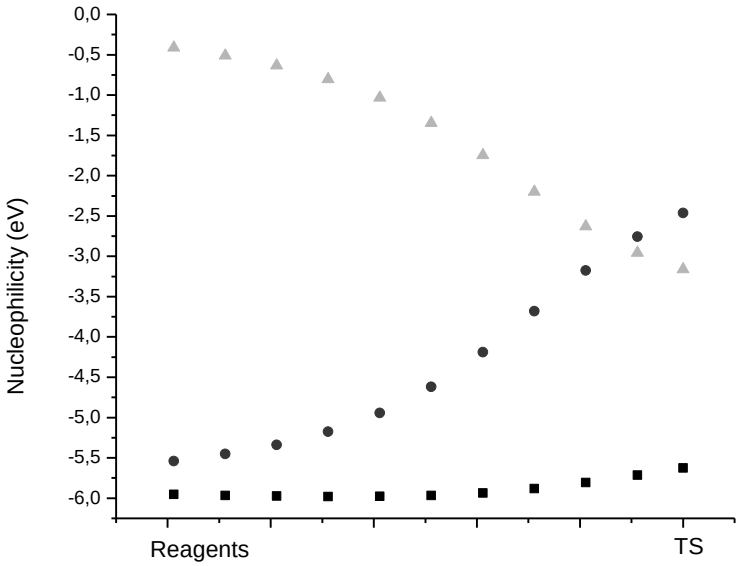

Fig F2. The IRC- nucleophilicity profile for the isolated TS for the reaction acrolein + CP. Global nucleophilicity (filled squares); Dienophile moiety nucleophilicity (filled triangles); Diene moiety nucleophilicity (filled circles).

Cartesian coordinates, energy and number of imaginary frequencies for the cations-anions ion pair structures, optimized at the B3LYP/6–311+G(d,p) level of theory

$Bm_2im[NTf_2]$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.038735	-0.548928	-0.186969
2	6	0	-0.136485	-0.252310	2.016921
3	6	0	1.119526	-0.661674	1.711299
4	7	0	1.164668	-0.835847	0.341006
5	1	0	-0.544089	0.030373	2.972550
6	1	0	1.980814	-0.783348	2.352694
7	6	0	2.363328	-1.249178	-0.401498
8	1	0	2.461036	-0.648823	-1.305310
9	1	0	3.226492	-1.073625	0.239914
10	1	0	2.296243	-2.307034	-0.662440
11	7	0	-0.846145	-0.182957	0.828506
12	6	0	-2.263708	0.202544	0.736195
13	6	0	-3.216530	-0.982914	0.913905
14	1	0	-2.421028	0.697277	-0.223574
15	1	0	-2.430148	0.952600	1.511369
16	6	0	-4.686844	-0.550491	0.865903
17	1	0	-3.022494	-1.728124	0.133469
18	1	0	-3.003578	-1.471297	1.870659
19	6	0	-5.654520	-1.723402	1.044801
20	1	0	-4.869074	0.196129	1.647396
21	1	0	-4.889951	-0.050610	-0.088908
22	1	0	-6.692395	-1.384262	1.010084
23	1	0	-5.522821	-2.471431	0.257167
24	1	0	-5.499606	-2.221228	2.006327
25	6	0	-0.381323	-0.597210	-1.634223
26	1	0	0.069869	-1.471809	-2.106042
27	1	0	-1.458734	-0.656828	-1.780218
28	1	0	-0.014924	0.292574	-2.156844
29	8	0	1.016023	0.543130	4.777396
30	16	0	2.404706	1.016364	4.745976
31	8	0	2.671109	2.402277	4.382782
32	7	0	3.245089	-0.098552	3.936044
33	16	0	4.671611	0.096144	3.198252
34	8	0	5.458058	1.275399	3.526747
35	8	0	4.515125	-0.285170	1.784334
36	6	0	5.605246	-1.370934	3.941492
37	9	0	6.823600	-1.435841	3.391558
38	9	0	5.736822	-1.230739	5.261771
39	9	0	4.966817	-2.521993	3.692339
40	6	0	2.982141	0.846148	6.539624
41	9	0	2.279285	1.682854	7.312435
42	9	0	4.277473	1.146405	6.644970
43	9	0	2.791292	-0.402471	6.978869

Total Energy (a.u.) = **-2290.33925921;** NIMAG = **0**

Bmim[BF_4]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.064628	0.535210	-0.007985
2	6	0	0.205413	-0.270580	2.026681
3	6	0	1.433514	-0.168418	1.450836
4	7	0	1.242272	0.336727	0.177274
5	1	0	-0.524017	0.875139	-0.921646
6	1	0	-0.085279	-0.625433	2.999770
7	1	0	2.410806	-0.412951	1.828996
8	6	0	2.271690	0.558146	-0.845723
9	1	0	2.796519	1.494881	-0.652850
10	1	0	2.973961	-0.274073	-0.819892
11	1	0	1.780357	0.580055	-1.817405
12	7	0	-0.717237	0.178663	1.099154
13	6	0	-2.190371	0.121498	1.217257
14	6	0	-2.710284	-1.317479	1.216303
15	1	0	-2.583884	0.658820	0.355107
16	1	0	-2.469398	0.656935	2.128607
17	6	0	-4.242743	-1.357017	1.224390
18	1	0	-2.326471	-1.819330	0.324244
19	1	0	-2.322473	-1.853837	2.091198
20	6	0	-4.790436	-2.786974	1.233538
21	1	0	-4.624817	-0.812110	2.097113
22	1	0	-4.614191	-0.830535	0.338821
23	1	0	-5.883364	-2.789367	1.226917
24	1	0	-4.450021	-3.341534	0.354885
25	1	0	-4.461566	-3.333902	2.123002
26	9	0	-2.222885	0.100522	-1.984534
27	5	0	-1.253591	-0.754269	-2.604929
28	9	0	-0.835304	-1.697496	-1.625560
29	9	0	-1.763781	-1.367921	-3.724211
30	9	0	-0.123528	0.067788	-2.921381

Total Energy (a.u.) = **-848.100391518;** NIMAG = **0**

Bmim[NTf_2]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.023992	0.676022	0.566774
2	6	0	0.323827	-1.066560	1.887647
3	6	0	1.530739	-0.723523	1.361911
4	7	0	1.322630	0.370452	0.546069
5	1	0	-0.420026	1.475661	-0.014057
6	1	0	0.053270	-1.855124	2.567275
7	1	0	2.504683	-1.161706	1.494214
8	6	0	2.319360	1.012265	-0.321264
9	1	0	1.892499	1.933816	-0.710752
10	1	0	3.215181	1.223745	0.262199
11	1	0	2.540553	0.347485	-1.155131
12	7	0	-0.605979	-0.176664	1.380338
13	6	0	-2.061265	-0.187365	1.637767
14	6	0	-2.743416	-1.447390	1.102790
15	1	0	-2.463801	0.703779	1.153689
16	1	0	-2.206044	-0.076365	2.715865
17	6	0	-4.261572	-1.396987	1.314387
18	1	0	-2.519507	-1.547216	0.037232
19	1	0	-2.333265	-2.329753	1.608520
20	6	0	-4.963842	-2.652563	0.789982
21	1	0	-4.485844	-1.267319	2.380719
22	1	0	-4.665272	-0.516054	0.802548
23	1	0	-6.044722	-2.588237	0.937720
24	1	0	-4.777637	-2.785970	-0.278863
25	1	0	-4.610040	-3.550193	1.306670
26	8	0	-2.042298	-1.277720	-2.236613
27	16	0	-1.034179	-0.385006	-2.804923
28	8	0	0.326413	-0.432729	-2.243780
29	7	0	-1.652026	1.087233	-2.926876
30	16	0	-0.768877	2.439553	-2.879669
31	8	0	0.190180	2.637517	-3.960359
32	8	0	-0.314849	2.773723	-1.510079
33	6	0	-2.195346	3.633991	-3.203732
34	9	0	-1.698339	4.875994	-3.198117
35	9	0	-2.755185	3.398365	-4.387502
36	9	0	-3.126547	3.543194	-2.250274
37	6	0	-0.845230	-0.978933	-4.590299
38	9	0	-0.382768	-2.236243	-4.584828
39	9	0	0.012771	-0.206870	-5.254906
40	9	0	-2.024627	-0.958032	-5.213084

Total Energy (a.u.) = **-2251.01780670;** NIMAG = **0**

BmimOTf

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.049817	-0.060147	-0.028783
2	6	0	-0.053506	0.246147	2.157127
3	6	0	1.242874	0.164288	1.748809
4	7	0	1.221558	-0.027489	0.378510
5	1	0	-0.371770	-0.183711	-1.054171
6	1	0	-0.472122	0.398255	3.136816
7	1	0	2.161485	0.233040	2.305325
8	6	0	2.375018	-0.153529	-0.523670
9	1	0	3.016055	0.721062	-0.412404
10	1	0	2.932529	-1.058414	-0.280152
11	1	0	1.995028	-0.207209	-1.543812
12	7	0	-0.844288	0.108216	1.030382
13	6	0	-2.322637	0.112888	0.961611
14	6	0	-2.926258	-1.246970	1.315455
15	1	0	-2.576176	0.393708	-0.061839
16	1	0	-2.671254	0.894682	1.640234
17	6	0	-4.456362	-1.226763	1.215263
18	1	0	-2.524612	-1.998754	0.627953
19	1	0	-2.623077	-1.541116	2.327855
20	6	0	-5.086420	-2.583502	1.540929
21	1	0	-4.856670	-0.464176	1.894477
22	1	0	-4.742295	-0.922449	0.203044
23	1	0	-6.175292	-2.539281	1.461479
24	1	0	-4.735077	-3.356381	0.851268
25	1	0	-4.839603	-2.904835	2.557831
26	9	0	-0.279015	2.093737	-4.985629
27	6	0	-1.120825	1.903961	-3.960986
28	9	0	-2.332108	2.346317	-4.324042
29	9	0	-0.694676	2.668535	-2.930709
30	16	0	-1.180236	0.089253	-3.452377
31	8	0	-1.636756	-0.616460	-4.644249
32	8	0	-2.111587	0.103220	-2.291278
33	8	0	0.222220	-0.175040	-3.023707

Total Energy (a.u.) = **-1385.14613554;** NIMAG = **0**

Bmim[PF_6]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.132952	0.653132	0.255755
2	6	0	0.058750	-0.525763	2.109449
3	6	0	1.303867	-0.358013	1.588855
4	7	0	1.161941	0.383480	0.430193
5	1	0	-0.550594	1.168130	-0.593121
6	1	0	-0.268035	-1.042492	2.994682
7	1	0	2.263255	-0.701200	1.935051
8	6	0	2.223781	0.729501	-0.522607
9	1	0	2.896314	1.463687	-0.077635
10	1	0	2.770257	-0.175781	-0.784205
11	1	0	1.757629	1.126875	-1.421592
12	7	0	-0.826102	0.117726	1.262051
13	6	0	-2.301391	0.096977	1.350429
14	6	0	-2.881415	-1.275748	1.005460
15	1	0	-2.662752	0.846342	0.646651
16	1	0	-2.573310	0.412406	2.361042
17	6	0	-4.414493	-1.256173	1.016745
18	1	0	-2.521938	-1.562447	0.014254
19	1	0	-2.515543	-2.022518	1.720530
20	6	0	-5.018691	-2.620191	0.672561
21	1	0	-4.774845	-0.931898	2.001391
22	1	0	-4.765086	-0.511584	0.293867
23	1	0	-6.110700	-2.578138	0.679612
24	1	0	-4.703393	-2.947931	-0.321598
25	1	0	-4.710139	-3.385160	1.392083
26	9	0	-1.961637	0.557818	-4.121591
27	15	0	-1.103925	-0.302929	-3.054975
28	9	0	-0.207245	1.064312	-2.672615
29	9	0	-0.223270	-1.117160	-1.896720
30	9	0	-0.007864	-0.708858	-4.175421
31	9	0	-2.163389	0.143819	-1.839988
32	9	0	-1.980634	-1.637021	-3.332052

Total Energy (a.u.) = **-1364.30779436;** NIMAG = **0**

Bmpy[NTf_2]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.324799	0.001883	0.011239
2	6	0	-0.556657	-0.050303	1.528737
3	6	0	0.862900	-0.115171	2.161116
4	6	0	1.839741	-0.155346	0.981637
5	7	0	1.090635	0.511204	-0.167670
6	1	0	-1.006944	0.653190	-0.534821
7	1	0	-1.102447	0.827919	1.876571
8	1	0	0.998089	-0.999953	2.782674
9	1	0	2.063419	-1.173561	0.675694
10	1	0	1.046699	0.751537	2.797301
11	1	0	-1.160881	-0.921635	1.782622
12	1	0	-0.360738	-0.992650	-0.428168
13	1	0	2.783467	0.361012	1.141750
14	6	0	1.662011	0.202700	-1.552890
15	1	0	0.987344	0.704233	-2.252233
16	1	0	2.626638	0.707507	-1.596659
17	6	0	1.129262	2.007186	0.009906
18	1	0	2.170395	2.328207	-0.013329
19	1	0	0.565298	2.465304	-0.801927
20	1	0	0.678049	2.269643	0.964354
21	6	0	1.833036	-1.265641	-1.927114
22	1	0	0.876788	-1.800213	-1.901596
23	1	0	2.517988	-1.762493	-1.237319
24	6	0	2.424119	-1.368260	-3.345171
25	1	0	3.378078	-0.833297	-3.365741
26	1	0	1.760695	-0.866023	-4.060376
27	6	0	2.639976	-2.821482	-3.774971
28	1	0	1.698452	-3.380290	-3.786309
29	1	0	3.067790	-2.870341	-4.779258
30	1	0	3.327110	-3.331489	-3.094814
31	8	0	4.371893	2.265544	0.066149
32	16	0	5.247938	1.164297	-0.361173
33	8	0	5.063931	0.645688	-1.721551
34	7	0	5.247333	0.065766	0.798602
35	16	0	5.508455	-1.521582	0.556550
36	8	0	6.685590	-1.876836	-0.225139
37	8	0	4.250260	-2.239676	0.298954
38	6	0	5.923503	-1.937145	2.352383
39	9	0	6.150515	-3.252584	2.435854
40	9	0	7.011155	-1.285640	2.759170
41	9	0	4.903052	-1.631561	3.166028
42	6	0	6.977683	1.928145	-0.338324
43	9	0	7.032011	2.914865	-1.240973
44	9	0	7.896723	1.014061	-0.638253
45	9	0	7.242643	2.434624	0.868519

Total Energy (a.u.) = **-2237.36660839;** NIMAG = **0**

Emim[NTf_2]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.184401	0.183281	0.540862
2	6	0	0.236272	0.067929	2.708534
3	6	0	1.363115	0.508303	2.087427
4	7	0	1.080537	0.575030	0.736403
5	1	0	-0.683346	0.127227	-0.427431
6	1	0	0.032268	-0.109714	3.750086
7	1	0	2.324178	0.785244	2.484766
8	6	0	2.015951	0.983786	-0.322451
9	1	0	2.595935	1.833682	0.035428
10	1	0	2.681976	0.153987	-0.562252
11	1	0	1.440956	1.281517	-1.198659
12	7	0	-0.718196	-0.127457	1.727986
13	6	0	-2.096501	-0.624525	1.948228
14	6	0	-2.124301	-2.115485	2.265615
15	1	0	-2.653044	-0.424984	1.034174
16	1	0	-2.520063	-0.029244	2.759673
17	1	0	-1.722100	-2.693403	1.431941
18	1	0	-1.562567	-2.355070	3.172395
19	1	0	-3.160603	-2.425032	2.415257
20	8	0	-0.091643	2.084147	-2.433898
21	16	0	-1.264620	1.465455	-3.066245
22	8	0	-2.468334	2.253958	-3.270174
23	7	0	-1.460698	0.051075	-2.299198
24	16	0	-2.781997	-0.895738	-2.337977
25	8	0	-3.830785	-0.548263	-3.282045
26	8	0	-3.130162	-1.227168	-0.949703
27	6	0	-2.014547	-2.503571	-2.976282
28	9	0	-2.953360	-3.453138	-3.014421
29	9	0	-1.511782	-2.342464	-4.200835
30	9	0	-1.030059	-2.912900	-2.159545
31	6	0	-0.644083	1.025189	-4.800932
32	9	0	-0.350948	2.150280	-5.459113
33	9	0	-1.569744	0.351502	-5.481141
34	9	0	0.464351	0.276541	-4.719204

Total Energy (a.u.) = **-2172.36802449;** NIMAG = **0**

Hbim[NTf_2]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.144206	-1.442512	0.873114
2	6	0	0.748720	-0.892854	2.054600
3	6	0	2.678072	0.026463	1.478470
4	1	0	0.676580	-2.185064	0.250483
5	1	0	-0.126226	-1.066975	2.656104
6	1	0	3.561904	0.652623	1.478633
7	7	0	2.343968	-0.856519	0.539361
8	7	0	1.720741	0.027199	2.414487
9	1	0	2.908614	-1.040358	-0.320465
10	6	0	1.741986	0.849075	3.637724
11	1	0	2.450766	1.658769	3.457405
12	1	0	0.750892	1.294982	3.749356
13	6	0	2.131721	0.046563	4.881134
14	1	0	3.115430	-0.406722	4.718340
15	1	0	1.423275	-0.777541	5.022975
16	6	0	2.163557	0.923028	6.139153
17	1	0	2.875772	1.742419	5.990391
18	1	0	1.181961	1.390143	6.282974
19	6	0	2.544059	0.135795	7.396140
20	1	0	3.535184	-0.315758	7.295283
21	1	0	2.563004	0.785056	8.274548
22	1	0	1.828850	-0.668652	7.592236
23	8	0	5.013827	2.113667	1.212347
24	16	0	5.629720	1.776923	-0.079807
25	8	0	5.486752	2.687830	-1.202509
26	7	0	5.215883	0.235157	-0.343902
27	16	0	5.127722	-0.557111	-1.740939
28	8	0	5.529146	0.112571	-2.964233
29	8	0	3.829842	-1.277555	-1.719611
30	6	0	6.373004	-1.955045	-1.467292
31	9	0	6.343482	-2.779035	-2.516800
32	9	0	7.604985	-1.463153	-1.334075
33	9	0	6.063088	-2.649585	-0.366218
34	6	0	7.481628	1.722880	0.300722
35	9	0	7.883453	2.932404	0.699047
36	9	0	8.165747	1.373034	-0.788737
37	9	0	7.736321	0.842059	1.274043

Total Energy (a.u.) = **-2211.70401370;** NIMAG = **0**

Omim[NTf_2]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.075471	0.117960	0.394364
2	6	0	-0.013139	0.004961	2.600925
3	6	0	1.267817	0.088852	2.150937
4	7	0	1.207836	0.160173	0.772110
5	1	0	-0.428611	0.145004	-0.636845
6	1	0	-0.404021	-0.055979	3.601662
7	1	0	2.201868	0.114356	2.684884
8	6	0	2.356545	0.244823	-0.142007
9	1	0	3.095979	0.918345	0.289697
10	1	0	2.790891	-0.746518	-0.277180
11	1	0	2.013269	0.647377	-1.094410
12	7	0	-0.836338	0.026889	1.490936
13	6	0	-2.313243	-0.070354	1.502728
14	6	0	-2.802195	-1.501612	1.728016
15	1	0	-2.661844	0.293530	0.537329
16	1	0	-2.668984	0.604443	2.284819
17	6	0	-4.333244	-1.574243	1.708565
18	1	0	-2.396247	-2.135934	0.934402
19	1	0	-2.419599	-1.883518	2.682560
20	6	0	-4.867016	-2.996191	1.917120
21	1	0	-4.742558	-0.916139	2.486358
22	1	0	-4.691038	-1.188366	0.748252
23	1	0	-4.455347	-3.651550	1.139886
24	6	0	-6.397259	-3.076492	1.887881
25	1	0	-6.759100	-2.684970	0.929125
26	1	0	-6.809677	-2.416223	2.662007
27	1	0	-4.501318	-3.388022	2.875493
28	6	0	-6.940275	-4.495141	2.092695
29	1	0	-6.529028	-5.155466	1.318274
30	1	0	-6.577423	-4.888681	3.051553
31	6	0	-8.470670	-4.576527	2.062682
32	1	0	-8.833156	-4.186060	1.104247
33	1	0	-8.882264	-3.915476	2.835217
34	6	0	-9.005302	-5.996687	2.269461
35	1	0	-10.098203	-6.020168	2.242404
36	1	0	-8.639693	-6.674112	1.491308
37	1	0	-8.688399	-6.402213	3.235732
38	8	0	0.899675	1.808544	-2.521873
39	16	0	-0.283142	1.462829	-3.321636
40	8	0	-1.228430	2.503100	-3.691938
41	7	0	-0.910971	0.154619	-2.599923
42	16	0	-2.396795	-0.461150	-2.834180
43	8	0	-3.179755	0.072579	-3.936416
44	8	0	-3.018915	-0.637650	-1.514874
45	6	0	-1.937458	-2.229283	-3.327847
46	9	0	-3.054368	-2.950496	-3.465132
47	9	0	-1.267683	-2.246423	-4.480618
48	9	0	-1.176277	-2.802707	-2.381731
49	6	0	0.452041	0.842300	-4.953117
50	9	0	1.077205	1.852580	-5.564210
51	9	0	-0.501881	0.371667	-5.754441
52	9	0	1.341720	-0.132183	-4.719698

Total Energy (a.u.) = **-2408.31548029;** NIMAG = **0**

Mepip[TFA]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.035743	-0.029149	0.089709
2	6	0	0.155114	0.069895	1.602606
3	6	0	1.640506	0.033955	1.980309
4	6	0	2.307874	-1.212526	1.387878
5	6	0	2.086044	-1.307489	-0.120467
6	1	0	-0.316138	0.994005	1.948830
7	1	0	0.391321	0.841971	-0.420763
8	1	0	-1.093800	-0.092989	-0.171693
9	1	0	2.139144	0.936443	1.604190
10	1	0	1.752240	0.042094	3.067500
11	1	0	3.385200	-1.206692	1.574727
12	1	0	1.906876	-2.112076	1.864628
13	1	0	2.578646	-0.481103	-0.645809
14	1	0	2.454844	-2.254507	-0.515735
15	1	0	-0.372590	-0.760254	2.082632
16	7	0	0.626137	-1.252408	-0.459430
17	1	0	0.142548	-2.155787	0.014327
18	6	0	0.411487	-1.398008	-1.921580
19	1	0	0.820674	-2.359895	-2.228485
20	1	0	-0.659358	-1.380727	-2.124774
21	1	0	0.901890	-0.580861	-2.455344
22	9	0	0.108340	-6.773220	0.131295
23	6	0	-0.475100	-5.689284	0.664262
24	6	0	0.106894	-4.354566	0.102642
25	9	0	-0.305849	-5.760119	2.006582
26	9	0	-1.802363	-5.785394	0.421383
27	8	0	1.032359	-4.410788	-0.703469
28	8	0	-0.469743	-3.323167	0.575455

Total Energy (a.u.) = **-818.28888222;** NIMAG = **0**

Cartesian coordinates, energy and number of imaginary frequencies for the TS---Cation/Anion complexes structures for reaction acrolein-CP, optimized at the B3LYP/6–311+G(d,p) level of theory

TS1-Hbim$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.048284	0.077248	-0.812641
2	6	0	0.202058	0.702127	0.432187
3	6	0	1.570467	0.989505	0.551671
4	6	0	2.155814	0.862290	-0.843745
5	6	0	1.114587	0.045997	-1.539718
6	1	0	-0.997008	-0.341810	-1.117696
7	1	0	-0.536999	0.864858	1.205526
8	1	0	1.941127	1.717808	1.263103
9	1	0	2.163217	1.865977	-1.296715
10	1	0	3.173370	0.479686	-0.911850
11	1	0	1.240063	-0.386438	-2.523422
12	1	0	1.640298	-0.725894	2.265824
13	6	0	2.307449	-0.677661	1.414539
14	6	0	2.257928	-1.735678	0.493988
15	1	0	3.273137	-0.231543	1.624286
16	6	0	1.151268	-2.607570	0.435408
17	1	0	3.081277	-1.927611	-0.182510
18	8	0	0.125493	-2.500444	1.159624
19	1	0	1.206858	-3.433303	-0.291389
20	1	0	-4.380024	-6.125688	1.076413
21	6	0	-3.496183	-5.581041	1.360689
22	6	0	-2.762485	-4.651208	0.685513
23	7	0	-2.897885	-5.746024	2.596771
24	1	0	-2.897729	-4.237872	-0.299007
25	7	0	-1.730309	-4.264888	1.508888
26	6	0	-1.831547	-4.936295	2.652804
27	6	0	-3.328591	-6.687299	3.651621
28	1	0	-0.955827	-3.530886	1.294043
29	1	0	-1.167663	-4.841604	3.495912
30	1	0	-2.866582	-6.352516	4.582178
31	1	0	-4.408712	-6.573186	3.764082
32	6	0	-2.951882	-8.137640	3.341248
33	1	0	-1.866434	-8.206887	3.208827
34	1	0	-3.405205	-8.437242	2.389836
35	6	0	-3.404435	-9.094006	4.452589
36	1	0	-2.954386	-8.785299	5.403335
37	1	0	-4.489391	-9.010618	4.584114
38	6	0	-3.034534	-10.550819	4.161425
39	1	0	-1.952545	-10.673427	4.058751
40	1	0	-3.366971	-11.205485	4.969590
41	1	0	-3.500970	-10.902468	3.236721

Total Energy (a.u.) =**-770.107672151;** NIMAG = **1 ,** ν_i (cm^{-1}) = **328i**

TS1-Emim$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.009453	1.255047	-1.198204
2	6	0	-3.234726	-0.086626	-1.567397
3	6	0	-4.210840	-0.651278	-0.723837
4	6	0	-4.916034	0.519117	-0.059302
5	6	0	-3.890787	1.599483	-0.198378
6	1	0	-2.230570	1.888714	-1.599088
7	1	0	-2.677685	-0.627221	-2.321263
8	1	0	-4.744039	-1.554551	-0.996921
9	1	0	-5.780217	0.787516	-0.686890
10	1	0	-5.293075	0.350914	0.948141
11	1	0	-3.948613	2.560003	0.295728
12	1	0	-2.427212	-1.923373	0.296008
13	6	0	-3.153887	-1.320652	0.826528
14	6	0	-2.670997	-0.220037	1.552523
15	1	0	-3.973086	-1.888639	1.253811
16	6	0	-1.377637	0.325587	1.322521
17	1	0	-3.258722	0.223601	2.346729
18	8	0	-0.555298	-0.097737	0.484067
19	1	0	-1.103254	1.190683	1.951830
20	1	0	4.241650	3.625808	0.694096
21	6	0	4.208110	2.539150	0.795556
22	6	0	3.521339	1.942414	-0.428973
23	1	0	3.663932	2.298431	1.711110
24	1	0	5.234966	2.181590	0.896620
25	7	0	3.429421	0.467445	-0.364526
26	1	0	2.500671	2.311948	-0.531054
27	1	0	4.055373	2.190666	-1.347924
28	6	0	2.317258	-0.228704	-0.101470
29	6	0	4.479692	-0.418612	-0.529495
30	7	0	2.626174	-1.530022	-0.096246
31	1	0	1.314322	0.155672	0.088758
32	6	0	3.975562	-1.670591	-0.362665
33	1	0	5.479911	-0.090453	-0.754526
34	6	0	1.668863	-2.617626	0.153184
35	1	0	4.454201	-2.633521	-0.415851
36	1	0	1.656704	-3.291175	-0.703572
37	1	0	1.964662	-3.162838	1.049513
38	1	0	0.684520	-2.173872	0.294061

Total Energy (a.u.) =**-730.768885465;** NIMAG = **1 ,** ν_i (cm^{-1}) = **362i**

TS1-Bmim$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.287137	0.444791	0.496582
2	6	0	0.719200	0.377425	1.836650
3	6	0	2.114601	0.190524	1.874163
4	6	0	2.623426	0.567911	0.492931
5	6	0	1.385896	0.405888	-0.331830
6	1	0	-0.745029	0.465159	0.175429
7	1	0	0.068846	0.375788	2.701451
8	1	0	2.691874	0.397349	2.767897
9	1	0	2.880987	1.638345	0.513675
10	1	0	3.503042	0.034288	0.136847
11	1	0	1.368525	0.428256	-1.413158
12	1	0	1.678673	-2.077457	2.589447
13	6	0	2.322804	-1.788970	1.768113
14	6	0	1.954112	-2.212483	0.481367
15	1	0	3.378859	-1.781010	2.015093
16	6	0	0.637396	-2.661712	0.183536
17	1	0	2.681316	-2.252995	-0.320275
18	8	0	-0.304972	-2.726028	0.999052
19	1	0	0.463390	-2.975406	-0.861112
20	1	0	-5.550269	-5.641421	-4.606268
21	6	0	-5.179142	-5.966996	-3.632303
22	6	0	-5.137611	-4.797295	-2.645296
23	1	0	-4.184397	-6.396188	-3.782536
24	1	0	-5.837762	-6.764378	-3.276470
25	6	0	-4.613988	-5.210156	-1.263295
26	1	0	-6.141665	-4.370001	-2.541436
27	1	0	-4.503620	-3.999503	-3.049308
28	6	0	-4.588792	-4.029743	-0.290085
29	1	0	-3.602819	-5.621804	-1.354958
30	1	0	-5.243979	-6.008285	-0.855261
31	7	0	-4.069435	-4.400151	1.043566
32	1	0	-3.949654	-3.227498	-0.662050
33	1	0	-5.588204	-3.614149	-0.144344
34	6	0	-2.854208	-4.095573	1.513113
35	6	0	-4.736779	-5.152026	1.994486
36	7	0	-2.727795	-4.627433	2.734035
37	1	0	-2.070012	-3.519531	1.021029
38	6	0	-3.896462	-5.292882	3.054659
39	1	0	-5.739511	-5.512606	1.842379
40	6	0	-1.530855	-4.509333	3.579214
41	1	0	-4.031189	-5.797639	3.996015
42	1	0	-1.801163	-4.038667	4.524390
43	1	0	-1.117717	-5.501034	3.763758
44	1	0	-0.804152	-3.894974	3.049685

Total Energy (a.u.) = **-809.418938327 ;** NIMAG = **1 ,** ν_i (cm^{-1}) = **358i**

TS1-Omim$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.088350	-2.182475	-1.524192
2	6	0	5.220416	-1.356647	-1.372167
3	6	0	6.044421	-1.868141	-0.350997
4	6	0	5.601300	-3.306028	-0.137485
5	6	0	4.211401	-3.270742	-0.689902
6	1	0	3.236288	-1.961258	-2.151807
7	1	0	5.384709	-0.423007	-1.893792
8	1	0	7.083764	-1.574695	-0.259074
9	1	0	6.212616	-3.944167	-0.794466
10	1	0	5.700013	-3.699331	0.872810
11	1	0	3.491987	-4.070666	-0.577394
12	1	0	5.315347	-0.005356	1.006853
13	6	0	5.296274	-1.046677	1.303555
14	6	0	4.040200	-1.619240	1.559816
15	1	0	6.126704	-1.343599	1.934842
16	6	0	2.832651	-1.021008	1.103259
17	1	0	3.949545	-2.518893	2.156053
18	8	0	2.755505	0.040607	0.451938
19	1	0	1.903515	-1.559311	1.362369
20	1	0	-8.196644	-1.832239	-1.035148
21	6	0	-7.786837	-2.260715	-0.112568
22	6	0	-6.772238	-1.282522	0.490247
23	1	0	-7.268651	-3.180932	-0.408436
24	6	0	-8.933039	-2.605562	0.842464
25	6	0	-5.617929	-0.937233	-0.457722
26	1	0	-6.365726	-1.709403	1.416269
27	1	0	-7.290548	-0.360221	0.782601
28	1	0	-9.637938	-3.302345	0.381882
29	1	0	-8.558626	-3.070771	1.759623
30	1	0	-9.492697	-1.710165	1.130116
31	6	0	-4.604888	0.041406	0.146721
32	1	0	-5.100119	-1.860221	-0.748447
33	1	0	-6.024827	-0.511377	-1.383648
34	6	0	-3.447766	0.376754	-0.802750
35	1	0	-4.200225	-0.381694	1.074688
36	1	0	-5.120012	0.967259	0.431474
37	6	0	-2.436004	1.353980	-0.191531
38	1	0	-3.851192	0.801506	-1.730236
39	1	0	-2.932889	-0.549348	-1.087247
40	6	0	-1.291526	1.661281	-1.159991
41	1	0	-2.020917	0.934694	0.731574
42	1	0	-2.942114	2.285717	0.084112
43	7	0	-0.297636	2.597986	-0.593495
44	1	0	-0.748685	0.753447	-1.427495
45	1	0	-1.663290	2.107526	-2.084755
46	6	0	0.894451	2.253296	-0.093522
47	6	0	-0.462177	3.963894	-0.446813
48	7	0	1.495525	3.357555	0.363843
49	1	0	1.336507	1.257761	-0.039962
50	6	0	0.662610	4.440459	0.151220
51	1	0	-1.348982	4.474585	-0.780720
52	6	0	2.828194	3.390676	0.982812
53	1	0	0.937918	5.442219	0.433647
54	1	0	3.476601	4.053360	0.409734
55	1	0	2.743415	3.750617	2.008196
56	1	0	3.228709	2.378131	0.975128

Total Energy (a.u.) = **-966.716990408 ;** NIMAG = **1 ,** ν_i (cm^{-1}) = **359i**

TS1-Bm_2im^+

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.522558	-0.057896	1.395844
2	6	0	4.118920	-1.389915	1.613345
3	6	0	4.568475	-2.198908	0.550458
4	6	0	5.655415	-1.399724	-0.149630
5	6	0	5.305809	-0.004974	0.264136
6	1	0	4.212046	0.791713	1.987987
7	1	0	3.480598	-1.723338	2.420820
8	1	0	4.629724	-3.277051	0.645068
9	1	0	6.616877	-1.662986	0.318128
10	1	0	5.764460	-1.563448	-1.220427
11	1	0	5.749533	0.885210	-0.160927
12	1	0	2.278444	-2.320424	-0.196936
13	6	0	3.126944	-2.038974	-0.808499
14	6	0	3.139095	-0.733204	-1.324456
15	1	0	3.502873	-2.836764	-1.439976
16	6	0	2.316455	0.295886	-0.778411
17	1	0	3.745747	-0.478204	-2.184856
18	8	0	1.529442	0.155109	0.175555
19	1	0	-7.590851	-3.281315	-0.510880
20	6	0	-7.008637	-2.558480	0.064289
21	6	0	-5.912186	-1.929192	-0.799443
22	1	0	-6.584766	-3.083874	0.924989
23	1	0	-7.700945	-1.800850	0.442358
24	6	0	-5.069998	-0.903421	-0.029924
25	1	0	-6.365816	-1.444455	-1.671575
26	1	0	-5.257778	-2.716599	-1.191485
27	6	0	-3.977769	-0.290845	-0.910187
28	1	0	-4.611007	-1.381306	0.842855
29	1	0	-5.714872	-0.104599	0.352529
30	7	0	-3.169911	0.727455	-0.207043
31	1	0	-3.297584	-1.054156	-1.290379
32	1	0	-4.410933	0.208783	-1.778256
33	6	0	-2.091680	0.505680	0.571266
34	6	0	-3.447998	2.083674	-0.218193
35	7	0	-1.684154	1.698249	1.044073
36	6	0	-1.450048	-0.796454	0.880769
37	6	0	-2.519018	2.688917	0.563204
38	1	0	-4.267728	2.493156	-0.782493
39	6	0	-0.521451	1.908800	1.920571
40	1	0	-1.591158	-1.049868	1.936256
41	1	0	-1.882640	-1.596339	0.282935
42	1	0	-0.375539	-0.738700	0.678058
43	1	0	-2.374811	3.726425	0.809783
44	1	0	0.360282	1.457615	1.460220
45	1	0	-0.376721	2.981168	2.033380
46	1	0	-0.713346	1.469624	2.900627
47	1	0	2.406872	1.287604	-1.257882

Total Energy (a.u.) = **-848.749317682;** NIMAG = **1 ,** ν_i (cm^{-1}) = **360i**

TS1-Bmpy^{+}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.329375	-0.369798	1.909490
2	6	0	1.060383	-1.557034	1.711437
3	6	0	1.865744	-1.428589	0.562293
4	6	0	1.950341	0.062346	0.279591
5	6	0	0.719470	0.560415	0.970333
6	1	0	-0.453293	-0.232425	2.642819
7	1	0	0.950759	-2.462954	2.293102
8	1	0	2.706002	-2.088793	0.380656
9	1	0	2.825771	0.454148	0.820667
10	1	0	2.060735	0.353596	-0.763475
11	1	0	0.327576	1.563406	0.868453
12	1	0	0.319530	-2.921922	-0.553146
13	6	0	0.651329	-1.959515	-0.923326
14	6	0	-0.323163	-0.961561	-1.079716
15	1	0	1.440675	-2.018163	-1.664861
16	6	0	-1.611111	-1.054453	-0.469299
17	1	0	-0.147465	-0.109003	-1.724463
18	8	0	-2.011862	-1.993838	0.239616
19	1	0	-2.290702	-0.204566	-0.667626
20	1	0	-3.609922	-4.540174	-4.992409
21	6	0	-3.592890	-3.985329	-4.052075
22	6	0	-4.205499	-4.813949	-2.920176
23	1	0	-2.552544	-3.726111	-3.836414
24	1	0	-4.145211	-3.054115	-4.206747
25	6	0	-4.184622	-4.072593	-1.571991
26	1	0	-5.237350	-5.078469	-3.178988
27	1	0	-3.660390	-5.759622	-2.820940
28	6	0	-4.868614	-4.915405	-0.500226
29	1	0	-3.152235	-3.843630	-1.297474
30	1	0	-4.700493	-3.114970	-1.685662
31	7	0	-4.737850	-4.444266	0.945303
32	1	0	-4.473752	-5.934333	-0.503215
33	1	0	-5.940967	-4.977896	-0.696771
34	6	0	-5.024233	-2.963671	1.152623
35	6	0	-3.319918	-4.575696	1.489130
36	6	0	-5.675990	-5.274966	1.776709
37	6	0	-4.438140	-2.643749	2.530020
38	1	0	-4.469142	-2.431317	0.384717
39	1	0	-6.094235	-2.788064	1.043598
40	6	0	-3.271067	-3.654628	2.717401
41	1	0	-3.123401	-5.628279	1.691111
42	1	0	-2.649705	-4.206175	0.717236
43	1	0	-6.699251	-5.073362	1.463880
44	1	0	-5.442620	-6.327284	1.621545
45	1	0	-5.557669	-5.025963	2.828082
46	1	0	-4.086858	-1.613319	2.544934
47	1	0	-5.184200	-2.747509	3.319586
48	1	0	-3.377460	-4.214051	3.647793
49	1	0	-2.309174	-3.146305	2.738086

Total Energy (a.u.) = **-795.766202936;** NIMAG = **1 ,** ν_i (cm^{-1}) = **371i**

TS1-Mepip^{+}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.507956	0.341463	0.206491
2	6	0	0.866420	0.223506	0.514948
3	6	0	1.488287	1.477234	0.397085
4	6	0	0.369623	2.503925	0.376200
5	6	0	-0.806396	1.664775	-0.007764
6	1	0	-1.200170	-0.484070	0.116158
7	1	0	1.378743	-0.704211	0.733724
8	1	0	2.445891	1.685268	0.859380
9	1	0	0.216945	2.850797	1.410261
10	1	0	0.533110	3.391742	-0.232728
11	1	0	-1.775321	2.063538	-0.276949
12	1	0	2.586565	0.580641	-1.580363
13	6	0	2.048092	1.518835	-1.534177
14	6	0	0.905605	1.648671	-2.339465
15	1	0	2.679586	2.390782	-1.405676
16	6	0	0.257952	0.528181	-2.906025
17	1	0	0.503909	2.624651	-2.582128
18	8	0	0.612859	-0.667756	-2.743139
19	1	0	-0.616240	0.742816	-3.542553
20	1	0	0.260708	-3.221582	-6.341022
21	6	0	0.272842	-2.369554	-5.661217
22	7	0	0.309558	-2.854621	-4.251504
23	1	0	-0.624584	-1.769699	-5.808089
24	1	0	1.155131	-1.759151	-5.848831
25	6	0	1.566136	-3.642981	-3.973876
26	6	0	-0.928790	-3.641988	-3.905034
27	1	0	0.338214	-1.988117	-3.631623
28	6	0	1.615747	-4.115934	-2.523965
29	1	0	1.572100	-4.487001	-4.669833
30	1	0	2.406230	-2.990241	-4.214306
31	6	0	-0.899159	-4.117044	-2.454871
32	1	0	-1.783643	-2.992554	-4.100587
33	1	0	-0.973479	-4.486363	-4.598978
34	6	0	0.367799	-4.926279	-2.154675
35	1	0	2.522578	-4.712203	-2.395586
36	1	0	1.709559	-3.245378	-1.866986
37	1	0	-1.797557	-4.713533	-2.277454
38	1	0	-0.957062	-3.249250	-1.789437
39	1	0	0.351859	-5.863385	-2.723404
40	1	0	0.396398	-5.202001	-1.098393

Total Energy (a.u.) = **-677.82438187;** NIMAG = **1 ,** ν_i (cm^{-1}) = **335i**

TS1-BF_4^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.568210	-0.840321	-0.080847
2	6	0	-0.449992	-0.373505	1.239636
3	6	0	0.656920	0.503691	1.333617
4	6	0	0.973845	0.922543	-0.092277
5	6	0	0.383838	-0.215616	-0.863681
6	1	0	-1.227799	-1.636146	-0.400897
7	1	0	-1.028793	-0.737260	2.078844
8	1	0	0.788502	1.205888	2.148813
9	1	0	0.398706	1.838984	-0.295843
10	1	0	2.016044	1.167800	-0.279691
11	1	0	0.545485	-0.391446	-1.919613
12	1	0	1.791326	-1.215835	2.524301
13	6	0	2.151428	-0.672445	1.657842
14	6	0	2.393168	-1.442374	0.501349
15	1	0	2.844369	0.133464	1.878248
16	6	0	1.826171	-2.746840	0.326145
17	1	0	3.071809	-1.086399	-0.265377
18	8	0	1.057922	-3.310626	1.111127
19	1	0	2.115266	-3.262349	-0.616658
20	9	0	3.657253	2.293852	1.212154
21	5	0	2.947320	3.334038	1.879131
22	9	0	2.285453	2.775360	3.006152
23	9	0	1.980538	3.868089	0.994530
24	9	0	3.840432	4.334972	2.290381

Total Energy (a.u.) = **-810.802273989;** NIMAG = **1 ,** ν_i (cm^{-1}) = **360i**

TS1-PF_6^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.045513	0.026577	-0.061962
2	6	0	0.036805	-0.032423	1.342437
3	6	0	1.367524	-0.042352	1.822004
4	6	0	2.224178	0.466965	0.674812
5	6	0	1.351516	0.144367	-0.497849
6	1	0	-0.822569	-0.107182	-0.693719
7	1	0	-0.845037	-0.188235	1.950279
8	1	0	1.626983	0.195886	2.846436
9	1	0	2.295836	1.560251	0.782750
10	1	0	3.243588	0.090647	0.654924
11	1	0	1.669628	0.194021	-1.531305
12	1	0	1.048498	-2.349246	2.343831
13	6	0	1.861509	-1.917588	1.771168
14	6	0	1.958703	-2.327047	0.426941
15	1	0	2.784307	-1.777903	2.324055
16	6	0	0.858220	-2.941765	-0.258602
17	1	0	2.899440	-2.252310	-0.106388
18	8	0	-0.266295	-3.130957	0.211653
19	9	0	3.517794	0.107632	4.313484
20	15	0	5.006512	0.583059	3.771765
21	9	0	4.284588	1.769725	2.883278
22	9	0	6.472297	1.048499	3.208494
23	9	0	4.840651	-0.451158	2.487776
24	9	0	5.145242	1.609040	5.040111
25	9	0	5.704920	-0.615312	4.642456
26	1	0	1.070220	-3.251324	-1.305785

Total Energy (a.u.) = **-1327.01587534;** NIMAG = **1 ,** ν_i (cm^{-1}) = **377i**

TS1-NTf_2^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.003643	-0.012174	-0.025050
2	6	0	-0.018198	0.010882	1.380458
3	6	0	1.309579	0.028081	1.865215
4	6	0	2.173451	0.465602	0.693862
5	6	0	1.304093	0.077715	-0.461860
6	1	0	-0.869633	-0.180726	-0.651222
7	1	0	-0.901853	-0.107945	1.993923
8	1	0	1.556810	0.318570	2.880107
9	1	0	2.237610	1.564827	0.731320
10	1	0	3.194580	0.091028	0.688115
11	1	0	1.628086	0.069261	-1.494468
12	1	0	0.971789	-2.262078	2.493672
13	6	0	1.794198	-1.866541	1.909186
14	6	0	1.909087	-2.333647	0.587706
15	1	0	2.709874	-1.712347	2.469041
16	6	0	0.814421	-2.982338	-0.079150
17	1	0	2.857496	-2.283036	0.065938
18	8	0	-0.312414	-3.153356	0.390503
19	1	0	1.036612	-3.339331	-1.108516
20	8	0	5.583616	-0.494316	1.297616
21	16	0	5.855155	-0.096059	2.679231
22	8	0	6.292374	-1.104060	3.640270
23	7	0	4.645182	0.847672	3.147684
24	6	0	7.344885	1.062551	2.502547
25	16	0	4.248798	1.243542	4.661774
26	9	0	8.397514	0.373123	2.029630
27	9	0	7.690155	1.600881	3.676606
28	9	0	7.082338	2.058682	1.642960
29	8	0	5.268613	1.079059	5.694160
30	8	0	2.874581	0.827517	4.949400
31	6	0	4.101082	3.115185	4.426734
32	9	0	3.737457	3.679420	5.591089
33	9	0	5.269409	3.653068	4.051765
34	9	0	3.177983	3.430521	3.507856

Total Energy (a.u.) = **-2213.72665226;** NIMAG = **1 ,** ν_i (cm^{-1}) = **380i**

TS1-OTf $^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.118682	-0.593900	-0.624500
2	6	0	-0.317650	0.118962	0.571121
3	6	0	0.845051	0.866402	0.873590
4	6	0	1.633331	0.946328	-0.422082
5	6	0	1.111246	-0.250995	-1.151100
6	1	0	-0.780262	-1.359378	-1.007862
7	1	0	-1.171836	0.004137	1.225804
8	1	0	0.850426	1.704148	1.559627
9	1	0	1.318050	1.866655	-0.936302
10	1	0	2.712527	1.016500	-0.311689
11	1	0	1.545147	-0.656432	-2.056125
12	1	0	1.253374	-0.687653	2.628012
13	6	0	1.947147	-0.370242	1.857348
14	6	0	2.399563	-1.381790	0.985951
15	1	0	2.650551	0.393923	2.174158
16	6	0	1.700072	-2.625403	0.848603
17	1	0	3.324481	-1.266322	0.432417
18	8	0	0.647618	-2.925042	1.419885
19	1	0	2.167570	-3.354511	0.150570
20	8	0	2.509701	4.103896	0.269147
21	16	0	3.308800	3.997783	1.506083
22	8	0	3.537131	5.253285	2.236726
23	8	0	2.994320	2.817620	2.342716
24	6	0	5.031796	3.572577	0.845156
25	9	0	5.927691	3.415361	1.840062
26	9	0	5.020403	2.418286	0.136198
27	9	0	5.506740	4.533293	0.026914

Total Energy (a.u.) = **-1347.85036727;** NIMAG = **1 ,** ν_i (cm^{-1}) = **360i**

TS1-TFA$^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.597346	-0.083616	0.189757
2	6	0	1.862363	-0.017225	-0.418480
3	6	0	2.248152	1.338458	-0.550940
4	6	0	1.355931	2.117249	0.396478
5	6	0	0.208864	1.188417	0.560691
6	1	0	0.004620	-0.982324	0.294727
7	1	0	2.401809	-0.862658	-0.825515
8	1	0	3.289651	1.608250	-0.695411
9	1	0	1.826804	2.223994	1.393964
10	1	0	1.085073	3.128415	0.093715
11	1	0	-0.699860	1.473618	1.071680
12	1	0	1.974670	1.163481	-2.913879
13	6	0	1.497590	1.888537	-2.263339
14	6	0	0.090875	1.839510	-2.212751
15	1	0	1.963476	2.869226	-2.278427
16	6	0	-0.610270	0.650596	-2.586525
17	1	0	-0.491844	2.693158	-1.887248
18	8	0	-0.080858	-0.399695	-2.969901
19	1	0	-1.716857	0.705418	-2.506018
20	9	0	1.669890	3.979655	5.890477
21	6	0	0.520260	3.810619	5.192875
22	6	0	0.713375	3.223518	3.736226
23	9	0	-0.269337	3.009307	5.964103
24	9	0	-0.086230	5.032056	5.173473
25	8	0	-0.357119	3.095247	3.119243
26	8	0	1.891219	2.977106	3.419717

Total Energy (a.u.) = **-912.56556650;** NIMAG = **1 ,** ν_i (cm^{-1}) = **360i**