Supplementary material for "Nucleophilic identity substitution reactions. The reaction between hydrogen fluoride and protonated alkyl fluorides" by Jon K. Laerdahl, Pervin U. Civcir, Lihn Bache-Andreassen, and Einar Uggerud.

SUPPLEMENTARY MATERIAL, HF + RFH+:

Cartesian coordinates:

HF:

F	0.000000	-0.000000	-0.092650
H	0.000000	0.000000	0.833850

H2F+:

H	-0.098183	0.000000	-0.914338
F	-0.079886	0.000000	0.054727
H	0.817155	-0.000000	0.421795

(HF)2:

F	-0.230158	-0.000000	-1.436624
H	-0.230158	-0.000000	-0.504603
F	0.141479	-0.000000	1.315561
H	1.028276	0.000000	1.594161

HF--H--FH+:

H	-1.192753	-0.475779	-1.279226
F	-1.062452	-0.050228	-0.439046
H	0.000000	0.000000	0.000000
F	1.062452	0.050228	0.439046
H	1.192753	0.475780	1.279226

A1, CH3FH+:

C	-0.045740	0.026408	-0.850364
F	-0.028558	0.016488	0.780110
H	0.860592	0.570578	-1.074765
H	-0.063840	-1.030584	-1.074764
H	-0.974862	0.562837	-0.977404
H	0.709573	-0.409672	1.208126

A2, HF--CH3FH+:

C	-0.298539	0.004766	-0.000006
F	2.136908	0.213106	-0.002518
H	3.024964	0.497905	-0.005596
H	-0.295182	1.083151	-0.011170
H	-0.055224	-0.501441	-0.920872
H	-0.054953	-0.482269	0.931072
F	-1.970410	-0.166305	0.002009
H	-2.326850	-1.047146	0.011180

A3, CH3FH--FH+:

C	-0.826535	1.397876	-0.186774
F	-0.699378	-0.143513	-0.310058
F	1.342440	-1.050974	0.443119
H	-0.728419	1.577853	0.874427
H	-1.818971	1.544409	-0.586619
H	-0.022916	1.770466	-0.806081
H	0.179540	-0.562253	0.010931
H	1.562418	-1.967343	0.430439

A4, CH3+:

C	-0.000001	0.000000	0.000006
H	0.939443	0.543006	-0.026045
H	-0.000537	-1.085085	-0.026045
H	-0.938902	0.542076	0.052053

TS(A2,A2'), HF--CH3--FH+:

C	-0.000993	0.008627	-0.017086
F	2.016567	-0.001013	-0.095892
F	-2.014554	-0.016475	0.130522
H	-0.013640	0.593613	0.887192
H	-0.056759	0.493276	-0.976858
H	0.067816	-1.064439	0.045205
H	2.641087	0.693969	0.000232
H	-2.659256	-0.536072	-0.312924

Imaginary Frequency: 236.5i cm-1

TS(A3,A3'), HF--CH3--FH+:

C	-0.165613	1.441064	-0.004668
F	-1.353559	-0.696674	-0.029865
F	1.411872	-0.477691	0.032644
H	-0.620317	1.321054	0.968974
H	-0.775281	1.347750	-0.892689
H	0.875139	1.716993	-0.086602
H	-1.285242	-1.627465	-0.044293
H	2.274557	-0.835429	0.057606

Imaginary Frequency: 286.0i cm-1

TS(A2,A3), HF--CH3FH+:

C	0.071147	-0.340525	0.024730
F	-0.143236	-0.199208	1.647677
F	2.748324	0.398863	-0.663945
H	0.761154	-1.170142	0.049895
H	0.500685	0.618159	-0.223577
H	-0.939298	-0.549029	-0.295957
H	3.610745	0.581842	-0.964416
H	-0.589004	0.582725	1.957796

Imaginary Frequency: 47.9i cm-1

B1, CH3CH2FH+:

C	0.081880	-0.108898	-0.915426
C	-1.098265	0.602803	-0.805842
F	0.836344	-0.406254	1.486938
H	1.033819	0.405868	-0.928950
H	0.066772	-1.185892	-1.026477
H	1.218179	-0.671023	2.295152
H	-1.077194	1.676908	-0.670336
H	-0.621795	0.381960	-1.956540
H	-2.048567	0.085033	-0.767685

B2, HF--CH3CH2--FH+:

C	0.228072	-0.126442	0.291889
C	-0.129625	1.152360	-0.078809
F	2.759302	-0.361326	-0.110581
F	-2.739261	-0.447569	-0.088405
H	-3.636027	-0.704813	-0.068392
H	0.576143	-0.329179	1.296047
H	0.133859	-0.948671	-0.404910
H	3.648976	-0.599972	-0.250052
H	-0.020593	1.973937	0.617508
H	-0.463272	1.358529	-1.087635
H	-1.010137	0.374714	0.409827

B3, CH3CH2FH--FH+:

C	-0.941703	0.620516	-0.000020
C	-2.235244	-0.089105	-0.000070
F	0.172876	-0.594300	-0.000003
F	2.463937	0.143236	0.000078
H	-0.648442	1.125426	0.912214
H	-0.648385	1.125452	-0.912221

H	1.133534	-0.324058	0.000031
H	3.232792	-0.397085	0.000094
H	-2.987885	0.707703	-0.000082
H	-2.375599	-0.683153	-0.898276
H	-2.375655	-0.683179	0.898110

B4, CH3CH2+:

C	0.162298	-0.675241	0.000037
C	-0.281138	0.635022	-0.000034
H	-0.466099	1.153031	0.933716
H	-0.466102	1.152929	-0.933841
H	0.329902	-1.199022	0.933844
H	0.329899	-1.199124	-0.933714
H	0.985437	0.333501	-0.000020

B5, CH2CH2:

C	0.165712	-0.648734	0.000035
C	-0.165711	0.648733	-0.000035
H	-0.305413	1.195693	0.922258
H	-0.305416	1.195593	-0.922388
H	0.305415	-1.195592	0.922388
H	0.305412	-1.195693	-0.922259

TS(B2,B2'), HF--(CH3)CH2--FH+:

C	-0.002297	-0.184447	-0.018556
C	-0.001738	1.250423	0.039497
F	-2.301890	-0.494981	-0.010031
F	2.297058	-0.496733	-0.011068
H	-0.002335	-0.807065	0.864917
H	-0.002706	-0.689346	-0.975092
H	-3.025838	-1.082121	0.058289
H	3.020584	-1.084432	0.056919
H	-0.861390	1.595021	-0.552210
H	-0.001352	1.667864	1.037678
H	0.857905	1.594369	-0.552602

Imaginary Frequency: 173.9i cm-1

TS(B2,B3), HF--(CH3)CH2--FH+:

C	-0.400107	0.141341	0.357385
F	0.255521	-0.703455	2.462682
F	2.565901	0.297019	1.087053
C	-0.401309	1.527829	0.402546
H	-1.298131	-0.417570	0.588929
H	0.456156	-0.386696	-0.040678
H	1.133276	-0.746147	2.776693
H	3.495073	0.343747	1.026290
H	-0.783677	1.097301	-0.664538
H	-1.241653	2.054038	0.836942
H	0.515092	2.068378	0.205745

Imaginary Frequency: 88.1i cm-1

C1, (CH3)2CHFH+:

C	0.093623	0.064322	-0.733352
C	-1.101159	0.867591	-0.752288
F	0.762621	0.387653	1.758706
H	1.048931	0.582688	-0.751356
C	0.118854	-1.375337	-0.722711
H	1.105774	0.493974	2.619451
H	-1.137012	1.179087	0.313196
H	-0.988145	1.793905	-1.313166
H	-2.010931	0.320126	-0.977638
H	0.987998	-1.788624	-0.217225
H	-0.821978	-1.841095	-0.445455
H	0.283867	-1.568394	-1.806058

C2, HF--(CH3)2CH--FH+:

C	-0.117334	-1.270579	0.724182
C	0.006315	-0.000063	0.054251
C	0.129212	1.269631	0.725877
F	2.517847	-0.305799	-0.648527
F	-2.504426	0.306536	-0.650973
H	0.006923	0.000602	-1.030824
H	-3.358945	0.466469	-0.987506
H	3.372744	-0.465321	-0.984294
H	0.320900	-2.092951	0.164775
H	0.164701	-1.250440	1.772551
H	-1.215850	-1.413098	0.668098
H	1.227791	1.412219	0.671199
H	-0.308395	2.092688	0.166988
H	-0.153998	1.248207	1.773904

C3, (CH3)2CH--FH--FH+:

C	-0.479831	-0.775873	-1.124776
C	-0.223196	0.098066	0.010711
H	-0.068112	-0.371491	0.976924
C	-0.510224	1.523986	0.009471
F	1.864913	0.319862	-0.125622
H	-1.549279	-1.021721	-1.000032
H	-0.359268	-0.281182	-2.083699
H	0.057861	-1.717928	-1.063527
H	0.071322	2.059630	0.755546
H	-0.452813	1.977953	-0.974540
H	-1.558430	1.560869	0.354490
H	2.537855	-0.342939	-0.253676
F	3.531100	-1.597673	-0.500135
H	4.465282	-1.622613	-0.499133

C4, (CH3)2CH+:

C	0.093616	0.401422	-0.212524
C	0.080804	0.402569	1.225287
H	1.178604	0.379092	1.416703
H	-0.357043	-0.480057	1.680793
H	-0.250943	1.345141	1.658271
C	-0.160233	-0.743159	-1.044969
H	0.313476	1.344171	-0.711643
H	-1.212183	-0.523079	-1.340472
H	0.393762	-0.732739	-1.982495
H	-0.150791	-1.697516	-0.527922

C5, CH3CHCH2:

C	-0.460424	-0.009079	-0.137120
C	-0.492892	-0.008447	1.203582
H	0.418689	0.009823	1.787923
H	-1.428368	-0.026121	1.745325
H	-1.398780	-0.027834	-0.683206
C	0.795110	0.014556	-0.955272
H	1.676559	0.032292	-0.314661
H	0.857642	-0.863452	-1.600433
H	0.823498	0.893115	-1.602086

D1a, (CH3)3C--FH+:

C	-0.724956	-0.712469	-1.209234
C	-0.610119	0.023462	0.047974
C	-0.662560	1.481191	0.037670
C	-0.524972	-0.687385	1.321865
F	2.088043	-0.095172	-0.164035
H	-1.814077	-0.836953	-1.338236
H	-0.379363	-0.131407	-2.061534

H	-0.278783	-1.701083	-1.171162
H	-0.088775	-1.677249	1.233684
H	-0.050737	-0.090187	2.097713
H	-1.580130	-0.807608	1.622714
H	0.403775	1.752552	-0.049271
H	-1.168018	1.887101	-0.835413
H	-1.025282	1.905005	0.971126
H	3.012636	-0.189039	-0.236157

D1b, (CH3)3C--FH+:

C	0.688635	0.000000	0.037976
C	0.504365	-0.000001	1.486015
C	0.755012	-1.268478	-0.681157
C	0.755015	1.268480	-0.681154
F	-2.170924	0.000002	-0.149558
H	0.028874	-0.905149	1.854960
H	0.028876	0.905147	1.854962
H	1.541742	-0.000002	1.865824
H	-0.305366	-1.472606	-0.909405
H	1.097662	-2.088891	-0.053681
H	1.292365	-1.207996	-1.622824
H	-0.305363	1.472610	-0.909403
H	1.097665	2.088891	-0.053677
H	1.292367	1.207998	-1.622822
H	-3.102845	0.000004	-0.167655

D2,HF--(CH3)3C--FH+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.460065
C	1.268424	0.000000	-0.721677
H	2.090455	-0.401312	-0.134681
H	1.196344	-0.454881	-1.706176
H	1.460073	1.076221	-0.867403
H	0.897452	0.454297	1.873922
H	0.045433	-1.074247	1.705189
H	-0.908740	0.408349	1.890404
F	0.202114	-2.886758	-0.016592
H	0.305754	-3.812278	-0.044008
F	-0.204627	2.724483	0.023554
H	-0.328406	3.647145	0.062527
C	-1.254026	-0.075131	-0.744019
H	-1.409878	-1.161438	-0.852670
H	-1.163884	0.330795	-1.749097
H	-2.100261	0.336964	-0.203822

D3a, (CH3)3C--FH--FH+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.459639
C	1.271183	0.000000	-0.721921
C	-1.266646	-0.107306	-0.721921
F	-0.109128	2.580946	-0.129790
H	-0.145886	3.450261	-0.494325
F	-0.208478	4.930437	-1.316990
H	-0.245945	5.816739	-1.029765
H	-0.045461	1.075133	1.699863
H	0.922640	-0.386439	1.886221
H	-0.886725	-0.462946	1.886221
H	2.066888	0.474775	-0.152316
H	1.530362	-1.070002	-0.792888
H	1.191595	0.393858	-1.729895
H	-1.434573	-1.195368	-0.792892
H	-1.220590	0.291867	-1.729894
H	-2.099590	0.298602	-0.152315

D3b, (CH3)3C--FH--FH+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.460222
C	1.268413	0.000000	-0.722027
C	-1.267784	0.039910	-0.722028
H	-0.897657	0.442446	1.883971
H	0.911137	0.413976	1.883971
H	-0.016938	-1.075990	1.707811
H	2.081452	-0.430160	-0.140736
H	1.487315	1.076959	-0.819745
H	1.200079	-0.419597	-1.721199
H	-2.093964	-0.364432	-0.140735
H	-1.212690	-0.381643	-1.721195
H	-1.452664	1.123226	-0.819764
F	0.043599	2.761145	0.092127
H	0.057385	3.660452	0.375062
F	0.080802	5.217887	1.058105
H	0.095209	6.078510	0.699914

D4, (CH3)3C+:

C	-0.015852	-0.000257	-0.000901
C	-0.014165	-0.002656	1.460896
H	1.052205	0.005576	1.739688
H	-0.491283	-0.870211	1.904155
H	-0.412466	0.934047	1.855829
C	-0.304988	-1.224451	-0.742318
C	0.310300	1.226522	-0.720278
H	-0.491290	-1.061432	-1.799751
H	0.623181	-1.815392	-0.647380
H	-1.082219	-1.820705	-0.266077
H	0.819047	1.034215	-1.664120
H	-0.683489	1.625679	-0.993120
H	0.814544	1.973279	-0.113618

D5, (CH3)2CCH2:

C	-0.000055	0.000764	0.118898
C	-0.000672	0.009402	1.462658
H	0.922544	0.047144	2.026188
H	-0.924404	-0.021098	2.025778
C	-1.272695	-0.051408	-0.680450
C	1.273320	0.042664	-0.679886
H	2.149530	0.079202	-0.033664
H	1.353217	-0.837692	-1.321799
H	1.288343	0.918179	-1.333116
H	-2.149498	-0.079641	-0.034616
H	-1.351998	0.820622	-1.333701
H	-1.287124	-0.935249	-1.322384

TS(D1a,D1b), (CH3)3C--FH+:

C	0.010431	-0.037564	0.000620
C	0.004117	-0.025249	1.462475
C	1.259472	-0.014094	2.205108
C	-1.265404	-0.039069	2.184344
F	0.085090	2.760921	1.468613
H	-0.599918	-0.872830	-0.355626
H	-0.527077	0.864497	-0.319707
H	1.003108	-0.054822	-0.436030
H	1.600820	-1.062705	2.145230
H	1.147676	0.250259	3.252152
H	2.022669	0.577098	1.701934
H	-1.202202	-0.645929	3.088712
H	-2.120922	-0.302106	1.570597
H	-1.378321	0.999244	2.533913
H	0.160129	3.689922	1.474125

Imaginary Frequency: 92.7i cm-1

TS(D2,D2'), HF--(CH3)3C--FH+:

C	0.061634	-0.146485	1.444454
C	-0.000434	0.002098	-0.007228
C	-0.002199	1.339329	-0.599588
C	-0.059002	-1.182138	-0.855036
F	-2.810220	0.002866	0.027456
F	2.809484	-0.015788	-0.019011
H	-0.325063	-2.089175	-0.320775
H	-0.672158	-1.020849	-1.739268
H	0.981900	-1.278290	-1.207794
H	0.643701	-1.021937	1.729761
H	-0.980411	-0.365546	1.725198
H	0.386837	0.749867	1.962660
H	-3.740743	-0.018811	-0.013294
H	3.740963	-0.004803	-0.003995
H	-0.855059	1.879122	-0.171538
H	-0.060655	1.339227	-1.682556
H	0.887322	1.870668	-0.250022

Imaginary Frequency: 110.4i cm-1