Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

σ-Hole promotes the Concertedness in Nucleophilic Aromatic Substitution reactions of nitroarenes.

Sebastián Gallardo-Fuentes,[a] *Rodrigo Ormazábal-Toledo*[a,b]*

[a]Departamento de Química, Facultad de Ciencias, Universidad de Chile, Las Palmeras 3425, Casilla 653, Santiago de Chile.

[b] Centro Integrativo de Biología y Química Aplicada (CIBQA), Universidad Bernardo O Higgins, Santiago 8370854, Chile

Contents:

1. Expulsion of fluoride assisted by acetonitrile

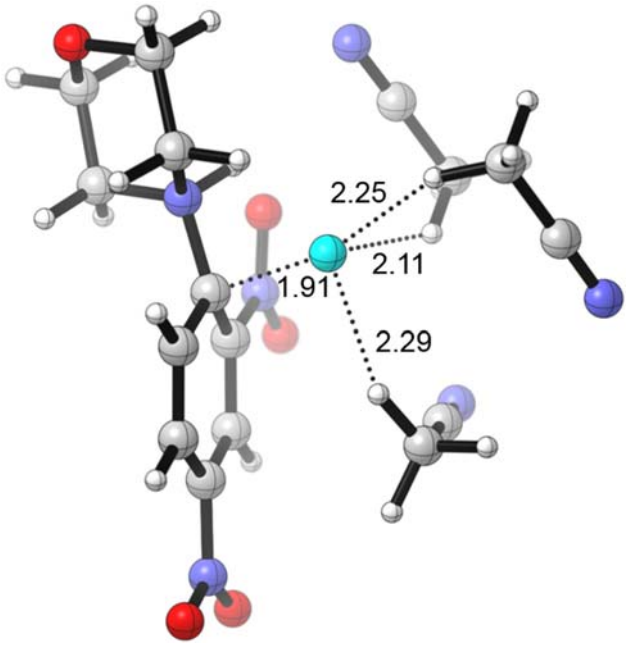

Figure S1. Expulsion of fluoride assisted by three molecules of solvent.

2. Leaving group nucleofugalities

Table S1. Nucleofugalities of leaving groups calculated at the M06-2x/6-31+G(d,p) level of theory.

Substrate	Group	Nucleofugality (eV)
1a	-F	0.02
1b	-Cl	0.02
1c	-Br	0.02
1d	-I	0.96
1e	-NO_2	0.08
1f	-OPh	0.51

3. NBO analysis.

Table S2. NBO population analysis for structures **1a**, **1b**, **1c** and **1d.** Charges are expressed in units of *e*.

		1a	**1b**	**1c**	**1d**
Reactants	%s	68.58	81.92	84.46	88.69
	%p	31.40	18.07	15.54	11.31
	q (X)	-0.31	0.10	0.18	0.32
TS1	%s	67.49	81.52	84.93	88.22
	%p	32.50	18.47	15.07	11.78
	q (X)	-0.33	0.10	-0.02	0.32
MC	%s	71.63	86.48	88.83	91.60
	%p	28.37	13.52	11.17	8.40
	q (X)	-0.39	-0.14	-0.08	0.02
TS2	%s	81.73	88.12	89.35	92.11
	%p	18.27	11.88	10.65	7.89
	q (X)	-0.70	-0.28	-0.27	-0.25
Products	%s	61.82	87.42	88.62	93.80
	%p	38.16	12.58	11.38	6.20
	q (X)	-0.65	-0.85	-0.83	-0.87

By using the same argument by Politzer, the *s* unshared electrons have a little *p* character in the **1b-d** cases. For **1a**, the *p* character is almost double than other substrates. In the same line, natural charge over the leaving group is negative for fluorine and positive for Cl, Br and I. Passing through **TS1**, the *s* and *p* character of the unshared electrons remains similar, with a negative change of natural charge of bromine. At the **MC-Z** stage, the charge over iodine is still positive, with a similar s character. For fluorine, the s unshared pair have a less important *p* character, which at **TS2** displays similar values than **1b-d**. At the products stage, the situation turns back due to the stabilization of fluoride by hydrogen bonds.

4. Cartesian coordinates for main TS structures.

TS1-1a in acetonitrile

1	6	0	0.005675	-0.036623	0.033010
2	6	0	0.048597	-0.046537	1.448505
3	6	0	1.250772	-0.024760	2.110432
4	6	0	2.445680	0.088047	1.376334
5	6	0	2.440916	0.199554	-0.001666
6	6	0	1.222674	0.172688	-0.665400
7	1	0	-0.892152	-0.083412	1.986687
8	1	0	1.281196	-0.059843	3.193456
9	1	0	3.361250	0.305303	-0.564031
10	7	0	3.712571	0.113188	2.076191
11	8	0	3.698890	0.010580	3.296354
12	8	0	4.739539	0.233581	1.420189
13	7	0	1.234604	0.221722	-2.109739
14	8	0	2.243610	0.629793	-2.668951
15	8	0	0.238306	-0.167952	-2.705785
16	9	0	-1.155270	0.357959	-0.518568
17	1	0	1.316127	-4.971595	-0.437325
18	6	0	0.418350	-4.370794	-0.602287
19	8	0	-0.551407	-4.806283	0.339020
20	6	0	0.724324	-2.888852	-0.421080
21	1	0	0.049968	-4.553503	-1.623993
22	6	0	-1.763082	-4.078406	0.201024
23	7	0	-0.491871	-2.077938	-0.482848
24	1	0	1.424523	-2.554427	-1.193440
25	1	0	1.181491	-2.720529	0.563821
26	6	0	-1.524477	-2.589003	0.419955
27	1	0	-2.185021	-4.247796	-0.802101
28	1	0	-2.458570	-4.470536	0.947123
29	1	0	-0.845635	-2.022898	-1.438600
30	1	0	-2.448614	-2.024776	0.264242
31	1	0	-1.179487	-2.427682	1.449241

SCF Done: E(RM062X) = -1027.92442563 A.U. after 1 cycles

Frequencies -- -197.2435 cm^{-1}

TS2-1a in acetonitrile

1	6	0	0.002312	-0.002459	-0.001592
2	6	0	0.002045	-0.018014	1.412722
3	6	0	1.175902	-0.011465	2.129661
4	6	0	2.398067	-0.063613	1.450329
5	6	0	2.453059	-0.140330	0.073508
6	6	0	1.264258	-0.155853	-0.643536
7	1	0	-0.936663	0.017110	1.948664
8	1	0	1.152240	0.017724	3.212944
9	1	0	3.400931	-0.189544	-0.447780
10	7	0	3.641048	-0.060130	2.203384
11	8	0	3.572339	0.006515	3.422290
12	8	0	4.693806	-0.123405	1.584658
13	7	0	1.386259	-0.178216	-2.089503
14	8	0	2.499950	-0.246795	-2.580556
15	8	0	0.362407	-0.129505	-2.768912
16	9	0	-0.425428	1.815688	-0.517885
17	1	0	-2.566830	-3.305944	-1.924591

18	6	0	-2.501611	-2.225334	-1.786454
19	8	0	-3.695987	-1.799001	-1.159193
20	6	0	-1.280090	-1.912596	-0.936484
21	1	0	-2.400816	-1.747472	-2.773221
22	6	0	-3.672221	-0.400025	-0.932942
23	7	0	-1.241616	-0.425088	-0.685331
24	1	0	-0.366599	-2.207111	-1.454697
25	1	0	-1.327174	-2.394413	0.042780
26	6	0	-2.526337	-0.018393	-0.012260
27	1	0	-3.589716	0.136955	-1.889942
28	1	0	-4.614503	-0.127877	-0.454647
29	1	0	-1.214140	0.059283	-1.593724
30	1	0	-2.477133	1.055407	0.160401
31	1	0	-2.604591	-0.569291	0.925333

SCF Done: E(RM062X) = -1027.92427441 A.U. after 1 cycles
Frequencies -- -338.9986 cm^{-1}

TS1-cat-1a in acetonitrile

1	6	0	0.405455	0.354819	0.537541
2	6	0	0.422936	-0.000950	1.903265
3	6	0	1.582278	-0.446316	2.490405
4	6	0	2.770142	-0.472307	1.738879
5	6	0	2.809747	-0.048892	0.423779
6	6	0	1.632522	0.393149	-0.165277
7	1	0	-0.503512	0.071977	2.462320
8	1	0	1.591886	-0.746005	3.532038
9	1	0	3.730809	-0.058347	-0.146753
10	7	0	3.995421	-0.936139	2.360596
11	8	0	3.941055	-1.321738	3.520921
12	8	0	5.025179	-0.922686	1.699476
13	7	0	1.672398	0.769851	-1.561239
14	8	0	2.763765	0.978235	-2.073529
15	8	0	0.612599	0.840454	-2.170124
16	9	0	-0.630665	1.101621	0.130225
17	1	0	0.497796	-4.431844	-1.576999
18	6	0	-0.253085	-3.666100	-1.366207
19	8	0	-1.138498	-4.210435	-0.397741
20	6	0	0.399686	-2.391080	-0.843956
21	1	0	-0.808875	-3.447619	-2.292435
22	6	0	-2.161936	-3.285104	-0.058668
23	7	0	-0.598621	-1.414481	-0.421629
24	1	0	1.035095	-1.954147	-1.622627
25	1	0	1.031037	-2.632649	0.023248
26	6	0	-1.562738	-2.000453	0.504338
27	1	0	-2.762651	-3.055503	-0.953968
28	1	0	-2.801595	-3.775288	0.680099
29	1	0	-1.103003	-1.003210	-1.220902
30	1	0	-2.354393	-1.269840	0.704448
31	1	0	-1.048058	-2.225099	1.448947
32	1	0	-2.324942	0.031410	-5.898294
33	6	0	-2.486925	0.456927	-4.903982
34	8	0	-3.891122	0.632725	-4.757256
35	6	0	-1.938464	-0.456367	-3.815706
36	1	0	-1.987397	1.438725	-4.852553
37	6	0	-4.211174	1.187203	-3.486910
38	7	0	-2.269082	0.027018	-2.471544
39	1	0	-0.850664	-0.545333	-3.907729

40	1	0	-2.375508	-1.456963	-3.931605
41	6	0	-3.706607	0.293590	-2.361311
42	1	0	-3.757906	2.188583	-3.400145
43	1	0	-5.299414	1.291041	-3.453650
44	1	0	-1.752956	0.889041	-2.292251
45	1	0	-3.913814	0.757082	-1.391357
46	1	0	-4.234486	-0.668102	-2.401294

SCF Done: E(RM062X) = -1315.62722927 A.U. after 2 cycles
Frequencies -- -338.9986 cm^{-1}

TS2-cat-1a in acetonitrile

1	6	0	0.002359	-0.057867	-0.004340
2	6	0	0.014504	-0.050621	1.489735
3	6	0	1.133789	0.015235	2.237956
4	6	0	2.421150	0.105689	1.618503
5	6	0	2.514590	0.222295	0.248011
6	6	0	1.377031	0.166118	-0.543756
7	1	0	-0.955557	-0.052705	1.972570
8	1	0	1.062809	0.028474	3.319878
9	1	0	3.477901	0.360885	-0.228083
10	7	0	3.595547	0.144239	2.411158
11	8	0	3.477911	0.071867	3.637929
12	8	0	4.694920	0.247459	1.859482
13	7	0	1.551230	0.333548	-1.935941
14	8	0	2.655761	0.641584	-2.388313
15	8	0	0.573239	0.149578	-2.674418
16	9	0	-0.860970	0.998707	-0.412912
17	1	0	0.101900	-4.423389	-1.574386
18	6	0	-0.577923	-3.578663	-1.447465
19	8	0	-1.623560	-3.997130	-0.589457
20	6	0	0.194061	-2.406136	-0.863769
21	1	0	-0.989414	-3.304716	-2.430650
22	6	0	-2.534830	-2.930769	-0.394617
23	7	0	-0.724997	-1.265293	-0.593226
24	1	0	0.954747	-2.093329	-1.579571
25	1	0	0.675376	-2.689981	0.079954
26	6	0	-1.847141	-1.747413	0.269219
27	1	0	-2.978085	-2.646403	-1.360375
28	1	0	-3.329386	-3.291630	0.261644
29	1	0	-2.553307	-0.924848	0.414440
30	1	0	-1.447468	-2.067207	1.235273
31	1	0	-1.304180	-0.870549	-1.577093
32	1	0	-1.579237	0.562314	-2.768406
33	7	0	-2.117075	-0.291444	-2.599768
34	6	0	-3.489461	0.097402	-2.215332
35	1	0	-4.036445	-0.809210	-1.934901
36	1	0	-3.437767	0.761464	-1.347869
37	6	0	-2.128982	-1.084407	-3.844213
38	1	0	-1.095315	-1.277566	-4.146270
39	1	0	-2.618337	-2.040922	-3.627438
40	6	0	-4.198926	0.784377	-3.372667
41	1	0	-5.241488	0.990087	-3.118727
42	1	0	-3.696696	1.736645	-3.606761
43	6	0	-2.885800	-0.356810	-4.943929
44	1	0	-2.354736	0.570555	-5.212675
45	1	0	-2.971160	-0.983346	-5.834995
46	8	0	-4.207971	-0.044835	-4.526786

SCF Done: E(RM062X) = -1315.65035761   A.U. after   1 cycles
Frequencies --   -338.9986 cm^{-1}

TS3-cat-1a in acetonitrile

1	6	0	0.020223	0.051957	0.023271
2	6	0	-0.015913	-0.012005	1.485477
3	6	0	1.098875	-0.073459	2.256307
4	6	0	2.383526	-0.103713	1.648931
5	6	0	2.507553	-0.064933	0.276357
6	6	0	1.372204	-0.014832	-0.523999
7	1	0	-0.985457	0.004860	1.966086
8	1	0	1.015788	-0.121244	3.336300
9	1	0	3.485666	-0.063084	-0.188261
10	7	0	3.556639	-0.182229	2.459868
11	8	0	3.419802	-0.184862	3.683377
12	8	0	4.658840	-0.246039	1.915546
13	7	0	1.603155	0.154987	-1.926518
14	8	0	2.747894	0.035723	-2.363443
15	8	0	0.655075	0.433103	-2.662820
16	9	0	-0.380721	1.769780	-0.191789
17	1	0	-1.748119	-3.152962	-2.709988
18	6	0	-1.912240	-2.165994	-2.271498
19	8	0	-3.155115	-2.214145	-1.590344
20	6	0	-0.776893	-1.818819	-1.326014
21	1	0	-1.960255	-1.417092	-3.079176
22	6	0	-3.436501	-0.957604	-0.996718
23	7	0	-1.049106	-0.516781	-0.698535
24	1	0	0.150636	-1.791741	-1.897052
25	1	0	-0.688124	-2.599940	-0.553070
26	6	0	-2.346120	-0.550359	-0.016739
27	1	0	-3.556532	-0.202299	-1.788137
28	1	0	-4.386903	-1.058932	-0.467266
29	1	0	-2.568404	0.442690	0.384588
30	1	0	-2.340168	-1.275184	0.813827
31	1	0	-1.814763	0.994697	-2.758615
32	1	0	-0.982123	1.942145	-1.718957
33	7	0	-1.656784	1.980853	-2.520435
34	6	0	-2.918316	2.616182	-2.039127
35	1	0	-3.667558	2.507853	-2.826938
36	1	0	-3.243461	2.088492	-1.140453
37	6	0	-1.096690	2.717652	-3.691300
38	1	0	-0.146965	2.256547	-3.962827
39	1	0	-1.812216	2.615083	-4.510691
40	6	0	-2.640393	4.079696	-1.740807
41	1	0	-3.567900	4.576672	-1.451191
42	1	0	-1.919318	4.164118	-0.913738
43	6	0	-0.913188	4.175199	-3.310223
44	1	0	-0.162258	4.263476	-2.510227
45	1	0	-0.571349	4.739471	-4.179552
46	8	0	-2.139242	4.749617	-2.886482

SCF Done: E(RM062X) = -1315.64944542   A.U. after   1 cycles
Frequencies --   -338.9986 cm^{-1}

TS1-1a+3 acetonitrile molecules

1	6	0	-1.167491	-0.072444	-0.659138
2	6	0	-1.189673	0.336852	0.698328
3	6	0	-0.019344	0.505942	1.394560

4	6	0	1.211536	0.351692	0.730690
5	6	0	1.276165	0.071112	-0.622095
6	6	0	0.088927	-0.107419	-1.319886
7	1	0	-2.155824	0.488930	1.167776
8	1	0	-0.037937	0.786456	2.441635
9	1	0	2.227513	-0.016686	-1.135647
10	7	0	2.442222	0.520125	1.469668
11	8	0	2.369220	0.843295	2.649526
12	8	0	3.504491	0.334853	0.887856
13	7	0	0.164567	-0.488882	-2.711089
14	8	0	1.213337	-0.291139	-3.311114
15	8	0	-0.819397	-1.009798	-3.218458
16	9	0	-2.285747	0.174828	-1.363987
17	1	0	-0.049312	-4.975265	0.333221
18	6	0	-0.914241	-4.411946	-0.025301
19	8	0	-1.929916	-4.536331	0.959053
20	6	0	-0.546738	-2.949389	-0.244163
21	1	0	-1.260184	-4.855385	-0.972213
22	6	0	-3.102769	-3.833431	0.575816
23	7	0	-1.723183	-2.147033	-0.580785
24	1	0	0.194197	-2.867195	-1.045773
25	1	0	-0.116972	-2.530950	0.676127
26	6	0	-2.803021	-2.350429	0.386900
27	1	0	-3.501621	-4.258573	-0.358469
28	1	0	-3.837278	-3.978149	1.371720
29	1	0	-2.045533	-2.350823	-1.527837
30	1	0	-3.695170	-1.816649	0.047049
31	1	0	-2.478493	-1.924958	1.345119
32	6	0	1.571175	2.799806	-3.410754
33	1	0	2.048966	2.460033	-4.332090
34	1	0	1.745037	3.869615	-3.274558
35	1	0	1.989707	2.259086	-2.558975
36	6	0	-1.859451	3.574692	-0.507614
37	1	0	-2.131150	4.457217	-1.091034
38	1	0	-2.273582	3.660536	0.499500
39	1	0	-2.259019	2.682785	-0.994603
40	6	0	3.868866	3.418349	0.990241
41	1	0	4.479307	2.809398	1.660147
42	1	0	2.809214	3.282739	1.219826
43	1	0	4.128181	4.472245	1.113582
44	6	0	0.137896	2.540865	-3.477815
45	7	0	-0.998333	2.320894	-3.511854
46	6	0	-0.406336	3.475205	-0.427217
47	7	0	0.747115	3.399166	-0.362833
48	6	0	4.113852	3.019094	-0.390958
49	7	0	4.310704	2.708444	-1.488404

SCF Done: E(RM062X) = -1426.07697396 A.U. after 1 cycles
Frequencies -- -192.0672 cm^{-1}

TS2-1a+3 acetonitrile molecules

1	6	0	-0.017214	-0.070756	0.221048
2	6	0	-0.484124	-0.247588	1.547780
3	6	0	0.383804	-0.322726	2.610854
4	6	0	1.764197	-0.294754	2.377249
5	6	0	2.274507	-0.215350	1.098072
6	6	0	1.392819	-0.155354	0.026928
7	1	0	-1.547814	-0.273117	1.741196

8	1	0	0.001595	-0.412485	3.621289
9	1	0	3.342328	-0.195900	0.918131
10	7	0	2.684971	-0.334951	3.499114
11	8	0	2.213040	-0.401268	4.625620
12	8	0	3.885158	-0.293886	3.267555
13	7	0	1.992281	-0.023904	-1.286145
14	8	0	3.206613	-0.023603	-1.380517
15	8	0	1.248510	0.079569	-2.261987
16	9	0	-0.320699	1.770225	-0.198189
17	1	0	-1.658583	-3.160700	-2.774402
18	6	0	-1.704803	-2.104176	-2.505076
19	8	0	-3.058371	-1.784745	-2.244719
20	6	0	-0.832207	-1.870938	-1.282632
21	1	0	-1.330669	-1.505099	-3.350137
22	6	0	-3.185964	-0.419977	-1.881308
23	7	0	-0.951976	-0.422646	-0.876968
24	1	0	0.211626	-2.089578	-1.509103
25	1	0	-1.161410	-2.463411	-0.425908
26	6	0	-2.403799	-0.118479	-0.614411
27	1	0	-2.845554	0.225323	-2.703422
28	1	0	-4.243467	-0.227638	-1.692293
29	1	0	-0.662373	0.169647	-1.670850
30	1	0	-2.471818	0.931392	-0.331621
31	1	0	-2.741352	-0.768913	0.193145
32	6	0	1.070045	3.048412	-2.662085
33	1	0	1.969397	2.622789	-3.113276
34	1	0	1.028926	4.120174	-2.871837
35	1	0	1.076080	2.871635	-1.581889
36	6	0	-1.370319	4.642837	-0.922219
37	1	0	-1.269976	3.559621	-0.786748
38	1	0	-1.485482	4.881058	-1.982457
39	1	0	-2.240941	5.007830	-0.372713
40	6	0	1.572658	3.086023	2.015718
41	1	0	2.005642	2.608352	2.898353
42	1	0	0.657222	2.568040	1.711945
43	1	0	1.350850	4.131511	2.240102
44	6	0	-0.109807	2.391232	-3.210352
45	7	0	-1.050325	1.859690	-3.627869
46	6	0	-0.165660	5.283262	-0.407291
47	7	0	0.799806	5.774890	0.000342
48	6	0	2.518059	3.017876	0.907418
49	7	0	3.259314	2.949727	0.020496

SCF Done: E(RM062X) = -1426.07738168 A.U. after 1 cycles
Frequencies -- -326.7415 cm^{-1}

TS1-1b in acetonitrile

1	6	0	0.012109	-0.039381	0.024106
2	6	0	0.031624	-0.025804	1.451889
3	6	0	1.210489	0.007870	2.151306
4	6	0	2.430413	0.119898	1.458999
5	6	0	2.462220	0.215368	0.080617
6	6	0	1.266708	0.164768	-0.621158
7	1	0	-0.914994	-0.046959	1.980123
8	1	0	1.201017	-0.009875	3.235323
9	1	0	3.397586	0.323813	-0.455935
10	7	0	3.671123	0.172837	2.195109

11	8	0	3.620662	0.104442	3.417663
12	8	0	4.718967	0.282456	1.568831
13	7	0	1.357110	0.189987	-2.065443
14	8	0	2.337623	0.711309	-2.579612
15	8	0	0.457343	-0.340362	-2.705679
16	1	0	1.365298	-4.912291	-0.291424
17	6	0	0.469039	-4.324257	-0.502371
18	8	0	-0.535444	-4.756289	0.401526
19	6	0	0.757548	-2.837231	-0.326520
20	1	0	0.148355	-4.521675	-1.537015
21	6	0	-1.744420	-4.040477	0.202727
22	7	0	-0.464425	-2.042125	-0.456047
23	1	0	1.486723	-2.509290	-1.073397
24	1	0	1.165656	-2.650877	0.675996
25	6	0	-1.527104	-2.546181	0.415165
26	1	0	-2.122565	-4.224258	-0.814894
27	1	0	-2.468146	-4.425944	0.924603
28	1	0	-0.774067	-2.005240	-1.428766
29	1	0	-2.449749	-1.993741	0.216209
30	1	0	-1.219494	-2.369352	1.453171
31	17	0	-1.463111	0.616076	-0.694407

SCF Done: E(RM062X) = -1388.27536431 A.U. after 1 cycles
Frequencies -- -225.0263 cm^{-1}

TS1-1c in acetonitrile

1	6	0	0.010769	-0.031206	0.010720
2	6	0	0.015031	-0.008941	1.435632
3	6	0	1.187524	0.025020	2.147557
4	6	0	2.411972	0.131212	1.464144
5	6	0	2.458912	0.202245	0.084722
6	6	0	1.268670	0.149884	-0.627001
7	1	0	-0.934077	-0.023344	1.959413
8	1	0	1.167936	0.015504	3.231544
9	1	0	3.400448	0.295504	-0.443887
10	7	0	3.647387	0.185494	2.211629
11	8	0	3.585441	0.124031	3.433653
12	8	0	4.700539	0.290138	1.594115
13	7	0	1.372223	0.146666	-2.072154
14	8	0	2.373889	0.626402	-2.586126
15	8	0	0.460133	-0.364305	-2.710194
16	1	0	1.270386	-4.936876	-0.240878
17	6	0	0.388023	-4.337109	-0.475745
18	8	0	-0.639512	-4.739896	0.415726
19	6	0	0.697213	-2.852514	-0.313405
20	1	0	0.082744	-4.542670	-1.513416
21	6	0	-1.832977	-4.007855	0.185386
22	7	0	-0.508159	-2.039100	-0.474993
23	1	0	1.446143	-2.545063	-1.049669
24	1	0	1.088621	-2.661178	0.694990
25	6	0	-1.595103	-2.514639	0.380708
26	1	0	-2.195768	-4.199893	-0.836303
27	1	0	-2.575396	-4.371450	0.899597
28	1	0	-0.796906	-2.005461	-1.454066
29	1	0	-2.506255	-1.952590	0.157415
30	1	0	-1.305655	-2.328570	1.422594
31	35	0	-1.582129	0.710675	-0.774958

SCF Done: E(RM062X) = -3499.91939854 A.U. after 1 cycles

Frequencies -- -213.5855 cm^{-1}

TS1-1d in acetonitrile

1	6	0	0.012180	-0.010434	0.014331
2	6	0	0.014566	-0.013559	1.440236
3	6	0	1.184020	0.000659	2.159408
4	6	0	2.414617	0.103088	1.489954
5	6	0	2.466811	0.195261	0.112763
6	6	0	1.280205	0.155114	-0.604287
7	1	0	-0.934701	-0.029547	1.963032
8	1	0	1.160181	-0.025554	3.242827
9	1	0	3.410950	0.291213	-0.409701
10	7	0	3.644085	0.144869	2.246234
11	8	0	3.569846	0.085614	3.465593
12	8	0	4.698955	0.236844	1.633682
13	7	0	1.400920	0.167453	-2.047673
14	8	0	2.384457	0.692430	-2.546167
15	8	0	0.518349	-0.379789	-2.695460
16	1	0	1.280861	-4.901715	-0.420792
17	6	0	0.384781	-4.300534	-0.595036
18	8	0	-0.592617	-4.732452	0.331845
19	6	0	0.696076	-2.817877	-0.410457
20	1	0	0.034005	-4.477623	-1.624000
21	6	0	-1.796468	-4.005030	0.175825
22	7	0	-0.519310	-2.009246	-0.492919
23	1	0	1.405700	-2.484017	-1.172826
24	1	0	1.132312	-2.648847	0.583059
25	6	0	-1.557942	-2.515670	0.402579
26	1	0	-2.208973	-4.166340	-0.832623
27	1	0	-2.505033	-4.394207	0.911340
28	1	0	-0.853341	-1.952815	-1.456768
29	1	0	-2.477266	-1.944171	0.245040
30	1	0	-1.210090	-2.359381	1.431057
31	53	0	-1.758153	0.892063	-0.851187

SCF Done: E(RM062X) = -939.380423661   A.U. after   1 cycles

Frequencies -- -212.3271 cm^{-1}