A Theoretical Study of Substituent effects on Allylic Ion and Ion Pair S_N2 Reactions

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Figure S1. Ion pair SN2 barriers vs σ^+ constants. Lines are: NaF, $33.90 \pm 0.53 + (14.58 \pm 1.61) \sigma^+$, $R^2 = 0.965$; LiF, $29.31 \pm 0.59 + (17.77 \pm 1.77) \sigma^+$, $R^2 = 0.971$; LiCl, $12.96 \pm 0.59 + (18.80 \pm 1.78) \sigma^+$, $R^2 = 0.974$. Similar plots are found vs σ : NaF, $32.43 \pm 0.46 + (16.74 \pm 1.42) \sigma$, $R^2 = 0.979$; LiF, $27.52 \pm 0.54 + (20.35 \pm 1.69) \sigma$, $R^2 = 0.980$; LiCl, $11.08 \pm 0.68 + (21.42 \pm 2.09) \sigma$, $R^2 = 0.972$.

Table S1. Optimized coordinates of the ionic, ion pair transition structures and reactants, their Hartree-Fock energies and zero point energies (au) at 6-31+G*. All transition structures have one imaginary frequency. All normal structures have all frequencies real.

Ionic transition structures

allyl chloride + chloride ion

-1035.501003 au

0.0759537 au

6	.000000	.273235	.000000
6	-.506264	-1.098845	.000000
6	.293502	-2.150973	.000000
1	-1.574137	-1.212617	.000000
1	-.661330	1.101714	.000000
1	1.045952	.464756	.000000
1	-.099108	-3.151945	.000000
1	1.363619	-2.045659	.000000
17	.035341	.667743	2.465192
17	.035341	.667743	-2.465192

(trans)methyl allyl chloride+chloride ion

-1074.541672

0.105911 au

6	0.000000	0.715674	0.000000
6	-0.492987	-0.651154	0.000000
6	0.326392	-1.691054	0.000000
1	-1.559944	-0.781004	0.000000
1	-0.666409	1.541056	0.000000
1	1.043946	0.918527	0.000000
1	1.389368	-1.512564	0.000000
17	0.060780	1.142347	2.493760
17	0.060780	1.142347	-2.493760
6	-0.107252	-3.125087	0.000000
1	-1.187855	-3.213767	0.000000
1	0.278729	-3.641161	-0.876030
1	0.278729	-3.641161	0.876030

(trans)SiH3 allyl chloride + chloride ion

-1325.5844182

0.0925068 au

H	-2.6445727	0.0004911	0.6964600
C	-1.8672815	-0.0015566	-0.0243553
H	-2.1301410	-0.0051820	-1.0546307
Cl	-2.2033914	2.4417101	-0.0183555
Cl	-2.1985393	-2.4415991	-0.0063862
C	-0.4556213	0.0028834	0.3853738
C	0.5536697	-0.0005268	-0.4771778
H	0.3141723	-0.0062555	-1.5303239
H	-0.2891801	0.0082261	1.4476465
Si	2.3447975	0.0005134	0.0384116
H	2.4537369	0.0034110	1.5125009
H	3.0621434	1.1849996	-0.4869705
H	3.0602075	-1.1871148	-0.4821928

(trans)OH allylchloride + chloride ion

-1110.36524771

0.081739 au

6	0.000000	0.632719	0.000000
6	-0.565273	-0.679868	0.000000
6	0.227872	-1.746987	0.000000
1	-1.636197	-0.776743	0.000000
1	-0.615441	1.497564	0.000000
1	1.053616	0.780586	0.000000
1	1.296972	-1.667507	0.000000
17	0.130164	1.122524	2.543816
17	0.130164	1.122524	-2.543816
8	-0.172511	-3.020110	0.000000
1	-1.120046	-3.073999	0.000000

(trans)F allyl chloride+chloride ion

-1134.359258

0.068286 au

6	0.000000	0.676356	0.000000
6	-0.534337	-0.673723	0.000000
6	0.277931	-1.705934	0.000000
1	-1.598026	-0.809759	0.000000
1	-0.647371	1.515929	0.000000
1	1.047990	0.853156	0.000000
1	1.347982	-1.663802	0.000000
17	0.087497	1.086205	2.471134
17	0.087497	1.086205	-2.471134
9	-0.176337	-2.956297	0.000000

(trans)CN allyl chloride + chloride ion

-1127.248479

0.075529 au

6	0.785810	-0.731264	0.000000
6	0.000000	0.512804	0.000000
6	-1.324362	0.521667	0.000000
1	0.558755	1.428699	0.000000
1	1.844622	-0.697596	0.000000
1	0.301458	-1.677105	0.000000
1	-1.898753	-0.385188	0.000000
17	0.994141	-0.878625	2.400104
17	0.994141	-0.878625	-2.400104
6	-2.078259	1.746889	0.000000
7	-2.700857	2.700552	0.000000

(trans)Cl allyl chloride + chloride ion

-1494.405167

0.066723 au

6	0.962741	-0.579921	0.000000
6	0.000000	0.521078	0.000000

6	-1.294488	0.287486	0.000000
1	0.390380	1.519891	0.000000
1	2.004339	-0.384678	0.000000
1	0.636996	-1.591446	0.000000
1	-1.725159	-0.692544	0.000000
17	1.260737	-0.783760	2.443702
17	1.260737	-0.783760	-2.443702
17	-2.481243	1.554397	0.000000

(cis)methyl allyl chloride + chloride ion
-1074.539823
0.106114 au

6	0.000000	0.610320	0.000000
6	-1.036675	-0.412786	0.000000
6	-0.817320	-1.721009	0.000000
1	-2.046498	-0.047148	0.000000
1	-0.264432	1.637855	0.000000
1	1.034057	0.372649	0.000000
1	-1.684928	-2.362250	0.000000
17	0.252638	0.943023	2.483025
17	0.252638	0.943023	-2.483025
6	0.500068	-2.435646	0.000000
1	1.345123	-1.763241	0.000000
1	0.575278	-3.072954	0.877686
1	0.575278	-3.072954	-0.877686

(cis) SiH3 allyl chloride + chloride ion
-1325.581827
0.092824 au

6	0.583022	-1.160418	1.041706
1	0.745948	-1.683574	1.973840
6	-0.193205	-0.084880	1.113936
1	-0.614754	0.216045	2.056280
6	-0.563263	0.782242	-0.015082
1	-0.377343	0.502048	-1.022312
1	-1.060096	1.702247	0.161896
17	-2.855535	-0.107299	-0.276217
17	1.476467	2.146647	-0.151960
14	1.471525	-1.876617	-0.445027
1	1.188291	-3.331423	-0.499479
1	1.067421	-1.279177	-1.725842
1	2.934008	-1.744108	-0.278362

(cis) OH allyl chloride + chloride ion
-1110.356213
0.081223 au

6	0.621724	1.797780	0.000000
1	0.508406	2.868050	0.000000
6	-0.441194	1.005669	0.000000
1	-1.414021	1.455241	0.000000

6	-0.350979	-0.432725	0.000000
1	0.593331	-0.921649	0.000000
1	-1.226501	-1.031502	0.000000
17	-0.441194	-0.864615	2.520213
17	-0.441194	-0.864615	-2.520213
8	1.882116	1.343630	0.000000
1	2.505157	2.053378	0.000000

(cis) F allyl chloride + chloride ion

-1134.356490

0.068675 au

6	0.609820	1.785035	0.000000
1	0.552235	2.854683	0.000000
6	-0.426158	0.976271	0.000000
1	-1.404603	1.413866	0.000000
6	-0.327184	-0.476997	0.000000
1	0.619873	-0.959108	0.000000
1	-1.202330	-1.074197	0.000000
9	1.865037	1.355294	0.000000
17	-0.426158	-0.827610	2.459950
17	-0.426158	-0.827610	-2.459950

(cis)CN allyl chloride + chloride ion

-1127.243875

0.075859 au

6	0.324039	1.699273	0.000000
1	0.110163	2.751148	0.000000
6	-0.664379	0.815782	0.000000
1	-1.673907	1.177785	0.000000
6	-0.518581	-0.648543	0.000000
1	0.443808	-1.102817	0.000000
1	-1.378490	-1.265989	0.000000
17	-0.664379	-0.854535	2.398908
17	-0.664379	-0.854535	-2.398908
6	1.723327	1.363619	0.000000
7	2.842984	1.159041	0.000000

(cis)Cl allyl chloride + chloride ion

-1494.401913

0.067155 au

6	0.275642	1.651558	0.000000
1	0.105971	2.708551	0.000000
6	-0.716084	0.783987	0.000000
1	-1.714090	1.179237	0.000000
6	-0.598116	-0.674987	0.000000
1	0.352211	-1.150535	0.000000
1	-1.469812	-1.276268	0.000000
17	-0.716084	-0.977466	2.434935
17	-0.716084	-0.977466	-2.434935
17	1.959055	1.247618	0.000000

Ion Pair Transition structures

allyl fluoride + LiF

-322.828743

0.0795797 au

6	-.215278	.411751	.000000
6	-.215278	1.825437	.000000
6	.967385	2.463334	.000000
3	-.231824	-2.397416	.000000
9	-.215278	-1.585614	1.484749
9	-.215278	-1.585614	-1.484749
1	.689872	-.147100	.000000
1	-1.120428	-.147100	.000000
1	-1.144142	2.364036	.000000
1	1.897133	1.923621	.000000
1	1.027071	3.536721	.000000

2-F allyl fluoride + LiF

-421.673891 au

0.0712173 au

6	.000000	.071025	.000000
6	1.408799	.142841	.000000
6	2.159096	-.960391	.000000
3	-2.770823	-.282530	.000000
9	-1.923947	-.223242	1.469198
9	-1.923947	-.223242	-1.469198
1	-.483134	-.873581	.000000
1	-.603940	.948009	.000000
9	1.966932	1.344938	.000000
1	1.688875	-1.923948	.000000
1	3.231963	-.909836	.000000

2-Me allyl fluoride + LiF

-361.868201

0.1093294 au

6	.000000	.012939	.000000
6	-.793233	1.188972	.000000
6	-.098944	2.341986	.000000
3	1.633771	-2.276447	.000000
9	1.182529	-1.610357	1.488133
9	1.182529	-1.610357	-1.488133
1	1.062088	.060935	.000000
1	-.428778	-.961990	.000000
6	-2.300687	1.098588	.000000
1	.975463	2.344809	.000000
1	-.585209	3.301466	.000000
1	-2.749851	2.083920	.000000
1	-2.651679	.565863	-.876888
1	-2.651679	.565863	.876888

allyl chloride + LiCl
-1042.967082 au
0.0779054 au

6	-.157908	.996425	.000000
6	-.157908	2.403734	.000000
6	1.028150	3.042021	.000000
3	-.182839	-2.247053	.000000
17	-.157908	-1.245557	1.974735
17	-.157908	-1.245557	-1.974735
1	.751789	.439243	.000000
1	-1.067606	.439243	.000000
1	-1.086623	2.941969	.000000
1	1.957214	2.501278	.000000
1	1.088621	4.115290	.000000

2-F allyl chloride + LiCl
-1141.810803 au
0.069564 au

6	1.095252	2.661236	0.000000
1	2.020584	2.119390	0.000000
1	1.125959	3.734824	0.000000
6	-0.065557	1.997977	0.000000
6	-0.104352	0.592923	0.000000
17	0.067414	-1.571459	1.958367
17	0.067414	-1.571459	-1.958367
3	0.067414	-2.621580	0.000000
1	-1.029716	0.061092	0.000000
1	0.805310	0.041974	0.000000
9	-1.218725	2.647139	0.000000

2-Me allyl chloride + LiCl
-1082.006962 au
0.107652 au

6	-2.536681	-0.000118	1.344956
1	-1.891441	-0.000282	2.204087
1	-3.595214	0.000098	1.535141
6	-2.036018	-0.000133	0.091893
6	-0.626153	-0.000069	0.016534
17	1.631272	-1.979143	-0.023011
17	1.631104	1.979231	-0.022937
3	2.620244	0.000064	-0.073144
1	-0.108514	0.000279	-0.917699
1	-0.025146	-0.000277	0.897170
6	-2.875035	0.000033	-1.164017
1	-2.663354	-0.877342	-1.764766
1	-2.663181	0.877439	-1.764660
1	-3.930945	0.000116	-0.924922

allyl fluoride + NaF
-477.196166 au

0.0783427 au

6	-.174448	.712365	.000000
6	-.174448	2.136288	.000000
6	.998915	2.780498	.000000
11	-.207971	-2.264049	.000000
9	-.174448	-.998882	1.637964
9	-.174448	-.998882	-1.637964
1	.735209	.169406	.000000
1	-1.084105	.169406	.000000
1	-1.107194	2.668414	.000000
1	1.932779	2.248052	.000000
1	1.050942	3.854227	.000000

2-F allyl fluoride + NaF

-576.043213 au

0.070069 au

6	1.069574	2.447210	0.000000
1	2.019746	1.951030	0.000000
1	1.048654	3.520803	0.000000
6	-0.048587	1.730666	0.000000
6	-0.034551	0.307439	0.000000
9	0.076059	-1.326861	1.620969
9	0.076059	-1.326861	-1.620969
11	0.076059	-2.631684	0.000000
1	-0.944072	-0.235583	0.000000
1	0.895301	-0.194099	0.000000
9	-1.238217	2.319775	0.000000

2-Me allyl fluoride + NaF

-516.235485 au

0.108088 au

6	2.283596	-0.000768	1.325472
1	1.661477	-0.001247	2.201381
1	3.346928	-0.000925	1.487799
6	1.751538	-0.000033	0.095099
6	0.323595	-0.000028	0.040868
9	-1.395577	1.643087	-0.007122
9	-1.395623	-1.643092	-0.008410
11	-2.652200	0.000056	-0.065891
1	-0.192707	0.000390	-0.885172
1	-0.250007	-0.000405	0.931425
6	2.552813	0.000672	-1.183926
1	2.321817	0.878008	-1.778524
1	2.322095	-0.876199	-1.779320
1	3.616146	0.000751	-0.978068

(trans)F allyl fluoride + LiF

-421.681373

0.072102 au

6	0.458142	0.253046	0.000000
6	0.784676	-1.104719	0.000000
6	-0.260738	-1.954278	0.000000
3	-0.472945	2.934573	0.000000
9	-0.260738	2.146292	1.480952
9	-0.260738	2.146292	-1.480952
1	-0.551501	0.586230	0.000000
1	1.201061	1.016870	0.000000
1	1.794803	-1.466982	0.000000
9	-0.103694	-3.231632	0.000000
1	-1.291487	-1.652699	0.000000

(cis) F allyl fluoride + LiF

-421.686882

0.0722489 au

6	.000000	.560736	.000000
6	1.377286	.835757	.000000
6	2.274683	-.167527	.000000
3	-2.746826	-.013757	.000000
9	-1.950022	.147391	1.484596
9	-1.950022	.147391	-1.484596
1	-.372576	-.435110	.000000
1	-.720286	1.343000	.000000
1	1.747200	1.842628	.000000
9	1.937268	-1.411937	.000000
1	3.339313	-.028644	.000000

(trans)Cl allyl fluoride + LiF

-781.727594 au

0.070287 au

6	-0.250058	-1.429627	0.000000
6	0.772813	-0.551902	0.000000
6	0.427156	0.809144	0.000000
9	-0.250058	2.703149	1.482092
9	-0.250058	2.703149	-1.482092
3	-0.465132	3.489594	0.000000
1	-0.587461	1.126255	0.000000
1	1.795587	-0.876798	0.000000
1	1.162551	1.579686	0.000000
1	-1.273206	-1.104260	0.000000
17	-0.052970	-3.106826	0.000000

(cis) Cl allyl fluoride + LiF

-781.721751 au

0.070368 au

6	1.031428	-1.750766	0.000000
6	1.492791	-0.483173	0.000000
6	0.640217	0.638449	0.000000
9	-0.589758	2.207012	1.485286
9	-0.589758	2.207012	-1.485286

3	-1.078283	2.855769	0.000000
1	-0.418310	0.545494	0.000000
1	2.557845	-0.344588	0.000000
1	1.716472	-2.577259	0.000000
17	-0.589758	-2.233570	0.000000
1	1.033744	1.626465	0.000000

(trans)CN allyl fluoride + LiF

-414.549564 au

0.078738 au

6	-0.272637	-1.572307	0.000000
6	0.719600	-0.670262	0.000000
6	0.354263	0.707223	0.000000
9	-0.272637	2.534923	1.469318
9	-0.272637	2.534923	-1.469318
3	-0.504060	3.356955	0.000000
1	-0.666438	1.000126	0.000000
1	1.751817	-0.964687	0.000000
1	1.084441	1.480378	0.000000
1	-1.304208	-1.268900	0.000000
6	-0.034972	-2.990582	0.000000
7	0.136644	-4.112976	0.000000

(cis)CN allyl fluoride + LiF

-414.544885 au

0.078849 au

6	0.979963	-1.916375	0.000000
6	1.493264	-0.677644	0.000000
6	0.656822	0.482313	0.000000
9	-0.425129	2.051441	1.470456
9	-0.425129	2.051441	-1.470456
3	-0.930597	2.742480	0.000000
1	-0.403296	0.403256	0.000000
1	2.559538	-0.555100	0.000000
1	1.079501	1.455954	0.000000
1	1.628839	-2.773882	0.000000
6	-0.425129	-2.227193	0.000000
7	-1.521426	-2.521459	0.000000

(trans)Me allyl fluoride + LiF

-361.878012 au

0.109383 au

6	0.435754	0.304879	0.000000
6	0.763203	-1.054540	0.000000
6	-0.252684	-1.952408	0.000000
3	-0.455659	3.002934	0.000000
9	-0.252684	2.247402	1.494976
9	-0.252684	2.247402	-1.494976
1	-0.576212	0.632572	0.000000
1	1.175187	1.072729	0.000000

1	1.789503	-1.373429	0.000000
6	-0.102925	-3.430843	0.000000
1	-1.260520	-1.570978	0.000000
1	0.933266	-3.739901	0.000000
1	-0.603013	-3.842778	0.872433
1	-0.603013	-3.842778	-0.872433

(cis)Me allyl fluoride + LiF

-361.874023 au

0.1093873 au

6	.661140	-.348476	.000000
6	.222661	-1.675189	.000000
6	-1.102827	-1.981103	.000000
3	1.218699	2.460570	.000000
9	.990385	1.708385	1.492347
9	.990385	1.708385	-1.492347
1	.000000	.480481	.000000
1	1.699513	-.102122	.000000
1	.943584	-2.471572	.000000
6	-2.276842	-1.065197	.000000
1	-1.354147	-3.029807	.000000
1	-2.024941	-.017215	.000000
1	-2.885913	-1.286307	-.872304
1	-2.885913	-1.286307	.872304

(trans)SH allyl fluoride + LiF

-720.348859 au

0.079844 au

6	-0.233999	-1.423440	0.000000
6	0.830352	-0.566487	0.000000
6	0.542546	0.789846	0.000000
9	-0.233999	2.745963	1.497451
9	-0.233999	2.745963	-1.497451
3	-0.425526	3.494110	0.000000
1	-0.457367	1.152555	0.000000
1	1.842014	-0.928232	0.000000
1	1.305272	1.536492	0.000000
1	-1.228428	-1.014515	0.000000
16	-0.088940	-3.127860	0.000000
1	-1.383293	-3.409728	0.000000

(cis)SH allyl fluoride + LiF

-720.341777 au

0.079709 au

6	1.027463	-1.745109	0.000000
6	1.554959	-0.480362	0.000000
6	0.754305	0.653441	0.000000
9	-0.632558	2.215329	1.497080
9	-0.632558	2.215329	-1.497080
3	-1.091315	2.839085	0.000000

1	-0.309125	0.613403	0.000000
1	2.624557	-0.385663	0.000000
1	1.172989	1.634026	0.000000
1	1.715958	-2.571367	0.000000
16	-0.632558	-2.172980	0.000000
1	-0.443831	-3.483713	0.000000

(trans)OH allyl fluoride + LiF

-397.685158 au

0.084936 au

6	1.643900	-1.086032	0.000000
6	1.344224	0.247161	0.000000
6	0.000000	0.587063	0.000000
9	-2.098077	0.752860	1.497451
9	-2.098077	0.752860	-1.497451
3	-2.853999	0.910934	0.000000
1	-0.766532	-0.150373	0.000000
1	2.115073	0.995567	0.000000
1	-0.333707	1.600902	0.000000
1	0.838308	-1.798164	0.000000
8	2.976164	-1.605621	0.000000
1	2.736187	-2.576399	0.000000

(cis)OH allyl fluoride + LiF

-397.700505 au

0.085739 au

6	0.679874	-2.192614	0.000000
6	1.315912	-0.979108	0.000000
6	0.588227	0.197053	0.000000
9	-0.607626	1.924663	1.508432
9	-0.607626	1.924663	-1.508432
3	-1.009088	2.556877	0.000000
1	-0.476047	0.203781	0.000000
1	2.388621	-0.978418	0.000000
1	1.064457	1.150271	0.000000
1	1.254301	-3.104395	0.000000
8	-0.607626	-2.315254	0.000000
1	-0.909861	-3.215759	0.000000

(trans-anti)vinyl allyl fluoride +LiF

-399.730514 au

0.115709 au

6	0.115457	-1.502392	0.000000
6	1.014063	-0.473896	0.000000
6	0.517462	0.823942	0.000000
9	-0.489842	2.673933	1.502727
9	-0.489842	2.673933	-1.502727
3	-0.784940	3.374591	0.000000
1	-0.528067	1.021933	0.000000
1	2.071975	-0.662765	0.000000

1	1.151282	1.682060	0.000000
1	-0.933260	-1.256599	0.000000
6	0.458043	-2.904956	0.000000
1	1.499620	-3.172107	0.000000
6	-0.489842	-3.841246	0.000000
1	-1.535416	-3.588519	0.000000
1	-0.245255	-4.887276	0.000000

(cis-anti)vinyl allyl fluoride + LiF

-399.726050 au

0.115666 au

6	0.903426	-1.733374	0.000000
6	1.522125	-0.519352	0.000000
6	0.798568	0.679397	0.000000
9	-0.519740	2.322318	1.502727
9	-0.519740	2.322318	-1.502727
3	-0.933985	2.959817	0.000000
1	1.294307	1.620474	0.000000
1	-0.258681	0.710902	0.000000
1	2.595515	-0.484726	0.000000
1	1.537373	-2.605013	0.000000
6	-0.519740	-2.011762	0.000000
1	-1.217052	-1.196693	0.000000
6	-0.955712	-3.268903	0.000000
1	-0.280506	-4.106561	0.000000
1	-2.005687	-3.495605	0.000000

(trans-syn)vinyl allyl fluoride + LiF

-399.724736 au

0.115550 au

6	-0.383756	-1.515622	0.000000
6	0.648527	-0.619825	0.000000
6	0.325263	0.731081	0.000000
9	-0.383756	2.709263	1.502694
9	-0.383756	2.709263	-1.502694
3	-0.581482	3.443887	0.000000
1	-0.685072	1.065441	0.000000
1	1.675762	-0.930701	0.000000
1	1.066912	1.497487	0.000000
1	-1.377938	-1.102534	0.000000
6	-0.311064	-2.967261	0.000000
1	-1.251505	-3.487576	0.000000
6	0.824580	-3.662628	0.000000
1	0.809560	-4.736745	0.000000
1	1.793046	-3.198230	0.000000

(cis-syn)vinyl allyl fluoride + LiF

-399.644070 au

0.111662 au

6	-0.390060	-2.226960	0.000000
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6	-1.245810	-1.206256	0.000000
6	-0.979328	0.301374	0.000000
1	-1.818619	1.006219	0.000000
1	0.050731	0.675800	0.000000
1	-2.275869	-1.580681	0.000000
1	-0.765342	-3.256707	0.000000
6	1.132486	-2.387626	0.000000
1	1.577853	-3.389057	0.000000
6	2.371465	-1.488242	0.000000
1	3.372525	-1.934441	0.000000
1	2.257355	-0.398198	0.000000
9	-0.390060	2.318470	-1.502694
9	-0.390060	2.318470	1.502694
3	-0.236688	3.063618	0.000000

(trans)F allyl chloride + LiCl

-1141.824828 au

0.070430 au

6	-0.464509	-0.533231	0.000000
6	-1.847803	-0.668248	0.000000
6	-2.550195	0.486581	0.000000
3	2.748590	0.156499	0.000000
17	1.755708	0.012546	1.972006
17	1.755708	0.012546	-1.972006
1	0.000000	0.426366	0.000000
1	0.189292	-1.378197	0.000000
1	-2.344262	-1.619458	0.000000
1	-2.112372	1.467673	0.000000
9	-3.833052	0.499661	0.000000

(cis) F allyl chloride + LiCl

-1141.819776 au

0.0705671 au

6	-0.597022	0.564868	0.000000
6	-0.949779	1.917387	0.000000
6	0.005329	2.871633	0.000000
3	0.264321	-2.557484	0.000000
17	0.005329	-1.589997	1.975754
17	0.005329	-1.589997	-1.975754
1	0.422753	0.253777	0.000000
1	-1.341399	-0.198685	0.000000
1	-1.976165	2.228256	0.000000
9	1.262453	2.599861	0.000000
1	-0.192585	3.926932	0.000000

(trans)Cl allyl chloride + LiCl

-1501.865776 au

0.068602 au

6	-0.196437	-2.113986	0.000000
1	-1.211054	-1.761917	0.000000

6	0.851848	-1.259225	0.000000
6	0.545090	0.103544	0.000000
17	-0.196437	2.249114	1.972751
17	-0.196437	2.249114	-1.972751
3	-0.449048	3.218688	0.000000
1	1.305207	0.854003	0.000000
1	-0.465114	0.443802	0.000000
1	1.865755	-1.610280	0.000000
17	-0.039517	-3.790208	0.000000

(cis)Cl allyl chloride + LiCl

-1501.860403 au

0.068691 au

6	1.153397	-2.347546	0.000000
6	1.667494	-1.095445	0.000000
6	0.861481	0.050797	0.000000
17	-0.481399	1.838472	1.976782
17	-0.481399	1.838472	-1.976782
3	-1.060037	2.654247	0.000000
1	1.295794	1.024955	0.000000
1	-0.202251	-0.008078	0.000000
1	2.736762	-0.997579	0.000000
1	1.806905	-3.199326	0.000000
17	-0.481399	-2.761036	0.000000

(trans)CN allyl chloride + LiCl

-1134.686626 au

0.077108 au

6	0.888112	2.074276	0.000000
6	-0.338525	1.526852	0.000000
6	-0.428185	0.109976	0.000000
17	-0.428185	-2.028938	1.957892
17	-0.428185	-2.028938	-1.957892
3	-0.482782	-3.090268	0.000000
1	-1.370224	-0.388421	0.000000
1	0.451982	-0.488684	0.000000
1	-1.226686	2.129294	0.000000
1	1.774037	1.464717	0.000000
6	1.103438	3.494631	0.000000
7	1.289783	4.614769	0.000000

(cis)CN allyl chloride + LiCl

-1134.682282 au

0.077198 au

6	-2.598236	-0.000639	0.779398
6	-1.438919	-0.001146	1.457404
6	-0.180321	-0.000385	0.790004
17	1.704486	1.962199	-0.138946
17	1.704198	-1.962101	-0.140311
3	2.640915	0.000203	-0.645015

1	0.724478	-0.000848	1.349353
1	-0.117150	0.000331	-0.273814
1	-1.460784	-0.002144	2.530250
1	-3.535308	-0.001165	1.306689
6	-2.711573	0.000602	-0.653720
7	-2.843901	0.001564	-1.781226

(trans)Me allyl chloride + LiCl

-1082.017571 au

0.1076217 au

6	-.419034	-.548654	.000000
6	-1.795866	-.743042	.000000
6	-2.593949	.359318	.000000
3	2.774081	.264383	.000000
17	1.835672	.085035	1.988123
17	1.835672	.085035	-1.988123
1	.000000	.432282	.000000
1	.275067	-1.361899	.000000
1	-2.212118	-1.733398	.000000
6	-4.077775	.352001	.000000
1	-2.116874	1.325591	.000000
1	-4.486725	-.648629	.000000
1	-4.437343	.891989	.872100
1	-4.437343	.891989	-.872100

(cis)Me allyl chloride + LiCl

-1082.013739 au

0.1075562 au

6	-1.056269	.082868	.000000
6	-1.929150	1.162720	.000000
6	-1.461958	2.446652	.000000
3	1.495142	-2.058020	.000000
17	.832026	-1.363445	1.985316
17	.832026	-1.363445	-1.985316
1	.000000	.202340	.000000
1	-1.410572	-.927136	.000000
1	-2.989100	.990355	.000000
6	-.057127	2.933025	.000000
1	-2.206431	3.226608	.000000
1	.689115	2.155533	.000000
1	.084857	3.565938	-.872118
1	.084857	3.565938	.872118

(cis)SH allyl chloride + LiCl

-1440.482168 au

0.078040 au

6	1.149999	-2.361306	0.000000
6	1.768624	-1.128454	0.000000
6	1.052909	0.048489	0.000000
17	-0.527296	1.845110	1.994062

17	-0.527296	1.845110	-1.994062
3	-1.059176	2.612378	0.000000
1	1.539401	1.000930	0.000000
1	-0.013694	0.073022	0.000000
1	2.841955	-1.110020	0.000000
1	1.782068	-3.231508	0.000000
16	-0.527296	-2.666736	0.000000
1	-0.436605	-3.987902	0.000000

(trans)OH allyl chloride + LiCl

-1117.823565 au

0.083192 au

6	-2.641340	0.615327	0.000000
6	-1.881282	-0.533731	0.000000
6	-0.509382	-0.456119	0.000000
17	1.859363	-0.082553	2.004307
17	1.859363	-0.082553	-2.004307
3	2.761958	0.003290	0.000000
1	0.101569	-1.333205	0.000000
1	0.000000	0.481586	0.000000
1	-2.396156	-1.474489	0.000000
8	-4.068961	0.532877	0.000000
1	-2.210834	1.591761	0.000000
1	-4.255076	1.515405	0.000000

(cis)OH allyl chloride + LiCl

-1117.841604 au

0.084059 au

6	0.022457	2.908086	0.000000
6	-0.996568	1.980935	0.000000
6	-0.709658	0.637128	0.000000
17	0.022457	-1.646403	2.004307
17	0.022457	-1.646403	-2.004307
3	0.245590	-2.525185	0.000000
1	-1.482771	-0.101003	0.000000
1	0.295025	0.277445	0.000000
1	-2.005110	2.345577	0.000000
1	-0.203794	3.961707	0.000000
8	1.266132	2.575346	0.000000
1	1.869913	3.309878	0.000000

(trans-anti)vinyl allyl chloride +LiCl

-1119.871302 au

0.113953 au

6	0.293400	-2.182842	0.000000
6	1.251575	-1.198060	0.000000
6	0.823918	0.112915	0.000000
17	-0.445569	2.193563	2.000711
17	-0.445569	2.193563	-2.000711
3	-0.811762	3.030691	0.000000
1	1.502478	0.941007	0.000000

1	-0.214686	0.356582	0.000000
1	2.297392	-1.443800	0.000000
1	-0.739969	-1.878953	0.000000
6	0.559149	-3.596060	0.000000
1	1.582991	-3.923868	0.000000
6	-0.445569	-4.474606	0.000000
1	-1.473752	-4.158821	0.000000
1	-0.264661	-5.533469	0.000000

(trans-syn)vinyl allyl chloride + LiCl

-1119.86540 au

0.113913 au

6	1.031401	1.990664	0.000000
6	-0.269936	1.548675	0.000000
6	-0.478708	0.185203	0.000000
17	-0.478708	-2.224122	2.000341
17	-0.478708	-2.224122	-2.000341
3	-0.564452	-3.136557	0.000000
1	-1.458494	-0.244297	0.000000
1	0.336831	-0.503244	0.000000
1	-1.103205	2.224477	0.000000
1	1.795125	1.231788	0.000000
6	1.510241	3.357122	0.000000
1	2.576892	3.486763	0.000000
6	0.715077	4.427769	0.000000
1	1.130495	5.418355	0.000000
1	-0.356678	4.359377	0.000000

(trans)F allyl fluoride + NaF

-576.054066 au

0.0708054 au

6	.000000	.455061	.000000
6	1.259864	1.081321	.000000
6	2.323264	.265846	.000000
11	-2.636754	-1.006189	.000000
9	-1.499088	-.441115	1.631104
9	-1.499088	-.441115	-1.631104
1	-.083761	-.600924	.000000
1	-.898953	1.018212	.000000
1	1.377465	2.147907	.000000
9	3.535863	.715098	.000000
1	2.271596	-.806288	.000000

(cis)F allyl fluoride + NaF

-576.049058 au

0.0709671 au

6	-.248631	-.565900	.000000
6	-1.600558	-.985861	.000000
6	-2.597888	-.092411	.000000
11	2.586633	.316200	.000000

9	1.377529	-.062089	1.638952
9	1.377529	-.062089	-1.638952
1	.000000	.463329	.000000
1	.534830	-1.277995	.000000
1	-1.856753	-2.027426	.000000
9	-2.400370	1.188031	.000000
1	-3.640770	-.345761	.000000

(trans)Cl allyl fluoride + NaF

-936.095040 au

0.069026 au

6	-0.175422	-1.821443	0.000000
1	-1.213312	-1.548874	0.000000
6	0.800258	-0.902252	0.000000
6	0.399863	0.455966	0.000000
9	-0.175422	2.080904	1.631989
9	-0.175422	2.080904	-1.631989
11	-0.529909	3.303298	0.000000
1	1.114655	1.238997	0.000000
1	-0.626236	0.717961	0.000000
1	1.837217	-1.178396	0.000000
17	0.101534	-3.495051	0.000000

(cis)Cl allyl fluoride + NaF

-936.089579 au

0.069155 au

6	1.218739	-1.998400	0.000000
6	1.607244	-0.714833	0.000000
6	0.694717	0.375313	0.000000
9	-0.381749	1.676996	1.638884
9	-0.381749	1.676996	-1.638884
11	-1.188757	2.658775	0.000000
1	1.057735	1.369634	0.000000
1	-0.351236	0.214803	0.000000
1	2.663024	-0.517517	0.000000
1	1.943828	-2.789360	0.000000
17	-0.381749	-2.569559	0.000000

(trans)CN allyl fluoride + NaF

-568.919920 au

0.077683 au

6	-0.186493	-1.958310	0.000000
6	0.755931	-1.012653	0.000000
6	0.335803	0.362764	0.000000
9	-0.186493	1.882757	1.627806
9	-0.186493	1.882757	-1.627806
11	-0.561376	3.138411	0.000000
1	1.052907	1.140384	0.000000
1	-0.695998	0.593192	0.000000
1	1.801121	-1.257185	0.000000

1	-1.231861	-1.708313	0.000000
6	0.122492	-3.364730	0.000000
7	0.348493	-4.477522	0.000000

(cis)CN allyl fluoride + NaF

-568.916010 au

0.077911 au

6	-0.476833	-2.391363	0.000000
6	0.671986	-1.711570	0.000000
6	0.709196	-0.267554	0.000000
9	0.778584	1.283716	1.633085
9	0.778584	1.283716	-1.633085
11	0.778584	2.598754	0.000000
1	1.643274	0.224322	0.000000
1	-0.194509	0.281220	0.000000
1	1.598846	-2.252810	0.000000
1	-0.476035	-3.466273	0.000000
6	-1.786458	-1.790049	0.000000
7	-2.836839	-1.359491	0.000000

(trans)Me allyl fluoride + NaF

-516.243800 au

0.108103 au

6	.000000	.432667	.000000
6	1.312194	.943241	.000000
6	2.340426	.069532	.000000
11	-2.771250	-.770422	.000000
9	-1.620882	-.319268	1.648369
9	-1.620882	-.319268	-1.648369
1	-.176444	-.612763	.000000
1	-.849030	1.070001	.000000
1	1.481332	2.004635	.000000
6	3.784672	.429281	.000000
1	2.108128	-.982693	.000000
1	3.939977	1.499672	.000000
1	4.265959	-.002850	.873005
1	4.265959	-.002850	-.873005

(cis)Me allyl fluoride + NaF

-516.239759 au

0.108200 au

6	-.155555	-.711390	.000000
6	-1.442158	-1.284161	.000000
6	-2.562618	-.525771	.000000
11	2.559502	.638083	.000000
9	1.419517	.152311	1.645688
9	1.419517	.152311	-1.645688
1	.000000	.334047	.000000
1	.713838	-1.321835	.000000
1	-1.534475	-2.354483	.000000

6	-2.690772	.959964	.000000
1	-3.502500	-1.054534	.000000
1	-1.749033	1.484626	.000000
1	-3.263515	1.259905	-.873044
1	-3.263515	1.259905	.873044

(trans)SH allyl fluoride + NaF

-874.713870 au

0.078420 au

6	-0.166021	-1.831495	0.000000
6	0.839758	-0.919425	0.000000
6	0.480301	0.431004	0.000000
9	-0.166021	2.140229	1.648463
9	-0.166021	2.140229	-1.648463
11	-0.488134	3.326020	0.000000
1	1.209076	1.204833	0.000000
1	-0.536937	0.730370	0.000000
1	1.871481	-1.219242	0.000000
1	-1.183820	-1.485751	0.000000
16	0.079399	-3.533280	0.000000
1	-1.196567	-3.888572	0.000000

(cis)SH allyl fluoride + NaF

-874.707051 au

0.078303 au

6	1.217523	-2.007822	0.000000
6	1.653518	-0.719462	0.000000
6	0.776377	0.372632	0.000000
9	-0.418280	1.721003	1.647321
9	-0.418280	1.721003	-1.647321
11	-1.187540	2.687827	0.000000
1	1.143545	1.368657	0.000000
1	-0.277523	0.253694	0.000000
1	2.713613	-0.548485	0.000000
1	1.958331	-2.787225	0.000000
16	-0.418280	-2.553462	0.000000
1	-0.138016	-3.847503	0.000000

(trans)OH allyl fluoride + NaF

-552.072236 au

0.084236 au

6	-0.234577	-2.318610	0.000000
6	0.857562	-1.502217	0.000000
6	0.594315	-0.145068	0.000000
9	-0.132997	1.612447	1.654185
9	-0.132997	1.612447	-1.654185
11	-0.406392	2.792589	0.000000
1	1.370774	0.584342	0.000000
1	-0.396853	0.232567	0.000000
1	1.848963	-1.913175	0.000000

1	-1.226528	-1.899626	0.000000
8	-0.132997	-3.611708	0.000000
1	-0.971905	-4.057594	0.000000

(cis)OH allyl fluoride + NaF

-552.064992 au

0.084261 au

6	2.624909	-0.000237	0.144965
6	1.600269	-0.000750	1.041755
6	0.274989	-0.000048	0.613334
9	-1.455529	-1.664144	0.018766
9	-1.456070	1.664166	0.020185
11	-2.601692	-0.000070	-0.348650
1	-0.527124	-0.000583	1.308741
1	0.025042	0.000843	-0.417846
1	1.848683	-0.001802	2.085225
1	3.645720	-0.000862	0.489617
8	2.446666	0.000988	-1.142958
1	3.256347	0.001295	-1.637800

(trans-anti)vinyl allyl fluoride +NaF

-554.095228 au

0.114316 au

6	0.194251	-1.895245	0.000000
6	1.051679	-0.842505	0.000000
6	0.516575	0.451703	0.000000
9	-0.314973	2.079301	1.654366
9	-0.314973	2.079301	-1.654366
11	-0.786661	3.203402	0.000000
1	1.134364	1.316195	0.000000
1	-0.532241	0.610720	0.000000
1	2.115749	-0.993412	0.000000
1	-0.863107	-1.690079	0.000000
6	0.589462	-3.288962	0.000000
1	1.641515	-3.512594	0.000000
6	-0.314973	-4.264722	0.000000
1	-1.370743	-4.058220	0.000000
1	-0.024723	-5.299062	0.000000

(cis-anti)vinyl allyl fluoride + NaF

-554.090825 au

0.114350 au

6	1.061577	-2.036016	0.000000
6	1.624277	-0.795045	0.000000
6	0.846813	0.369464	0.000000
9	-0.347415	1.778116	1.648617
9	-0.347415	1.778116	-1.648617
11	-1.014914	2.805150	0.000000
1	1.299126	1.332166	0.000000
1	-0.210773	0.352729	0.000000

1	2.694971	-0.711512	0.000000
1	1.734609	-2.877842	0.000000
6	-0.347415	-2.379006	0.000000
1	-1.081166	-1.596581	0.000000
6	-0.725612	-3.654718	0.000000
1	-0.012914	-4.460717	0.000000
1	-1.764158	-3.929060	0.000000

(trans-syn)vinyl allyl fluoride + NaF

-554.089547 au

0.114223 au

6	-1.863765	-0.146923	0.552578
6	-1.075674	-0.047710	-0.548649
6	0.312217	-0.012246	-0.362768
9	2.150166	-1.627641	-0.124629
9	2.046592	1.670630	0.109095
11	3.307271	0.047799	0.158613
1	0.985749	0.072867	-1.179736
1	0.737258	-0.069374	0.607551
1	-1.485943	-0.007866	-1.539942
1	-1.366041	-0.221683	1.504413
6	-3.321424	-0.177034	0.599720
1	-3.757019	-0.513321	1.523654
6	-4.110968	0.221780	-0.392719
1	-5.179953	0.194830	-0.289563
1	-3.727158	0.604660	-1.320285

(cis-syn)vinyl allyl fluoride + NaF

-554.0110233 au

0.110277 au

6	2.391354	-0.977421	0.009011
6	1.178900	-1.528831	0.015970
6	-0.202463	-0.868698	0.011337
1	-1.106169	-1.488762	0.018563
1	-0.287636	0.223937	0.000796
1	1.264073	-2.621465	0.026511
1	3.283147	-1.614520	0.014058
6	2.953532	0.446554	-0.005606
1	4.037614	0.607720	-0.008593
6	2.418439	1.880938	-0.018892
1	3.116212	2.726068	-0.028043
1	1.337606	2.062645	-0.019252
9	-1.793101	-0.006888	-1.653421
9	-1.792554	0.045060	1.654334
11	-2.892048	0.549597	-0.007561

Reactants

Cl⁻

-459.539661 au

LiF

-106.946363 au

0.002114 au
 LiCl
 -467.011399 au
 0.001416 au
 NaF
 -261.321512 au
 0.001239 au
 Allyl fluoride
 -215.928943 au
 0.078642 au
 Allyl chloride
 -575.976092 au
 0.077036 au
 2-F allyl fluoride
 -314.784459 au
 0.070751 au

6	-1.550328	-0.829753	-0.192192
6	-0.542536	-0.034539	0.082134
6	0.837865	-0.434264	0.482633
1	1.104614	0.022125	1.426142
1	0.915268	-1.508518	0.554385
1	-2.517914	-0.435746	-0.439439
1	-1.418365	-1.894240	-0.178654
9	-0.694404	1.290421	0.050788
9	1.744004	-0.000675	-0.450553

2-Me allyl fluoride
 -254.968371 au
 0.108751 au

6	-1.456983	-1.027512	-0.184644
1	-1.224140	-2.078345	-0.182015
1	-2.476421	-0.762841	-0.404320
6	-0.539089	-0.108496	0.069768
6	0.862678	-0.513279	0.431313
1	1.012936	-1.577932	0.328744
1	1.109790	-0.208019	1.440865
9	1.770053	0.114120	-0.398873
6	-0.817846	1.372469	0.056659
1	-0.197331	1.871560	-0.679689
1	-0.590998	1.816273	1.023091
1	-1.856870	1.573139	-0.175391

2-F allyl chloride
 -674.831510 au
 0.069016 au

6	-1.923169	-0.823057	-0.351876
6	-0.973771	-0.034699	0.096936
6	0.310974	-0.446093	0.728116
1	0.441420	0.050646	1.677125
1	0.338495	-1.513548	0.866516
1	-2.827696	-0.419071	-0.765039
1	-1.805398	-1.888504	-0.316086
9	-1.114650	1.290105	0.046126

17 1.729460 -0.001022 -0.277453

2-Me allyl chloride

-615.014914 au

0.107111 au

6	-0.972874	-0.107529	0.091746
6	-1.808244	-1.040188	-0.338678
1	-1.564791	-2.087265	-0.293003
6	-1.283181	1.366278	0.035286
1	-2.268502	1.540642	-0.379292
1	-2.767226	-0.787630	-0.755454
1	-0.556906	1.892333	-0.574826
1	-1.249480	1.805103	1.029424
6	0.339779	-0.502581	0.710292
1	0.436334	-1.572366	0.791698
1	0.468218	-0.055554	1.684777
17	1.755852	0.056992	-0.264424

(trans)Me allyl chloride

-615.015906 au

0.107110 au

6	-1.599941	0.249421	-0.317165
6	-0.522849	0.152433	0.444062
1	-0.549880	-0.421329	1.356243
6	-2.929407	-0.380994	-0.015859
1	-1.543092	0.818809	-1.232904
1	-3.219564	-1.060728	-0.812230
1	-2.904405	-0.937637	0.913978
6	0.776885	0.816867	0.124485
1	1.111534	1.453011	0.929420
1	0.722538	1.391666	-0.786169
1	-3.706445	0.374647	0.059810
17	2.102423	-0.390870	-0.108311

(cis)Me allyl chloride

-615.0128563 au

0.107381 au

6	-0.482990	0.912451	0.051827
6	-1.714153	0.546024	-0.273506
1	-2.321620	1.283280	-0.774072
6	0.536215	0.086995	0.770847
1	0.164857	-0.871627	1.086778
1	0.929206	0.612584	1.627385
17	1.970445	-0.247988	-0.280257
1	-0.156775	1.904897	-0.209831
6	-2.396051	-0.774730	-0.045379
1	-2.749854	-1.176000	-0.990645
1	-3.266778	-0.644584	0.591552
1	-1.754728	-1.517194	0.410482

(trans)SiH3 allyl chloride

-866.057022 au

0.093561 au

6	-1.063422	0.487478	-0.320838
6	0.012291	0.202889	0.403365
1	-0.042207	-0.496095	1.222562
1	-0.950658	1.186230	-1.138794
6	1.361549	0.815622	0.181934
1	1.699234	1.350705	1.056843
1	1.368038	1.477182	-0.669159
17	2.607990	-0.449231	-0.126355
14	-2.759226	-0.254484	-0.009395
1	-3.738449	0.810261	0.284723
1	-3.226885	-0.987258	-1.201708
1	-2.678242	-1.177261	1.138341

(cis)SiH3 allyl chloride

-866.053392 au

0.093779 au

6	-1.171954	0.954071	-0.234032
1	-1.618747	1.829341	-0.685832
6	0.112460	1.076408	0.084449
1	0.623424	2.002407	-0.127273
6	0.971548	0.044444	0.748864
1	0.452877	-0.878163	0.940340
1	1.381571	0.422212	1.673448
14	-2.352570	-0.499033	-0.043679
1	-3.438378	-0.127143	0.883968
1	-2.949731	-0.801684	-1.357440
1	-1.680637	-1.705051	0.471156
17	2.393722	-0.364999	-0.281326

(trans)F allyl chloride

-674.829118 au

0.0694014 au

6	0.581154	0.135702	0.464755
6	1.629756	0.179954	-0.323442
1	1.685162	0.667933	-1.276856
6	-0.699663	0.814942	0.110172
1	-0.623532	1.365431	-0.814253
1	0.635294	-0.397311	1.397061
1	-1.022526	1.482845	0.893001
17	-2.043310	-0.368325	-0.102715
9	2.777154	-0.404551	0.004255

(cis)F allyl chloride

-674.8299012 au

0.069668 au

6	-0.566477	0.833364	0.135182
6	-1.770947	0.460382	-0.231998
6	0.457242	-0.072308	0.737888
1	0.097322	-1.082238	0.832354
1	-0.304728	1.865776	-0.006772
1	0.779104	0.287350	1.702694
17	1.943735	-0.138690	-0.279281
1	-2.517338	1.101843	-0.654472

9 -2.201863 -0.793736 -0.108051

(trans)Cl allyl chloride

-1034.8750504 au

0.067807 au

6	0.058338	0.201402	0.446223
6	1.104365	0.404415	-0.325790
1	1.080676	0.999239	-1.217691
6	-1.272000	0.820582	0.157728
1	-1.247175	1.439455	-0.724779
1	0.134853	-0.416336	1.323123
17	2.666927	-0.269094	-0.001388
1	-1.620144	1.406556	0.994198
17	-2.531187	-0.436042	-0.118837

(cis)Cl allyl chloride

-1034.874723 au

0.068066 au

6	-1.269100	0.898048	-0.208114
1	-1.830441	1.713961	-0.615679
6	-0.002983	1.017930	0.134779
1	0.451023	1.981404	-0.019612
6	0.870993	-0.040126	0.727156
1	0.375736	-0.992165	0.798914
1	1.225755	0.256156	1.702450
17	2.342177	-0.285316	-0.280214
17	-2.213679	-0.550829	-0.060315

(trans)CN allyl chloride

-667.711574 au

0.076461 au

6	1.239467	0.496918	-0.320544
6	0.188586	0.168296	0.414079
1	0.279115	-0.565874	1.195109
6	-1.158508	0.789546	0.227711
1	-1.166546	1.496503	-0.586172
1	-1.484334	1.279849	1.132494
17	-2.391436	-0.461996	-0.137780
1	1.179871	1.217387	-1.115851
6	2.538880	-0.088928	-0.101698
7	3.570823	-0.538419	0.057055

(cis)CN allyl chloride

-667.711293 au

0.076678 au

6	-0.084090	1.047783	0.149508
6	-1.360953	1.004487	-0.201077
6	0.710391	-0.096519	0.696251
1	0.162563	-1.023773	0.681995
1	0.439147	1.982098	0.050370
1	1.033915	0.114348	1.704594
17	2.201622	-0.338493	-0.271818
1	-1.862829	1.879878	-0.568074

6	-2.171102	-0.186985	-0.118958
7	-2.823692	-1.115826	-0.057476

(trans)OH allyl chloride

-650.832121 au

0.082267 au

6	0.562768	0.203048	0.479477
1	0.615580	-0.199011	1.475820
6	1.618015	0.138083	-0.310125
6	-0.717367	0.824859	0.039617
1	-0.635171	1.278999	-0.935428
1	-1.070832	1.561895	0.743068
17	-2.060010	-0.386833	-0.081819
1	1.598928	0.514295	-1.319312
8	2.788749	-0.394584	0.097285
1	3.421180	-0.419286	-0.605335

(cis)OH allyl chloride

-650.833299 au

0.082580 au

6	-0.540553	0.867460	0.093848
6	-1.750527	0.461661	-0.245149
6	0.480126	0.000361	0.751475
1	0.107808	-0.992742	0.933154
1	-0.273993	1.887306	-0.114011
1	0.834632	0.429180	1.675756
17	1.955561	-0.184023	-0.281705
1	-2.451950	1.131984	-0.709359
8	-2.193747	-0.796049	-0.023464
1	-3.045343	-0.935832	-0.409895

(trans)SH allyl chloride

-973.484745 au

0.077026 au

6	0.037860	0.184027	0.472986
1	0.096938	-0.472695	1.324479
6	1.095807	0.416767	-0.284211
1	1.025777	1.063712	-1.141586
6	-1.293202	0.811011	0.211927
1	-1.265197	1.480428	-0.632711
1	-1.660059	1.342305	1.076466
17	-2.551768	-0.431931	-0.155107
16	2.727181	-0.223168	-0.086263
1	2.504915	-0.971061	0.986156

(cis)SH allyl chloride

-973.482145 au

0.077266 au

6	-0.014744	1.265866	-0.085597
1	0.304597	2.212447	-0.486005
6	-1.247184	0.868817	-0.362423
6	0.988209	0.526923	0.741054
1	0.526139	-0.114405	1.473344

1	1.650309	1.211985	1.244657
17	2.059109	-0.536800	-0.258111
1	-1.889371	1.515966	-0.931662
16	-2.059961	-0.640791	0.070259
1	-0.994832	-1.417368	0.205213

(trans-anti)vinyl allyl chloride

-652.866367 au

0.113045 au

6	-0.001504	0.073045	0.573702
1	-0.035113	-0.660898	1.362016
6	1.135884	0.318653	-0.063174
6	-1.283941	0.776239	0.273943
1	-1.169343	1.506312	-0.511132
1	-1.692505	1.254612	1.150868
17	-2.559571	-0.379246	-0.276833
1	1.155554	1.046226	-0.859500
1	2.387300	-1.078939	1.034700
6	2.406574	-0.346277	0.244483
1	4.453863	-0.607598	-0.132391
6	3.544452	-0.095213	-0.388206
1	3.604153	0.628791	-1.182889

(trans-syn)vinyl allyl chloride

-652.861455 au

0.112986 au

6	0.141542	-0.112768	0.293764
1	0.294481	-1.177855	0.252995
6	1.117481	0.718459	-0.041923
6	-1.208365	0.345851	0.740259
1	-1.286234	1.421179	0.751284
1	-1.457974	-0.040356	1.716766
17	-2.509856	-0.255693	-0.358319
1	0.921371	1.779659	-0.054222
6	2.480032	0.313304	-0.442381
1	2.920676	0.888399	-1.241037
6	3.185097	-0.661771	0.111629
1	4.168945	-0.908417	-0.244811
1	2.811565	-1.234272	0.942360

(cis-anti)vinyl allyl chloride

-652.863077 au

0.113381 au

6	0.076572	1.020667	0.074878
1	0.498835	1.963143	-0.228581
6	-1.206927	0.791396	-0.182963
6	1.028635	0.099982	0.769001
1	0.571537	-0.811062	1.112373
1	1.502742	0.591705	1.604550
17	2.379395	-0.390607	-0.326628
1	-1.759403	1.576233	-0.673058
6	-1.981501	-0.419707	0.116745
1	-1.472772	-1.251129	0.571591

6	-3.273960	-0.535234	-0.158174
1	-3.816896	-1.435494	0.065164
1	-3.830671	0.264301	-0.616284

(cis-syn)vinyl allyl chloride

-652.858638 au

0.113253 au

6	-0.018146	0.929638	0.414089
1	0.541967	1.792491	0.730817
6	-1.263048	1.107647	-0.010257
6	0.721882	-0.369342	0.487727
1	0.212526	-1.165178	-0.026543
1	0.911231	-0.664017	1.509122
17	2.349630	-0.216842	-0.277648
1	-1.631210	2.120860	-0.037735
6	-2.219715	0.087951	-0.491397
1	-2.724443	0.332048	-1.413051
1	-3.258107	-1.718408	-0.288321
6	-2.535865	-1.039261	0.128076
1	-2.106313	-1.311282	1.076297

(trans)Me allyl fluoride

-254.968768 au

0.1087519 au

6	1.101750	0.371627	-0.160943
1	1.017024	1.311402	-0.686385
6	0.010406	-0.176523	0.346188
1	0.063494	-1.120143	0.866082
6	-1.345875	0.446300	0.263668
1	-1.332082	1.363235	-0.309102
1	-1.756582	0.642438	1.245734
9	-2.226526	-0.417403	-0.358367
6	2.485044	-0.206762	-0.070980
1	2.896753	-0.369627	-1.063040
1	2.486953	-1.152899	0.458108
1	3.155223	0.474377	0.446317

(cis)Me allyl fluoride

-254.965454 au

0.108967 au

6	-1.234831	0.638646	-0.073542
6	0.065786	0.771047	0.139925
1	0.494591	1.759461	0.115881
6	1.051124	-0.315424	0.438085
1	0.646125	-1.306948	0.311038
1	1.447352	-0.219320	1.441097
9	2.128712	-0.202664	-0.418542
1	-1.793323	1.543503	-0.254120
6	-2.061041	-0.618486	-0.094336
1	-2.614502	-0.684316	-1.026517
1	-2.792233	-0.602453	0.709465
1	-1.472647	-1.520648	0.009234

(trans)F allyl fluoride

-314.7826104 au

0.071096 au

6	1.141495	0.336352	-0.164011
1	1.166599	1.265152	-0.699822
6	0.079485	-0.218760	0.370624
1	0.164919	-1.163575	0.877758
6	-1.263914	0.430191	0.303736
1	-1.224600	1.386620	-0.199425
1	-1.687861	0.562867	1.289474
9	-2.139709	-0.370199	-0.396584
9	2.343992	-0.222886	-0.084536

(cis)F allyl fluoride

-314.782910 au

0.071267 au

6	-1.313941	0.529476	-0.078479
6	-0.040941	0.747614	0.155059
1	0.294905	1.768770	0.160354
6	0.979893	-0.312598	0.422420
1	0.597223	-1.302270	0.228721
1	1.346017	-0.257385	1.438970
9	2.066138	-0.112106	-0.401362
1	-2.052729	1.283074	-0.261219
9	-1.836747	-0.696687	-0.105397

(trans)Cl allyl fluoride

-674.828226 au

0.069477 au

6	0.605290	0.465240	-0.155555
1	0.552413	1.398069	-0.682001
6	-0.442885	-0.147793	0.350182
1	-0.338939	-1.090231	0.858586
6	-1.820461	0.430992	0.264326
1	-1.837472	1.350913	-0.302813
1	-2.232355	0.607117	1.249012
9	-2.658721	-0.462767	-0.361839
17	2.219599	-0.152447	-0.036467

(cis)Cl allyl fluoride

-674.8279529 au

0.069448 au

6	-0.775013	0.926926	-0.024664
6	0.529678	0.823101	0.107750
1	1.102004	1.734673	0.117605
6	1.319033	-0.440137	0.271425
1	0.865764	-1.277135	-0.236557
1	1.454640	-0.684357	1.317246
9	2.570872	-0.249720	-0.264945
1	-1.278800	1.866666	-0.121941
17	-1.866097	-0.426571	-0.048171

(trans)CN allyl fluoride

-307.664558 au

0.078077 au

6	0.726881	0.542975	-0.150987
6	-0.324977	-0.135370	0.277858
1	-0.209333	-1.121068	0.694224
6	-1.718464	0.410703	0.245456
1	-1.785137	1.314696	-0.342906
1	-2.077668	0.603360	1.248012
9	-2.555301	-0.522787	-0.312313
1	0.637558	1.522746	-0.584399
6	2.067875	0.018538	-0.065689
7	3.132057	-0.376534	-0.006277

(cis)CN allyl fluoride

-307.664408 au

0.078189 au

6	-0.826204	1.029465	-0.051928
6	0.477339	0.862161	0.110351
1	1.114106	1.729352	0.101482
6	1.176847	-0.443821	0.338628
1	0.611174	-1.286822	-0.028240
1	1.390314	-0.582065	1.390918
9	2.379523	-0.416370	-0.321929
1	-1.250113	2.007250	-0.181906
6	-1.768751	-0.063885	-0.057756
7	-2.519510	-0.917701	-0.060093

(trans)OH allyl fluoride

-290.785534 au

0.084007 au

6	0.053062	-0.260480	0.381957
1	0.131718	-1.233958	0.834114
6	1.127346	0.318874	-0.119257
6	-1.285437	0.394212	0.347464
1	-1.231513	1.398995	-0.050269
1	-1.743402	0.424682	1.326751
9	-2.154605	-0.316122	-0.460221
1	1.083520	1.286528	-0.590854
8	2.348523	-0.251429	-0.064208
1	2.993108	0.264644	-0.525076

(cis)OH allyl fluoride

-290.789459 au

0.085048 au

6	-0.025466	1.073127	-0.000437
1	-0.000159	2.148875	-0.001578
6	-1.219639	0.499788	-0.000394
6	1.319065	0.413105	0.001198
1	1.890592	0.670985	0.882998
1	1.893753	0.673935	-0.877650
9	1.201261	-0.969670	-0.001235
1	-2.108093	1.101587	-0.001498
8	-1.524172	-0.805860	0.000744

1 -0.737826 -1.337597 0.000683

(trans)SH allyl fluoride

-613.4379037 au

0.078551 au

6	-0.469315	-0.191163	0.289674
1	-0.385262	-1.198550	0.661595
6	0.598305	0.469403	-0.120134
6	-1.841079	0.406244	0.296016
1	-1.860514	1.374266	-0.184946
1	-2.227932	0.497253	1.302727
9	-2.708410	-0.418025	-0.386497
1	0.515587	1.469472	-0.509474
16	2.244533	-0.169674	0.035218
1	2.693810	0.227665	-1.148255

(cis)SH allyl fluoride

-613.434495 au

0.078372 au

6	0.560303	0.802255	0.110506
1	1.144345	1.705215	0.155096
6	-0.752269	0.911616	0.002340
6	1.355368	-0.465918	0.198851
1	0.956901	-1.246409	-0.435019
1	1.424774	-0.831802	1.216348
1	-1.197721	1.887870	-0.056277
16	-1.987178	-0.354595	-0.069596
1	-1.273230	-1.382111	0.365811
9	2.639928	-0.216329	-0.222511

(trans-anti)vinyl allyl fluoride

-292.819171 au

0.114684 au

6	-0.530735	-0.338116	0.293260
1	-0.562176	-1.403736	0.454918
6	0.624472	0.272207	0.066014
6	-1.843732	0.371408	0.364332
1	-1.747308	1.419682	0.118036
1	-2.297210	0.272231	1.342272
9	-2.730037	-0.187476	-0.533875
1	0.639533	1.337319	-0.106232
1	1.911003	-1.475699	0.193240
6	1.922852	-0.410435	0.029818
1	4.005365	-0.333706	-0.212456
6	3.075873	0.205498	-0.191156
1	3.128747	1.267815	-0.358506

(trans-syn) vinyl allyl fluoride

-292.814161 au

0.114673 au

6	0.376814	-0.049607	0.375051
1	0.169570	0.788245	1.019786
6	-0.613357	-0.723096	-0.191618

6	1.819469	-0.402557	0.202762
1	1.953368	-1.223660	-0.487476
1	2.285384	-0.647140	1.148584
9	2.510072	0.681308	-0.301994
1	-0.379193	-1.580579	-0.804228
6	-2.051857	-0.420332	-0.040376
1	-2.703508	-1.275414	0.044428
6	-2.580617	0.794025	-0.033773
1	-3.639127	0.938978	0.086935
1	-1.979865	1.677197	-0.162358

(cis-anti)vinyl allyl fluoride

-292.815755 au

0.114912 au

6	0.618689	0.793235	0.143348
1	1.128970	1.740731	0.100079
6	-0.700749	0.772932	-0.008933
6	1.519037	-0.374881	0.400898
1	1.045869	-1.328226	0.225033
1	1.908148	-0.352073	1.411148
1	-1.198638	1.716098	-0.164108
9	2.609352	-0.299778	-0.440713
6	-1.585048	-0.400378	0.012485
1	-1.138462	-1.371673	0.133681
6	-2.902509	-0.315393	-0.114775
1	-3.525608	-1.191053	-0.101089
1	-3.400964	0.631110	-0.236465

(cis-syn)vinyl allyl fluoride

-292.812053 au

0.114879 au

6	0.529280	0.830335	0.293334
1	1.192992	1.624957	0.590204
6	-0.744667	1.118518	0.058580
6	1.191421	-0.507419	0.175315
1	0.662359	-1.174903	-0.487643
1	1.315651	-0.982418	1.140593
1	-1.044412	2.149907	0.151849
6	-1.819539	0.193156	-0.354274
1	-2.475377	0.566760	-1.124882
1	-2.874823	-1.608882	-0.200455
6	-2.062147	-1.003877	0.159670
1	-1.480912	-1.409676	0.968987
9	2.459825	-0.327780	-0.337155

Table S2. Energy barriers (Kcal mol⁻¹) of identity ion-pair S_N2 reactions of MX with allyl X. The substituent (Y) on the central (β) and terminal (γ) allylic carbon atoms and the leaving and attacking nucleophile (X) are given. The reaction angle (X-C-X) and some important bond lengths are also given.

Y	M	X	ΔE^*	Reaction angle deg	Bond lengths, Å ^a			
					M-X	C-X	C _α -C _β	C _β -C _γ
H	Li	F	28.54	73.25	1.692	2.489	1.414	1.344
H	Li	Cl	12.49	82.75	2.214	2.988	1.407	1.347
H	Na	F	33.18	87.49	2.070	2.369	1.424	1.339
β -F	Li	F	34.78	74.10	1.697	2.439	1.411	1.334
β -Me	Li	F	28.32	73.08	1.692	2.500	1.419	1.346
β -F	Li	Cl	19.65	84.1	2.222	2.924	1.406	1.337
β -Me	Li	Cl	11.64	82.48	2.213	3.002	1.412	1.349
β -F	Na	F	38.28	89.40	2.081	2.304	1.423	1.328
β -Me	Na	F	33.04	87.38	2.069	2.379	1.429	1.340
Trans								
γ-F	Li	F	25.78	72.36	1.691	2.509	1.396	1.347
γ-Cl	Li	F	28.74	72.77	1.692	2.498	1.404	1.348
γ-CN	Li	F	37.67	74.50	1.699	2.427	1.425	1.341
γ-Me	Li	F	22.44	71.91	1.687	2.546	1.398	1.356
γ-SH	Li	F	21.75	70.86	1.685	2.583	1.387	1.367
γ-OH	Li	F	28.65	70.86	1.685	2.583	1.387	1.367
γ-vinyl(a)	Li	F	21.35	71.01	1.684	2.588	1.390	1.366
γ-vinyl(s)	Li	F	21.75	71.14	1.684	2.583	1.389	1.367
γ-F	Li	Cl	9.62	81.56	2.213	3.019	1.390	1.352
γ-Cl	Li	Cl	12.62	81.98	2.212	3.008	1.397	1.353
γ-CN	Li	Cl	22.37	84.94	2.228	2.900	1.420	1.343
γ-Me	Li	Cl	5.59	80.65	2.206	3.072	1.390	1.361
γ-OH	Li	Cl	12.24	79.78	2.200	3.125	1.374	1.378
γ-vinyl(a)	Li	Cl	3.76	78.76	2.199	3.153	1.379	1.374
γ-vinyl(s)	Li	Cl	4.39	79.40	2.200	3.131	1.379	1.374
γ-F	Na	F	30.53	86.09	2.067	2.390	1.407	1.340
γ-Cl	Na	F	33.35	86.87	2.070	2.374	1.416	1.340
γ-CN	Na	F	40.57	90.73	2.090	2.288	1.438	1.335
γ-Me	Na	F	28.08	85.39	2.060	2.431	1.408	1.349
γ-SH	Na	F	27.79	84.11	2.056	2.461	1.397	1.358
γ-OH	Na	F	21.26	82.03	2.050	2.521	1.382	1.364
γ-vinyl(a)	Na	F	27.60	84.30	2.055	2.465	1.400	1.358
γ-vinyl(s)	Na	F	27.97	84.49	2.056	2.460	1.401	1.358
Cis								
γ-F	Li	F	29.41	73.36	1.693	2.485	1.404	1.346
γ-Cl	Li	F	32.30	73.38	1.693	2.486	1.409	1.349
γ-CN	Li	F	40.51	75.30	1.702	2.407	1.430	1.341
γ-Me	Li	F	22.74	71.24	1.687	2.562	1.397	1.360
γ-SH	Li	F	24.08	71.26	1.685	2.570	1.388	1.370
γ-OH	Li	F	21.34	71.35	1.684	2.587	1.383	1.370

γ -vinyl(a)	Li	F	21.85	71.01	1.684	2.588	1.400	1.363
γ -vinyl(s)	Li	F	68.69	71.14	1.684	2.583	1.531	1.332
γ -F	Li	Cl	13.21	82.89	2.215	2.985	1.398	1.350
γ -Cl	Li	Cl	15.68	82.96	2.215	2.984	1.401	1.354
γ -CN	Li	Cl	24.84	86.07	2.232	2.875	1.425	1.343
γ -Me	Li	Cl	5.89	79.70	2.205	3.098	1.389	1.366
γ -SH	Li	Cl	6.76	79.62	2.202	3.115	1.377	1.379
γ -OH	Li	Cl	1.61	79.78	2.200	3.125	1.374	1.377
γ -F	Na	F	33.86	87.82	2.072	2.363	1.416	1.339
γ -Cl	Na	F	36.70	88.27	2.074	2.354	1.422	1.341
γ -CN	Na	F	43.00	92.89	2.097	2.253	1.444	1.335
γ -Me	Na	F	28.47	84.99	2.060	2.436	1.408	1.353
γ -SH	Na	F	27.69	84.88	2.059	2.441	1.401	1.360
γ -OH	Na	F	29.97	84.57	2.054	2.473	1.393	1.362
γ -vinyl(a)	Na	F	28.11	83.51	2.054	2.476	1.400	1.363
γ -vinyl(s)	Na	F	73.54	84.49	2.056	2.460	1.531	1.332

(a) Bond lengths calculated in addition for (a) allyl fluoride C-X= 1.379; C _{α} -C _{β} = 1.496; C _{β} -C _{γ} = 1.321 (b) Li-F=1.575 (c) Li-Cl = 2.066 (d) Na-F = 1.928

Table S3. Reduced natural charges on allylic carbon centers, attacking and leaving groups, X, and on the substituents, Y, for ion pair SN2 reactions of MX with allyl X.

Y	M	X	Reduced charges*					
			C _{α}	C _{β}	C _{γ}	M	X	Y
H	Li	F	0.768	-0.207	0.376	0.962	-0.950	
H	Li	Cl	0.688	-0.199	0.404	0.897	-0.895	
H	Na	F	0.767	-0.194	0.330	0.981	-0.942	
β -F	Li	F	0.766	0.217	0.322	0.963	-0.944	-0.380
β -Me	Li	F	0.777	-0.272	0.359	0.962	-0.951	0.077
β -F	Li	Cl	0.670	0.225	0.343	0.900	-0.881	-0.375
β -Me	Li	Cl	0.697	-0.271	0.388	0.897	-0.897	0.084
β -F	Na	F	0.761	0.241	0.262	0.981	-0.930	-0.385
β -Me	Na	F	0.779	-0.257	0.312	0.980	-0.943	0.070
Trans								
γ -F	Li	F	0.735	-0.264	0.824	0.962	-0.952	-0.353
γ -Cl	Li	F	0.754	-0.196	0.295	0.962	-0.951	0.088
γ -CN	Li	F	0.797	-0.106	0.228	0.963	-0.942	0.231
								-0.229
γ -Me	Li	F	0.732	-0.227	0.384	0.961	-0.956	0.061
γ -SH	Li	F	0.692	-0.222	0.152	0.961	-0.958	0.334
γ -OH	Li	F	0.702	-0.248	0.692	0.961	-0.958	-0.192
γ -vinyl(a)	Li	F	0.696	-0.214	0.344	0.961	-0.959	-0.098

								0.229
γ -vinyl(s)	Li	F	0.692	-0.218	0.358	0.961	-0.959	-0.111
								0.235
γ -F	Li	Cl	0.658	-0.252	0.845	0.897	-0.902	-0.345
γ -Cl	Li	Cl	0.671	-0.191	0.315	0.897	-0.899	0.105
γ -CN	Li	Cl	0.696	-0.097	0.241	0.901	-0.874	0.227
								-0.220
γ -Me	Li	Cl	0.659	-0.219	0.413	0.895	-0.908	0.069
γ -OH	Li	Cl	0.632	-0.240	0.724	0.893	-0.912	-0.183
γ -vinyl(a)	Li	Cl	0.615	-0.205	0.376	0.893	-0.916	-0.108
								0.262
γ -vinyl(s)	Li	Cl	0.615	-0.209	0.387	0.893	-0.915	-0.118
								0.263
γ -F	Na	F	0.745	-0.260	0.787	0.981	-0.946	-0.361
γ -Cl	Na	F	0.762	-0.188	0.264	0.981	-0.943	0.066
γ -CN	Na	F	0.783	-0.08	0.175	0.982	-0.924	0.247
								-0.257
γ -Me	Na	F	0.744	-0.220	0.345	0.980	-0.952	0.056
γ -SH	Na	F	0.719	-0.221	0.130	0.980	-0.955	0.304
γ -OH	Na	F	0.677	-0.267	0.711	0.980	-0.962	-0.176
γ -vinyl(a)	Na	F	0.721	-0.209	0.311	0.980	-0.956	-0.085
								0.194
γ -vinyl(s)	Na	F	0.721	-0.211	0.321	0.980	-0.956	-0.095
								0.195
<hr/>								
Cis								
γ -F	Li	F	0.772	-0.291	0.81	0.962	-0.950	-0.353
γ -Cl	Li	F	0.779	-0.221	0.286	0.962	-0.949	0.092
γ -CN	Li	F	0.811	-0.116	0.222	0.963	-0.939	0.218
								-0.222
γ -Me	Li	F	0.731	-0.240	0.39	0.962	-0.956	0.071
γ -SH	Li	F	0.705	-0.245	0.145	0.961	-0.957	0.347
γ -OH	Li	F	0.705	-0.301	0.718	0.961	-0.959	-0.163
γ -vinyl(a)	Li	F	0.707	-0.225	0.340	0.961	-0.958	-0.078
								0.211
γ -vinyl(s)	Li	F	0.801	-0.208	0.257	0.962	-0.955	-0.143
								0.242
γ -F	Li	Cl	0.687	-0.278	0.831	0.897	-0.895	-0.348
γ -Cl	Li	Cl	0.689	-0.213	0.306	0.897	-0.893	0.106
γ -CN	Li	Cl	0.703	-0.102	0.235	0.902	-0.866	0.213
								-0.214
γ -Me	Li	Cl	0.655	-0.232	0.424	0.910	-0.895	0.078
γ -SH	Li	Cl	0.617	-0.231	0.162	0.894	-0.912	0.383
γ -OH	Li	Cl	0.630	-0.285	0.744	0.893	-0.915	-0.151
γ -F	Na	F	0.773	-0.280	0.770	0.981	-0.941	-0.362
γ -Cl	Na	F	0.781	-0.204	0.252	0.981	-0.938	0.067

γ -CN	Na	F	0.786	-0.082	0.164	0.982	-0.916	0.239 -0.256
γ -Me	Na	F	0.748	-0.231	0.348	0.980	-0.952	0.061
γ -SH	Na	F	0.733	-0.239	0.122	0.980	-0.952	0.310
γ -OH	Na	F	0.726	-0.302	0.687	0.980	-0.957	-0.178
γ -vinyl(a)	Na	F	0.722	-0.221	0.316	0.980	-0.957	-0.068 0.186
γ -vinyl(s)	Na	F	0.806	-0.192	0.228	0.980	-0.950	-0.129 0.206

* Reduced charges calculated in addition for (a) allyl fluoride: $C_\alpha = 0.451$; $C_\beta = -0.033$ $C_\gamma = 0.027$; $X = -0.445$ (b) LiF: Li=0.979; F = -0.979 (c) LiCl: Li =0.941 ; Cl = -0.941 (d) NaF: Na =0.988, F=-0.988