

SUPPORTING INFORMATION FOR

Solvation Effects on Alternative Nucleophilic Substitution Reaction Paths for Chloride/Allyl Chloride and γ -Methylated Congeners

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Contents:

Pages S-1 to S-11: Cartesian coordinate ($\text{\AA}$) and energies (E_h) for all optimized structures in gas phase, carbon tetrachloride, and water. For gas-phase structures, E is the electronic energy. For solvated structures, E is the sum of the electronic energy, the solvation polarization free energy, and the non-electrostatic components of the solvation free energy.

Name: chloride anion	# of imaginary frequencies: 0		
Phase: gas	Cartesians:		
E: -460.2628998	C	.043478	.715878 .174446
# of imaginary frequencies: 0	C	-1.117020	-.168681 .429313
Cartesians:	C	-2.207960	-.163197 -.309639
Cl .000000 .000000 .000000	H	-3.042898	-.802426 -.083137
	H	-2.307786	.480517 -1.167891
Name: chloride anion	Cl	1.525470	-.225919 -.125159
Phase: CCl ₄ solution	H	.259118	1.345244 1.028021
E: -460.3340309	H	-.118405	1.342176 -.691558
# of imaginary frequencies: 0	H	-1.033997	-.828889 1.277541
Cartesians:	Name: allyl cation		
Cl .000000 .000000 .000000	Phase: gas		
	E: -116.9265506		
Name: chloride anion	# of imaginary frequencies: 0		
Phase: water solution	Cartesians:		
E: -460.3856787	C	1.172033	-.211120 .000000
# of imaginary frequencies: 0	C	.000000	.495876 .000000
Cartesians:	C	-1.172028	-.211135 .000000
Cl .000000 .000000 .000000	H	2.130287	.282975 .000000
	H	1.176013	-1.289594 .000000
Name: allyl chloride	H	-.000028	1.571541 .000000
Phase: gas	H	-2.130282	.282962 .000000
E: -577.4735728			

H -1.176015 -1.289610 .000000

Name: S_N2 TS structure for chloride/allyl chloride

Phase: gas

E: -1037.7306762

of imaginary frequencies: 1

Cartesians:

C	.000000	.339198	.000000
C	.423323	-1.053986	.000000
C	-.413792	-2.073789	.000000
Cl	.009479	.624853	2.338019
Cl	.009479	.624853	-2.338019
H	-1.036961	.588735	.000000
H	.710929	1.129661	.000000
H	1.486501	-1.218983	.000000
H	-.060564	-3.089955	.000000
H	-1.479378	-1.923002	.000000

Name: *syn* S_N2' TS structure for chloride/allyl chloride

Phase: gas

E: -1037.7175455

of imaginary frequencies: 1

Cartesians:

C	-.078821	1.107073	1.216070
C	.586977	1.172812	.000000
C	-.078821	1.107073	-1.216070
H	-1.152729	1.166119	1.198644
H	.374170	1.581393	2.066360
H	-1.152729	1.166119	-1.198644
H	.374170	1.581393	-2.066360
H	1.661003	1.253965	.000000
Cl	-.078821	-.796198	2.309654
Cl	-.078821	-.796198	-2.309654

Name: *anti* S_N2' TS structure for chloride/allyl chloride

Phase: gas

E: -1037.7241414

of imaginary frequencies: 1

Cartesians:

C	.000000	.000000	.829742
H	.000000	.000000	1.905925
C	.000000	1.203917	.153311
H	-.257437	2.108595	.668621
H	-.223200	1.203012	-.897143
C	.000000	-1.203917	.153311
H	.257437	-2.108595	.668621
H	.223200	-1.203012	-.897143
Cl	2.061945	2.075867	-.243149
Cl	-2.061945	-2.075867	-.243149

Name: allyl chloride

Phase: CCl_4 solution

E: -577.4790463

of imaginary frequencies: 0

Cartesians:

C	.037021	.717362	.171679
C	-1.120377	-.166755	.431156
C	-2.207432	-.166591	-.311098
H	-3.045393	-.800158	-.080195
H	-2.303302	.468603	-1.175994
Cl	1.529387	-.226140	-.123747
H	.256225	1.350646	1.020814
H	-.120547	1.337541	-.698986
H	-1.041832	-.816355	1.287638

Name: allyl cation

Phase: CCl_4 solution

E: -116.9892562

of imaginary frequencies: 0

Cartesians:

C	.000000	1.166682	-.211599
C	.000000	.000000	.498668
C	.000000	-1.166682	-.211599
H	.000000	2.126661	.276833
H	.000000	1.163580	-1.289747
H	.000000	-2.126661	.276833
H	.000000	-1.163580	-1.289747
H	.000000	.000000	1.573008

Name: S_N2 TS structure for chloride/allyl chloride

Phase: CCl_4 solution

E: -1037.7860683

of imaginary frequencies: 1

Cartesians:

C	.000000	.298956	.000000
C	.493821	-1.063693	.000000
C	-.301023	-2.116191	.000000
Cl	-.031145	.646192	2.378117
Cl	-.031145	.646192	-2.378117
H	-1.049060	.494805	.000000
H	.665735	1.128889	.000000
H	1.562773	-1.181924	.000000
H	.094681	-3.116204	.000000
H	-1.372001	-2.010526	.000000

Name: *syn* S_N2' TS structure for chloride/allyl chloride

Phase: CCl_4 solution

E: -1037.7753174

of imaginary frequencies: 1

Cartesians:

C	-.591414	1.223764	.000000
H	-1.663580	1.315565	.000000
C	.079732	1.178622	1.204587

H	-.381559	1.599656	2.076470
H	1.153755	1.206622	1.197969
C	.079732	1.178622	-1.204587
H	-.381559	1.599656	-2.076470
H	1.153755	1.206622	-1.197969
Cl	.079732	-.835711	2.313618
Cl	.079732	-.835711	-2.313618

Name: *anti* S_N2' TS structure for
chloride/allyl chloride

Phase: CCl₄ solution

E: -1037.7788275

of imaginary frequencies: 1

Cartesians:

C	.000000	.000000	.834100
H	.000000	.000000	1.909584
C	.000000	1.196055	.155614
H	-.205174	2.115691	.666730
H	-.182044	1.202665	-.902088
C	.000000	-1.196055	.155614
H	.205174	-2.115691	.666730
H	.182044	-1.202665	-.902088
Cl	2.178492	2.061469	-.244436
Cl	-2.178492	-2.061469	-.244436

Name: allyl chloride

Phase: water solution

E: -577.4743046

of imaginary frequencies: 0

Cartesians:

C	.032597	.725662	.156531
C	-1.122866	-.152738	.438174
C	-2.204456	-.178620	-.310909
H	-3.044343	-.803001	-.063469
H	-2.295082	.426907	-1.197091
Cl	1.530766	-.230599	-.118765
H	.257369	1.378181	.988727
H	-.122164	1.322875	-.729967
H	-1.050442	-.770594	1.318038

Name: allyl cation

Phase: water solution

E: -117.0331916

of imaginary frequencies: 0

Cartesians:

C	.000000	1.162531	-.212175
C	.000000	.000000	.502040
C	.000000	-1.162531	-.212175
H	.000000	2.124743	.269427
H	.000000	1.149800	-1.290085
H	.000000	-2.124743	.269427
H	.000000	-1.149800	-1.290085
H	.000000	.000000	1.575181

Name: S_N2 TS structure for chloride/allyl
chloride

Phase: water solution

E: -1037.8187754

of imaginary frequencies: 1

Cartesians:

C	.000000	.222529	.000000
C	.625944	-1.069122	.000000
C	-.079501	-2.188093	.000000
Cl	-.109675	.682163	2.441502
Cl	-.109675	.682163	-2.441502
H	-1.063979	.310079	.000000
H	.569444	1.121300	.000000
H	1.700531	-1.091972	.000000
H	.399683	-3.151286	.000000
H	-1.155394	-2.173558	.000000

Name: *syn* S_N2' TS structure for
chloride/allyl chloride

Phase: water solution

E: -1037.8123683

of imaginary frequencies: 1

Cartesians:

C	-.605270	1.323963	.000000
H	-1.674088	1.434052	.000000
C	.081852	1.321337	1.185307
H	-.384423	1.657501	2.090223
H	1.154678	1.282739	1.187533
C	.081852	1.321337	-1.185307
H	-.384423	1.657501	-2.090223
H	1.154678	1.282739	-1.187533
Cl	.081852	-.915128	2.425728
Cl	.081852	-.915128	-2.425728

Name: *anti* S_N2' TS structure for
chloride/allyl chloride

Phase: water solution

E: -1037.8118514

of imaginary frequencies: 1

Cartesians:

C	.000000	.000000	.851240
H	.000000	.000000	1.925620
C	.000000	1.184219	.165093
H	-.123408	2.123565	.666358
H	-.107212	1.194111	-.902265
C	.000000	-1.184219	.165093
H	.123408	-2.123565	.666358
H	.107212	-1.194111	-.902265
Cl	2.404026	2.105771	-.251246
Cl	-2.404026	-2.105771	-.251246

Name: Z-crotyl chloride

Phase: gas

E: -616.7845059

of imaginary frequencies: 0

Cartesians:

C	-.528681	.066687	.757706
C	.472857	.906521	.063269
C	1.702186	.546936	-.266226
H	2.312674	1.291443	-.753671
C	2.365553	-.765643	-.052999
Cl	-1.949770	-.238862	-.279031
H	-.911580	.562342	1.639709
H	-.142119	-.898179	1.046086
H	.142054	1.902664	-.181093
H	1.711721	-1.511812	.379196
H	3.227383	-.656829	.599681
H	2.734473	-1.155982	-.996877

Name: Z-crotyl cation

Phase: gas

E: -156.2578878

of imaginary frequencies: 0

Cartesians:

C	.736912	-1.432101	.000000
C	1.010453	-.105441	.000000
C	.000000	.850965	.000000
H	1.532493	-2.157825	.000000
H	-.266668	-1.819500	.000000
H	.325054	1.881718	.000000
C	-1.437867	.660238	.000000
H	2.031963	.230665	.000000
H	-1.847941	1.192075	.860169
H	-1.783947	-.361172	.000000
H	-1.847941	1.192075	-.860169

Name: S_N2 TS structure for chloride/Z-crotyl chloride

Phase: gas

E: -1077.0430964

of imaginary frequencies: 1

Cartesians:

C	-.140758	-.624096	.027405
C	-.071359	.480560	.967199
C	.255988	1.718031	.629706
Cl	2.161557	-1.149974	-.088942
Cl	-2.506200	-.592542	-.186428
H	-.091894	-.460159	-1.024250
H	-.278710	-1.622585	.368590
H	-.321217	.246573	1.986533
H	.258759	2.470700	1.401886
C	.637176	2.136882	-.746764
H	1.389689	1.462384	-1.145414
H	1.038895	3.144306	-.759027
H	-.222877	2.113277	-1.412305

Name: syn S_N2' TS structure for chloride/Z-crotyl chloride

Phase: gas

E: -1077.0275786

of imaginary frequencies: 1

Cartesians:

C	-1.105833	.852323	.345193
C	.106340	.782386	1.024158
C	1.337293	.996231	.429596
C	-1.166612	1.313900	-1.073732
H	-1.960370	1.107943	.944078
H	1.373086	1.436074	-.548768
H	2.155871	1.273443	1.065788
H	.078854	.531312	2.070560
Cl	-2.118599	-1.144789	.064999
Cl	2.522241	-.756116	-.276331
H	-.854174	2.355795	-1.135330
H	-2.171829	1.224574	-1.460646
H	-.510489	.717205	-1.694323

Name: anti S_N2' TS structure for chloride/Z-crotyl chloride

Phase: gas

E: -1077.0354892

of imaginary frequencies: 1

Cartesians:

C	.778928	.246309	.658591
C	-1.015776	-.933713	-.469441
C	-.083850	-.830872	.538255
H	1.296279	.347159	1.593461
H	-1.553622	-1.852093	-.601267
C	.560756	1.508959	-.094781
H	-.918003	-.337934	-1.355684
H	-.048650	-1.597059	1.292853
Cl	-3.013597	.131268	-.022776
Cl	2.913708	-.247506	-.204689
H	.512657	1.328061	-1.160473
H	1.362014	2.210850	.088322
H	-.392905	1.932974	.213942

Name: Z-crotyl chloride

Phase: CCl₄ solution

E: -616.7917391

of imaginary frequencies: 0

Cartesians:

C	-.527548	.107920	.762702
C	.478473	.916889	.042240
C	1.702804	.534761	-.279835
H	2.320334	1.261401	-.784969
C	2.352918	-.777070	-.035856
Cl	-1.945823	-.253225	-.276243
H	-.925511	.641840	1.614766
H	-.147377	-.843345	1.099801
H	.159625	1.910845	-.225444
H	1.694648	-1.510619	.410829
H	3.214781	-.660101	.615289

H 2.722605 -1.190197 -.969653

Name: Z-crotyl cation

Phase: CCl_4 solution

E: -156.3167355

of imaginary frequencies: 0

Cartesians:

C	.734078	-1.428345	.000000
C	1.009768	-.104234	.000000
C	.000000	.850536	.000000
H	1.528521	-2.154360	.000000
H	-.269392	-1.815226	.000000
H	.322228	1.881720	.000000
C	-1.434838	.656147	.000000
H	2.030429	.231901	.000000
H	-1.843284	1.188224	.859512
H	-1.779270	-.365107	.000000
H	-1.843284	1.188224	-.859512

Name: $\text{S}_\text{N}2$ TS structure for chloride/Z-crotyl chloride

Phase: CCl_4 solution

E: -1077.1002613

of imaginary frequencies: 1

Cartesians:

C	-.008170	-.606638	.066661
C	-.004111	.486315	1.006440
C	.014866	1.760223	.638391
Cl	2.388216	-.927518	-.147612
Cl	-2.408170	-.894850	-.153404
H	-.004817	-.434331	-.985050
H	-.016193	-1.618309	.398490
H	-.018846	.223642	2.048729
H	.013588	2.506445	1.416401
C	.037141	2.234385	-.769443
H	.900104	1.834550	-1.294504
H	.081539	3.315434	-.821672
H	-.854518	1.907125	-1.297413

Name: *syn* $\text{S}_\text{N}2'$ TS structure for chloride/Z-crotyl chloride

Phase: CCl_4 solution

E: -1077.087437

of imaginary frequencies: 1

Cartesians:

C	1.096351	.941645	-.319619
C	-.089651	.826026	-1.025346
C	-1.320717	1.065789	-.466648
C	1.147698	1.358411	1.103825
H	1.978459	1.139537	-.898019
H	-1.398478	1.464249	.525680
H	-2.151201	1.278937	-1.110227
H	-.031961	.583866	-2.071585
Cl	2.189033	-1.199360	-.072057

Cl -2.593703 -.803299 .273089

H .880373 2.411776 1.172689

H 2.143341 1.229271 1.501939

H .456778 .786344 1.708700

Name: *anti* $\text{S}_\text{N}2'$ TS structure for chloride/Z-crotyl chloride

Phase: CCl_4 solution

E: -1077.0921097

of imaginary frequencies: 1

Cartesians:

C	.740729	.291311	.650262
C	-.980150	-.948362	-.501079
C	-.074718	-.816952	.515490
H	1.278478	.389761	1.573551
H	-1.531075	-1.859947	-.622250
C	.562114	1.531600	-.134163
H	-.946343	-.311394	-1.362205
H	-.019735	-1.582481	1.268471
Cl	-3.138366	.108613	-.004741
Cl	3.034168	-.256999	-.174920
H	.510151	1.336100	-1.196618
H	1.373930	2.220904	.044755
H	-.381891	1.984028	.165474

Name: Z-crotyl chloride

Phase: water solution

E: -616.7857064

of imaginary frequencies: 0

Cartesians:

C	-.523930	.137129	.766868
C	.482699	.926340	.027610
C	1.702378	.526584	-.290514
H	2.326309	1.238589	-.807995
C	2.338572	-.787001	-.023709
Cl	-1.941092	-.263134	-.274230
H	-.933251	.693066	1.598448
H	-.145101	-.803656	1.132507
H	.172506	1.918899	-.253881
H	1.674219	-1.504368	.439403
H	3.203651	-.666088	.621753
H	2.701924	-1.221482	-.949850

Name: Z-crotyl cation

Phase: water solution

E: -156.3547563

of imaginary frequencies: 0

Cartesians:

C	.731297	-1.423166	.000000
C	1.010443	-.101036	.000000
C	.000000	.851322	.000000
H	1.522362	-2.151532	.000000
H	-.273728	-1.805070	.000000
H	.317375	1.883511	.000000

C -1.432578 .648720 .000000
H 2.030173 .235097 .000000
H -1.841132 1.178703 .859266
H -1.768883 -.374459 .000000
H -1.841132 1.178703 -.859266

Name: S_N2 TS structure for chloride/*Z*-crotyl chloride

Phase: water solution

E: -1077.0295548

of imaginary frequencies: 1

Cartesians:

C .000008 -.521247 .130056
C .000000 .593926 1.006780
C -.000018 1.865597 .597638
Cl 2.490833 -1.017478 -.156148
Cl -2.490811 -1.017512 -.156145
H .000006 -.411111 -.930127
H .000016 -1.516967 .507136
H .000007 .380818 2.059977
H -.000025 2.621718 1.368030
C -.000033 2.377343 -.783333
H .870226 3.010571 -.932256
H -.870322 3.010530 -.932252
H -.000017 1.605570 -1.538380

Name: *syn* S_N2' TS structure for chloride/*Z*-crotyl chloride

Phase: water solution

E: -1077.1281426

of imaginary frequencies: 1

Cartesians:

C 1.126325 1.247178 -.187411
C .069924 1.025450 -1.057514
C -1.209546 1.262968 -.687902
C 1.045883 1.620977 1.215121
H 2.111483 1.268829 -.618455
H -1.478045 1.574426 .302843
H -2.006773 1.241755 -1.405614
H .296628 .754245 -2.071128
Cl 2.714672 -1.441220 -.054401
Cl -3.204080 -.972084 .254115
H 1.268378 2.689644 1.263032
H 1.840418 1.124755 1.757414
H .092328 1.433078 1.683003

Name: *anti* S_N2' TS structure for chloride/*Z*-crotyl chloride

Phase: water solution

E: -1077.0813462

of imaginary frequencies: 1

Cartesians:

C .762050 .489341 .584102
C -.901920 -.819845 -.538999

C .014106 -.669214 .444547
H 1.415946 .543530 1.435655
H -1.468987 -1.724827 -.635603
C .653259 1.711386 -.198026
H -1.069381 -.078506 -1.295541
H .168967 -1.458659 1.155322
Cl -3.829115 -.057256 .030876
Cl 3.587785 -.396229 -.109936
H .096856 1.619286 -1.116993
H 1.645899 2.099237 -.387556
H .148328 2.439185 .438987

Name: *E*-crotyl chloride

Phase: gas

E: -616.7869609

of imaginary frequencies: 0

Cartesians:

C .772929 .805056 .127603
C -.512937 .146873 .445187
C -1.587113 .248461 -.315287
C -2.901158 -.375132 -.017539
H -1.525005 .824405 -1.227579
Cl 2.080847 -.386360 -.110342
H 1.106738 1.447114 .931835
H .707803 1.386910 -.780946
H -.542970 -.432129 1.355051
H -2.874069 -.935413 .909625
H -3.196573 -1.051658 -.814524
H -3.680654 .377350 .062563

Name: *E*-crotyl cation

Phase: gas

E: -156.2628611

of imaginary frequencies: 0

Cartesians:

C -1.290429 -1.382079 .000000
C -.067743 -.797285 .000000
C .000000 .587312 .000000
H -1.403751 -2.453190 .000000
H -2.195145 -.796252 .000000
C 1.219437 1.367051 .000000
H -.932824 1.133928 .000000
H .833202 -1.385581 .000000
H 1.204400 2.038475 .860856
H 1.204400 2.038475 -.860856
H 2.122134 .774149 .000000

Name: S_N2 TS structure for chloride/*E*-crotyl chloride

Phase: gas

E: -1077.0436329

of imaginary frequencies: 1

Cartesians:

C -.453302 -.636106 .000000

C	.000000	.742365	.000000
C	1.274822	1.089679	.000000
Cl	-.624604	-.887884	2.349670
Cl	-.624604	-.887884	-2.349670
H	.249760	-1.438221	.000000
H	-1.489524	-.874643	.000000
H	-.769599	1.495727	.000000
C	1.765457	2.489885	.000000
H	2.022073	.311270	.000000
H	.940859	3.194451	.000000
H	2.380550	2.692270	-.874421
H	2.380550	2.692270	.874421

Name: *syn* S_N2' TS structure for
chloride/*E*-crotyl chloride

Phase: gas

E: -1077.0277504

of imaginary frequencies: 1

Cartesians:

C	-1.094893	-.652705	.313108
C	.060491	-1.068947	-.338144
C	1.292124	-1.132206	.291723
H	-.999867	-.486686	1.372631
C	-2.403538	-1.228170	-.125435
H	1.319479	-.982522	1.356074
H	2.013560	-1.837410	-.074785
H	-.010044	-1.351279	-1.376222
Cl	-1.654765	1.478836	-.001456
Cl	2.756626	.480057	-.080937
H	-2.521474	-1.119812	-1.197031
H	-3.237497	-.740111	.359406
H	-2.420910	-2.291189	.113094

Name: *anti* S_N2' TS structure for
chloride/*E*-crotyl chloride

Phase: gas

E: -1077.0360603

of imaginary frequencies: 1

Cartesians:

C	.745996	.517586	-.166171
C	-1.121750	-.856995	.479013
C	-.167379	.086068	.780328
C	1.460167	1.809797	.012766
H	-1.678516	-1.332764	1.261868
H	.566686	.214712	-1.181665
H	-1.020749	-1.428841	-.423793
H	-.140683	.521029	1.765623
Cl	-3.124454	.010590	-.294136
Cl	2.647796	-.818758	-.191049
H	.744040	2.616463	-.140821
H	2.276150	1.917248	-.687120
H	1.854048	1.892261	1.018434

Name: *E*-crotyl chloride

Phase: CCl₄ solution

E: -616.7942812

of imaginary frequencies: 0

Cartesians:

C	.767697	.809826	.119873
C	-.516100	.155924	.446339
C	-1.586902	.238155	-.320792
C	-2.901779	-.375150	-.013747
H	-1.520741	.791730	-1.246475
Cl	2.084613	-.388417	-.106329
H	1.106692	1.459195	.915553
H	.707421	1.379483	-.796351
H	-.550780	-.398609	1.371122
H	-2.882464	-.914285	.925975
H	-3.196533	-1.067989	-.796788
H	-3.679512	.381043	.044508

Name: *E*-crotyl cation

Phase: CCl₄ solution

E: -156.3217008

of imaginary frequencies: 0

Cartesians:

C	-1.289425	-1.376192	.000000
C	-.065570	-.797884	.000000
C	.000000	.584787	.000000
H	-1.408618	-2.445855	.000000
H	-2.189948	-.784416	.000000
C	1.217830	1.363657	.000000
H	-.932643	1.131305	.000000
H	.834196	-1.386348	.000000
H	1.200258	2.034214	.860053
H	1.200258	2.034214	-.860053
H	2.119490	.770682	.000000

Name: S_N2 TS structure for chloride/*E*-
crotyl chloride

Phase: CCl₄ solution

E: -1077.1018721

of imaginary frequencies: 1

Cartesians:

C	.000000	.727786	.000000
C	.477600	-.630706	.000000
C	-.338673	-1.672914	.000000
Cl	-.052326	1.121595	2.402736
Cl	-.052326	1.121595	-2.402736
H	-1.046510	.936354	.000000
H	.671844	1.552866	.000000
H	1.544927	-.770700	.000000
C	.096151	-3.086544	.000000
H	-1.402188	-1.489817	.000000
H	1.176551	-3.172154	.000000
H	-.287996	-3.608251	-.873112
H	-.287996	-3.608251	.873112

Name: *syn* S_N2' TS structure for
chloride/*E*-crotyl chloride

Phase: CCl₄ solution

E: -1077.0874958

of imaginary frequencies: 1

Cartesians:

C	-1.120820	-.737981	.317941
C	.033608	-1.125168	-.337895
C	1.241160	-1.216342	.311711
H	-1.033339	-.524725	1.368309
C	-2.439220	-1.240219	-.146269
H	1.286571	-1.020965	1.366713
H	1.997443	-1.873877	-.068581
H	-.033882	-1.426421	-1.369837
Cl	-1.647948	1.563735	.005353
Cl	2.812123	.490611	-.086429
H	-2.535177	-1.140389	-1.220271
H	-3.258452	-.720091	.327667
H	-2.502489	-2.299150	.101380

Name: *anti* S_N2' TS structure for
chloride/*E*-crotyl chloride

Phase: CCl₄ solution

E: -1077.0933661

of imaginary frequencies: 1

Cartesians:

C	.707609	.582171	-.162627
C	-1.054869	-.882422	.509966
C	-.159388	.107863	.800687
C	1.421602	1.864609	.002559
H	-1.637534	-1.348207	1.279180
H	.572435	.224078	-1.166165
H	-.978096	-1.420605	-.414852
H	-.144822	.548490	1.782731
Cl	-3.231661	-.030116	-.300956
Cl	2.758760	-.831087	-.200294
H	.702004	2.661399	-.185850
H	2.243428	1.962358	-.690532
H	1.792169	1.979610	1.013229

Name: *E*-crotyl chloride

Phase: water solution

E: -616.7880811

of imaginary frequencies: 0

Cartesians:

C	.763039	.815613	.112038
C	-.517947	.163846	.448608
C	-1.585208	.229000	-.324823
C	-2.901959	-.375441	-.010915
H	-1.513506	.763332	-1.261107
Cl	2.086643	-.390798	-.102628
H	1.107745	1.473604	.897278
H	.703018	1.370699	-.812568
H	-.556083	-.368368	1.385982

H	-2.888672	-.895193	.939367
H	-3.195351	-1.082163	-.781438
H	-3.677640	.383538	.027713

Name: *E*-crotyl cation

Phase: water solution

E: -156.3596899

of imaginary frequencies: 0

Cartesians:

C	-1.288104	-1.371151	.000000
C	-.061589	-.800201	.000000
C	.000000	.580658	.000000
H	-1.415999	-2.438806	.000000
H	-2.182221	-.770002	.000000
C	1.215198	1.363303	.000000
H	-.934509	1.124219	.000000
H	.836795	-1.388987	.000000
H	1.192491	2.032187	.859602
H	1.192491	2.032187	-.859602
H	2.117916	.773550	.000000

Name: S_N2 TS structure for chloride/*E*-
crotyl chloride

Phase: water solution

E: -1077.1355064

of imaginary frequencies: 1

Cartesians:

C	.000000	.598403	.000000
C	.569791	-.692810	.000000
C	-.202736	-1.782584	.000000
Cl	-.147895	1.208766	2.523971
Cl	-.147895	1.208766	-2.523971
H	-1.060450	.728295	.000000
H	.595985	1.480618	.000000
H	1.641817	-.778027	.000000
C	.289040	-3.168328	.000000
H	-1.272640	-1.643221	.000000
H	1.369889	-3.220028	.000000
H	-.091370	-3.696881	-.870242
H	-.091370	-3.696881	.870242

Name: *syn* S_N2' TS structure for
chloride/*E*-crotyl chloride

Phase: water solution

E: N/A

of imaginary frequencies: N/A

Cartesians: N/A

Name: *anti* S_N2' TS structure for
chloride/*E*-crotyl chloride

Phase: water solution

E: N/A

of imaginary frequencies: N/A

Cartesians: N/A

Name: isoprenyl chloride

Phase: gas

E: -656.0973183

of imaginary frequencies: 0

Cartesians:

C	-1.027036	.186646	.792695
C	.201772	-.559091	.446815
C	1.357259	-.045532	.047200
C	2.519017	-.936297	-.241934
C	1.631308	1.406280	-.156153
Cl	-2.327869	-.098413	-.401392
H	-.879999	1.254099	.836103
H	-1.429847	-.142234	1.741010
H	.120265	-1.630757	.535916
H	2.281385	-1.979413	-.073418
H	3.370088	-.675395	.382184
H	2.840956	-.822865	-1.274018
H	1.996551	1.575938	-1.165315
H	2.413681	1.742673	.519430
H	.766767	2.038943	-.009967

Name: isoprenyl cation

Phase: gas

E: -195.5877617

of imaginary frequencies: 0

Cartesians:

C	2.026260	-.060127	.010089
C	.841239	-.696799	-.010565
C	-.394552	-.020627	-.008303
H	2.945892	-.619243	-.004491
H	2.119822	1.010596	.036454
C	-1.620772	-.819472	-.003369
C	-.547312	1.435084	.000580
H	.819789	-1.772384	-.039588
H	-2.469376	-.285398	-.411272
H	-1.846439	-1.014387	1.050144
H	-1.497684	-1.783305	-.480494
H	-.906191	1.721268	-.989820
H	.345583	1.997731	.221388
H	-1.340579	1.716771	.687089

Name: S_N2 TS structure for
chloride/isoprenyl chloride

Phase: gas

E: -1116.35627

of imaginary frequencies: 1

Cartesians:

C	.328446	-.900280	-.123582
C	-.017672	.370080	-.721929
C	-.487474	1.405216	-.037590
Cl	-1.836781	-1.881198	-.077211
Cl	2.673654	-.476838	.059713
H	.334865	-1.036866	.932719

H	.616074	-1.726806	-.729686
H	.136261	.451214	-1.783733
C	-.806970	2.695000	-.707462
C	-.727946	1.326318	1.433985
H	-.596551	2.658748	-1.770225
H	-.228110	3.509164	-.274550
H	-1.857048	2.950452	-.575786
H	.210992	1.212227	1.969941
H	-1.354796	.469531	1.664165
H	-1.218837	2.220939	1.804081

Name: syn S_N2' TS structure for chloride/
isoprenyl chloride

Phase: gas

E: -1116.3373567

of imaginary frequencies: 1

Cartesians:

C	-.991416	-.615120	.013447
C	.156818	-.886756	-.729492
C	1.399607	-1.146495	-.182584
C	-.923355	-.679361	1.507282
C	-2.286762	-1.072516	-.583972
H	1.477427	-1.351409	.867705
H	2.104284	-1.683743	-.787907
H	.059118	-.895959	-1.802372
Cl	-1.540647	1.606769	-.112406
Cl	2.880031	.513494	.002903
H	-2.334482	-.821913	-1.635899
H	-3.135750	-.626271	-.084341
H	-2.345353	-2.157412	-.486513
H	-1.838476	-.303740	1.944129
H	-.099254	-.087079	1.880974
H	-.786388	-1.715460	1.817678

Name: anti S_N2' TS structure for
chloride/isoprenyl chloride

Phase: gas

E: -1116.3467772

of imaginary frequencies: 1

Cartesians:

C	-.653854	.484993	-.079228
C	1.191981	-1.051965	-.465416
C	.214695	-.203163	-.918507
C	-1.348928	1.674972	-.648269
H	1.755132	-1.635626	-1.166599
C	-.392458	.525879	1.386276
H	1.150695	-1.452120	.527933
H	.153482	-.001427	-1.974613
Cl	3.182666	.027835	.136294
Cl	-2.692659	-.795829	.104297
H	-.631080	2.495724	-.673325
H	-2.199075	1.964463	-.047340
H	-1.684876	1.482679	-1.658709

H	-1.212770	.998199	1.909100
H	.528402	1.084287	1.547748
H	-.258649	-.464572	1.796612

Name: isoprenyl chloride
Phase: CCl_4 solution
E: -656.1055608
of imaginary frequencies: 0
Cartesians:

C	-1.023541	.143905	.812725
C	.208355	-.581821	.444351
C	1.354674	-.045714	.045948
C	2.528057	-.912551	-.262233
C	1.607852	1.411542	-.134968
Cl	-2.323510	-.083020	-.410597
H	-.884384	1.208873	.907535
H	-1.439619	-.230965	1.737489
H	.141443	-1.655561	.517865
H	2.312237	-1.962832	-.110267
H	3.377263	-.646134	.361856
H	2.844432	-.775817	-1.293092
H	1.973635	1.600864	-1.140335
H	2.385692	1.747516	.545856
H	.736596	2.033228	.018302

Name: isoprenyl cation
Phase: CCl_4 solution
E: -195.6435487
of imaginary frequencies: 0
Cartesians:

C	2.022612	-.058517	.007622
C	.840999	-.698239	-.006498
C	-.393317	-.021515	-.007629
H	2.943239	-.615091	-.007151
H	2.114005	1.012445	.027130
C	-1.619365	-.816595	-.006044
C	-.545791	1.431793	.002171
H	.819338	-1.773451	-.030951
H	-2.463971	-.279935	-.417379
H	-1.848153	-1.004925	1.047455
H	-1.496898	-1.782424	-.477686
H	-.893406	1.717476	-.991858
H	.343501	1.994630	.234498
H	-1.348483	1.709717	.678206

Name: $\text{S}_\text{N}2$ TS structure for
chloride/isoprenyl chloride
Phase: CCl_4 solution
E: -1116.4154808
of imaginary frequencies: 1
Cartesians:

C	-.876919	-.278284	.000000
C	.000000	.852756	.000000
C	1.328165	.746496	.000000

Cl	-1.145569	-.604960	2.424858
Cl	-1.145569	-.604960	-2.424858
H	-.505207	-1.276779	.000000
H	-1.934762	-.152891	.000000
H	-.462495	1.823892	.000000
C	2.195873	1.950416	.000000
C	2.015216	-.576499	.000000
H	1.622592	2.869424	.000000
H	2.845163	1.948962	-.872859
H	2.845163	1.948962	.872859
H	1.735921	-1.151116	-.878408
H	1.735921	-1.151116	.878408
H	3.093031	-.460006	.000000

Name: *syn* $\text{S}_\text{N}2'$ TS structure for chloride/
isoprenyl chloride
Phase: CCl_4 solution
E: -1116.3988821
of imaginary frequencies: 1
Cartesians:

C	-1.012393	-.728506	.022403
C	.124815	-.919696	-.753892
C	1.351329	-1.227734	-.231593
C	-.937915	-.760477	1.506854
C	-2.320858	-1.103258	-.576068
H	1.476688	-1.403724	.817932
H	2.090265	-1.677008	-.864645
H	.004859	-.911719	-1.823313
Cl	-1.595684	1.723988	-.101539
Cl	3.002105	.537767	.018791
H	-2.370844	-.835894	-1.622769
H	-3.148442	-.645740	-.054069
H	-2.413060	-2.187094	-.496027
H	-1.837314	-.344666	1.937394
H	-.087913	-.207226	1.879690
H	-.853264	-1.798732	1.826293

Name: *anti* $\text{S}_\text{N}2'$ TS structure for
chloride/isoprenyl chloride
Phase: CCl_4 solution
E: -1116.40578
of imaginary frequencies: 1
Cartesians:

C	-.598624	.540984	-.079414
C	1.116173	-1.127137	-.424573
C	.194203	-.250945	-.902978
C	-1.273284	1.712266	-.683152
H	1.693894	-1.732572	-1.094482
C	-.393659	.573821	1.386336
H	1.143092	-1.417599	.605912
H	.121258	-.096875	-1.965283
Cl	3.348866	-.007382	.123043
Cl	-2.878289	-.774045	.107376
H	-.538982	2.518759	-.705494

H	-2.123249	2.031923	-.099027
H	-1.589885	1.513945	-1.697849
H	-1.201720	1.096468	1.876924
H	.546583	1.091753	1.572351
H	-.319636	-.415477	1.812517

Name: isoprenyl chloride
Phase: water solution
E: -656.0984218
of imaginary frequencies: 0
Cartesians:

C	-1.018152	.131847	.820634
C	.212131	-.589361	.443378
C	1.354701	-.045406	.043887
C	2.531033	-.905211	-.268812
C	1.598413	1.413610	-.129169
Cl	-2.323948	-.079198	-.413074
H	-.880830	1.195771	.925070
H	-1.440374	-.253149	1.737728
H	.151467	-1.663367	.514882
H	2.319671	-1.956896	-.122589
H	3.378332	-.638129	.356764
H	2.847883	-.760640	-1.297998
H	1.961297	1.611524	-1.133489
H	2.376343	1.748937	.551152
H	.724566	2.029447	.031235

Name: isoprenyl cation
Phase: water solution
E: -195.6771756
of imaginary frequencies: 0
Cartesians:

C	2.017903	-.059939	.008857
C	.838769	-.702492	-.007627
C	-.392672	-.023234	-.006575
H	2.940088	-.612366	-.009598
H	2.103371	1.011240	.034114
C	-1.621076	-.811303	-.005380
C	-.538905	1.429345	.002117
H	.815468	-1.776871	-.036714
H	-2.450086	-.281247	-.454470
H	-1.875712	-.949829	1.049174

H	-1.495121	-1.794425	-.435565
H	-.841754	1.713778	-1.006398
H	.345695	1.984236	.267144
H	-1.366055	1.711227	.643959

Name: S_N2 TS structure for
chloride/isoprenyl chloride
Phase: water solution
E: -1116.4495552
of imaginary frequencies: 1
Cartesians:

C	-.012427	-.740221	-.207196
C	.008278	.535210	-.762830
C	.026397	1.679013	-.036345
Cl	-2.619431	-1.452159	.021856
Cl	2.570648	-1.532031	.021825
H	-.015774	-.914326	.844734
H	-.024861	-1.609824	-.823100
H	.012202	.606540	-1.835520
C	.049492	2.986299	-.724417
C	.028221	1.745161	1.438465
H	.083491	2.890244	-1.800685
H	.907077	3.564012	-.390383
H	-.831591	3.559550	-.447491
H	.938010	2.241201	1.765229
H	-.042740	.789683	1.932319
H	-.796256	2.371377	1.766257

Name: *syn* S_N2' TS structure for chloride/
isoprenyl chloride
Phase: water solution
E: N/A
of imaginary frequencies: N/A
Cartesians: N/A

Name: *anti* S_N2' TS structure for
chloride/isoprenyl chloride
Phase: water solution
E: N/A
of imaginary frequencies: N/A
Cartesians: N/A