

Supplementary material for "Nucleophilic identity substitution reactions. II. The reaction between ammonia and protonated amines" by Jon K. Laerdahl, Lihn Bache-Andreassen, and Einar Uggerud.

SUPPLEMENTARY MATERIAL, NH3 + RNH3+ :

Cartesian coordinates:

NH3:

N	0.000000	0.000000	-0.116597
H	-0.000965	0.939869	0.272059
H	-0.813468	-0.470770	0.272059
H	0.814433	-0.469099	0.272059

(NH3)2:

N	0.099580	-0.205490	-1.550699
N	-0.099581	0.205492	1.550703
H	0.496438	0.476769	-2.192612
H	-0.454652	0.315856	-0.873484
H	-0.552710	-0.764760	-2.095456
H	0.454630	-0.315834	0.873456
H	0.552726	0.764742	2.095461
H	-0.496423	-0.476786	2.192605

NH4+:

N	0.000002	0.000002	0.000002
H	-0.010032	-0.009717	1.028620
H	0.973096	-0.009707	-0.333531
H	-0.492664	-0.830129	-0.355585
H	-0.470417	0.849540	-0.339516

TS, H3N--H--NH3+:

N	0.000000	0.000000	0.000000
N	0.000000	0.000000	2.614306
H	0.950921	0.000000	-0.378487
H	-0.475460	0.823522	-0.378487
H	-0.475460	-0.823522	-0.378487
H	0.000000	-0.000000	1.307153
H	0.475463	0.823520	2.992793
H	0.475458	-0.823523	2.992793
H	-0.950921	0.000003	2.992793

Imaginary Frequency: 948.78i cm-1

H3N--HNH3+:

N	-0.001604	-0.000004	-1.372524
N	0.001590	0.000004	1.359237
H	0.939675	0.000703	-1.769511
H	-0.473557	0.815216	-1.767850
H	-0.472330	-0.815936	-1.767842
H	0.000286	0.000003	0.244540
H	0.481436	0.831981	1.717326
H	0.482809	-0.831180	1.717326
H	-0.958216	-0.000788	1.719014

A1, CH3NH3+:

C	0.000000	0.000000	0.800770
N	0.000000	0.000000	-0.709186
H	-0.895121	0.516798	1.140251
H	0.000000	-1.033597	1.140251
H	0.895121	0.516798	1.140251
H	0.000000	0.956516	-1.087025
H	0.828367	-0.478258	-1.087025
H	-0.828367	-0.478258	-1.087025

A2, H3N--CH3NH3+:

C	0.000000	0.000000	-0.525677
H	-0.000001	1.029471	-0.182494
H	-0.891548	-0.514736	-0.182494
H	0.891548	-0.514735	-0.182494
N	0.000000	0.000000	-2.045657
H	0.827535	0.477778	-2.423161
H	0.000001	-0.955555	-2.423161

H	-0.827536	0.477777	-2.423161
N	0.000000	0.000000	2.407119
H	-0.809655	0.467454	2.813600
H	0.000001	-0.934909	2.813600
H	0.809654	0.467455	2.813600

A3, CH3NH3--NH3+:

H	-1.211258	0.377102	-2.303761
C	-0.386491	0.234442	-1.607974
N	-0.921864	0.086176	-0.217072
N	1.177387	-0.280064	1.577648
H	0.277265	1.096731	-1.629103
H	0.166609	-0.668441	-1.859857
H	-1.457013	0.915540	0.062073
H	-1.559220	-0.714804	-0.151057
H	-0.116863	-0.057984	0.499634
H	1.734671	-1.111632	1.376491
H	1.835960	0.500148	1.586934
H	0.860131	-0.386098	2.542459

TS(A2,A3), H3N--CH3NH3+:

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.514746
N	1.282209	0.000000	-2.805497
H	1.019282	0.000005	-0.373663
H	-0.518253	0.894364	-0.336969
H	-0.518245	-0.894369	-0.336969
H	0.506374	0.000048	-3.466722
H	1.847633	0.810027	-3.056854
H	0.480650	0.827242	1.889392
H	0.480658	-0.827237	1.889392
H	-0.953582	-0.000005	1.897643
H	1.847553	-0.810075	-3.056879

Imaginary Frequency: 102.28i cm-1

TS(A3,A3'), CH3(NH3)2+:

C	0.000000	1.219866	0.007906
N	1.349321	-0.505032	-0.005445
N	-1.349321	-0.505032	-0.005445
H	-0.895959	1.555167	-0.492570
H	0.895958	1.555167	-0.492571
H	0.000000	1.307039	1.085345
H	1.205346	-1.182315	0.744552
H	2.296428	-0.135353	0.109743
H	1.336971	-1.015394	-0.890000
H	-1.205344	-1.182318	0.744550
H	-1.336974	-1.015392	-0.890002
H	-2.296427	-0.135353	0.109747

Imaginary Frequency: 762.34i cm-1

TS(A2,A2'), H3N--CH3--NH3+:

C	0.000000	0.000000	0.000000
H	0.000001	1.077029	0.000000
H	0.932735	-0.538515	0.000000
H	-0.932735	-0.538514	0.000000
N	0.000000	0.000000	2.002194
H	-0.821501	0.474295	2.382427
H	-0.000001	-0.948588	2.382427
H	0.821502	0.474294	2.382427
N	0.000000	0.000000	-2.002194
H	0.821502	0.474294	-2.382427
H	-0.000001	-0.948588	-2.382427
H	-0.821501	0.474295	-2.382427

Imaginary Frequency: 614.39i cm-1

A6, CH3+:

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.089010
H	0.943109	0.000000	-0.544506
H	-0.943109	0.000002	-0.544506

B1, CH3CH2NH3+:

C	-0.000148	0.614571	0.000000
C	-1.308127	-0.148989	0.000000
N	1.170562	-0.355544	0.000000
H	1.145733	-0.965584	0.827952
H	2.077385	0.130668	0.000000
H	1.145733	-0.965584	-0.827952
H	-1.413708	-0.772386	-0.891708
H	-1.413708	-0.772386	0.891708
H	-2.131168	0.568754	0.000000
H	0.122724	1.235916	0.888134
H	0.122724	1.235916	-0.888134

B2, H3N--CH2(CH3)NH3+:

C	-0.000420	0.536183	0.000000
C	-1.364974	-0.114647	0.000000
N	1.323076	-2.277842	0.000000
N	-0.156211	2.053948	0.000000
H	0.585169	0.281840	0.881297
H	0.585169	0.281840	-0.881297
H	0.751699	2.536172	0.000000
H	-0.677007	2.372109	-0.827189
H	-0.677007	2.372109	0.827189
H	1.105321	-2.857850	0.809652
H	1.105321	-2.857850	-0.809652
H	2.338907	-2.190939	0.000000
H	-1.942442	0.146929	-0.891105
H	-1.208373	-1.193250	0.000000
H	-1.942442	0.146929	0.891105

B3, CH3CH3NH3--NH3+:

C	2.355180	-0.068271	0.000001
C	0.904593	-0.509002	0.000000
N	-0.025925	0.674467	0.000000
N	-2.694943	-0.169161	0.000000
H	0.654208	-1.096279	0.885195
H	0.654210	-1.096277	-0.885199
H	0.139366	1.264445	0.823508
H	0.139365	1.264446	-0.823509
H	-1.065606	0.367651	0.000000
H	2.999582	-0.949845	0.000000
H	2.595697	0.519488	-0.889889
H	2.595695	0.519486	0.889892
H	-2.933564	-0.737103	-0.814075
H	-2.933638	-0.736871	0.814216
H	-3.357867	0.607358	-0.000140

B4, CH2CH2:

C	0.000003	0.000006	-0.668193
C	-0.000004	-0.000007	0.668193
H	0.922647	0.034076	1.238285
H	-0.922657	-0.034095	1.238281
H	-0.922645	-0.034071	-1.238291
H	0.922659	0.034100	-1.238276

TS(B2,B2'), H3N--CH2(CH3)--NH3+:

C	-0.000042	0.245710	0.000000
C	0.045490	-1.265187	0.000000
N	-2.052489	0.324281	0.000000
N	2.017388	0.596557	0.000000
H	-0.034622	0.805008	0.921336
H	-0.034622	0.805008	-0.921336
H	-2.381143	1.292411	0.000000
H	-2.461497	-0.127447	-0.820357
H	-2.461497	-0.127447	0.820357
H	2.477740	0.199320	0.821456
H	2.477740	0.199320	-0.821456
H	2.224040	1.597920	0.000000
H	-0.449689	-1.663025	-0.886954
H	1.066261	-1.647044	0.000000
H	-0.449689	-1.663025	0.886954

Imaginary Frequency: 595.94i cm-1

TS(B3,B3'), CH3CH2(NH3)2+:

C	-0.812246	-0.000135	0.741121
C	-1.676628	0.000077	-0.429640
N	1.020553	1.455701	-0.082313
N	1.020554	-1.455670	-0.082839
H	-0.666071	-0.914179	1.293694
H	-0.666071	0.913710	1.294025
H	0.784792	-2.448732	-0.025423
H	1.260442	-1.283338	-1.058946
H	1.884585	-1.345876	0.448462
H	1.260439	1.283724	-1.058483
H	0.784791	2.448742	-0.024535
H	1.884586	1.345714	0.448946
H	-2.685845	-0.000008	0.032226
H	-1.598079	0.903254	-1.031229
H	-1.598077	-0.902880	-1.031557

Imaginary Frequency: 559.20i cm-1

TS(B2,B3), H3N--CH2(CH3)NH3+:

C	-0.000220	-0.388493	0.399384
N	0.021829	-0.970233	1.808541
N	-1.209552	1.135966	-2.059704
H	-0.741042	0.407897	0.387721
H	-0.349518	-1.186784	-0.254778
C	1.379972	0.104980	0.028744
H	-0.995361	2.129414	-2.139801
H	-0.905924	0.725192	-2.941987
H	-0.901456	-1.317826	2.097641
H	0.315431	-0.262570	2.493875
H	0.684531	-1.753068	1.877723
H	-2.227390	1.079971	-2.076442
H	2.115275	-0.704113	0.009493
H	1.314260	0.533487	-0.971515
H	1.726745	0.889348	0.707449

Imaginary Frequency: 45.30i cm-1

B5, CH2CH2--NH4--NH3+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.342991
H	0.925521	0.000000	-0.568495
H	-0.922570	-0.068218	-0.569177
H	0.925515	-0.000033	1.911497
H	-0.922573	-0.068243	1.912157
H	-0.080822	2.276403	0.671631
N	-0.088551	3.313164	0.671299
H	0.419443	3.646304	1.496229
H	0.400832	3.645614	-0.165084
H	-1.111076	3.695081	0.682596
N	-2.686197	4.297471	0.699920
H	-3.215360	4.001525	1.521366
H	-3.234435	3.998483	-0.107800
H	-2.721629	5.317913	0.698432

TS(B3,B5), CH2CH2--H--NH3--NH3+:

C	-1.320994	-1.484136	-0.296359
C	-0.548751	-0.722592	0.581596
N	-0.954689	1.797132	-0.093789
N	2.459815	-0.103850	-0.061286
H	-2.282529	-1.874742	0.024860
H	-0.835066	-1.966245	-1.139842
H	-1.488093	-0.360295	-0.596530
H	-0.987875	-0.353248	1.502781
H	0.489112	-0.441186	0.341155
H	-1.338386	2.148571	-0.973005
H	-1.456899	2.302036	0.637603
H	0.004499	2.143704	-0.060530
H	2.956380	-0.993656	-0.010932
H	2.921434	0.497133	0.621418
H	2.700016	0.285324	-0.972884

Imaginary Frequency: 618.56i cm-1

TSb(B3,B5), H3N--CH2CH2--H--NH3+:

C	1.137163	0.959882	-0.000008
H	1.713600	0.911695	0.916271
C	-0.173690	1.418664	0.000006
H	-0.511782	1.892567	-0.920407
H	-0.977955	0.350455	0.000023
H	-0.511763	1.892563	0.920428
N	-2.021546	-0.574993	-0.000002
H	-2.899294	-0.049700	-0.000136
H	-2.026393	-1.173935	0.828089
H	-2.026216	-1.174090	-0.827980
N	1.359824	-1.268701	0.000003
H	1.003321	-1.755988	0.822809
H	2.370834	-1.414668	-0.000010
H	1.003286	-1.755999	-0.822782
H	1.713576	0.911683	-0.916301

Imaginary Frequency: 1145.61i cm-1

TS(B2,B5), H3N--CH2CH2--H--NH3+:

C	0.620594	-0.453115	0.000000
C	-0.179471	0.687005	0.000000
H	0.705383	-1.038110	-0.911512
H	0.705383	-1.038110	0.911512
H	-0.216560	1.276224	0.915446
H	-0.216560	1.276224	-0.915446
N	2.601116	-0.044572	0.000000
H	2.809119	0.523338	-0.822608
H	2.809119	0.523337	0.822609
H	3.238554	-0.844219	-0.000001
N	-2.801983	-0.164884	0.000000
H	-3.056381	-0.706332	-0.830739
H	-3.056381	-0.706333	0.830739
H	-3.348013	0.701194	0.000000
H	-1.614333	0.095637	0.000000

Imaginary Frequency: 842.11i cm-1

B6, (CH2CH2)H+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.381978
H	1.107393	0.000000	0.690989
H	-0.011106	-0.936068	1.936533
H	-0.011105	0.936068	1.936534
H	-0.011106	-0.936068	-0.554555
H	-0.011105	0.936068	-0.554555

B7, (CH2CH2)NH4+:

C	1.177419	0.871588	0.000460
C	1.393742	-0.456026	-0.000510
N	-1.885130	-0.304693	0.000036
H	-0.849543	-0.138186	0.000017
H	-2.380820	0.595045	-0.002501
H	-2.151515	-0.834883	0.838449
H	-2.150841	-0.839238	-0.835822
H	1.125753	1.439312	-0.924519
H	1.125951	1.437996	0.926257
H	1.524881	-1.009622	-0.926175
H	1.525080	-1.010945	0.924335

TS(B1,B7), CH2CH2--H--NH3+:

C	-1.443394	-0.092988	-0.699968
C	-0.835191	0.142734	0.529664
N	1.750918	-0.024272	0.197227
H	-0.273648	-0.170051	-0.857575
H	2.155199	-0.925017	-0.066239
H	2.106713	0.160036	1.137224
H	2.214821	0.662853	-0.400144
H	-1.785887	0.747641	-1.296805
H	-1.854350	-1.075705	-0.913403
H	-0.539846	1.142350	0.828470

H -0.607922 -0.670679 1.209703
Imaginary Frequency: 651.93i cm-1

C1, (CH3)2CHNH3+:

C	0.358943	-0.650063	1.274522
C	0.358943	0.173331	0.000000
C	0.358943	-0.650063	-1.274522
N	-0.896235	1.046830	0.000000
H	-1.743431	0.462334	0.000000
H	-0.939443	1.651987	-0.831082
H	-0.939443	1.651987	0.831082
H	-0.489171	-1.341398	-1.299459
H	0.339484	-0.023352	-2.170905
H	1.273595	-1.245631	-1.309780
H	1.273595	-1.245631	1.309780
H	0.339484	-0.023352	2.170905
H	-0.489171	-1.341398	1.299459
H	1.187180	0.887409	0.000000

C3, (CH3)2CHNH3--NH3+:

C	-2.202531	-0.549548	-0.151537
C	-0.813498	0.034505	-0.339700
C	-0.674810	1.454107	0.182574
N	0.195365	-0.835080	0.378616
N	2.846426	-0.034147	-0.145546
H	0.025891	-0.811357	1.391534
H	1.209835	-0.516629	0.193684
H	0.110375	-1.815685	0.085340
H	-0.939311	1.508123	1.243579
H	0.339371	1.839051	0.048804
H	-1.357386	2.108521	-0.363606
H	-2.927622	0.054120	-0.701662
H	-2.269205	-1.574070	-0.529556
H	-2.492039	-0.540686	0.904000
H	-0.521388	-0.011692	-1.393095
H	2.988791	0.297318	-1.100487
H	3.179072	0.716400	0.461152
H	3.506110	-0.803214	-0.019205

C4, CH3CHCH2:

C	-0.460345	-0.009027	-0.135579
C	-0.493125	-0.008501	1.202164
H	0.418959	0.009692	1.792472
H	-1.429515	-0.026170	1.749792
H	-1.400170	-0.027715	-0.686433
C	0.794679	0.014554	-0.955330
H	1.680221	0.032523	-0.314202
H	0.858798	-0.865849	-1.603617
H	0.824452	0.895364	-1.605546

TS(SNB), H3N--CH(CH3)2--NH3+:

C	0.000000	-1.303056	0.613465
C	0.000000	0.000000	-0.144005
C	0.000000	1.303059	0.613460
N	2.100320	-0.000001	-0.488013
N	-2.100321	-0.000001	-0.488012
H	0.000000	-0.000002	-1.219811
H	-2.387004	0.820094	-1.027032
H	-2.387004	-0.820097	-1.027030
H	-2.664142	0.000000	0.364340
H	2.664143	0.000000	0.364340
H	2.387004	-0.820098	-1.027030
H	2.387004	0.820093	-1.027034
H	-0.000002	-2.161395	-0.060564
H	0.873880	-1.366426	1.263763
H	-0.873879	-1.366425	1.263765
H	0.873880	1.366430	1.263759
H	0.000002	2.161395	-0.060573
H	-0.873880	1.366432	1.263758

Imaginary Frequency: 567.39i cm-1

TS(C3,C3'), (CH3)2CH(NH3)2+:

C	-0.666949	1.048459	1.288817
C	-0.666949	1.048459	-1.288817
C	0.000000	1.024212	0.000000
N	-0.974846	-1.692430	0.000000
N	2.105886	-0.768715	0.000000
H	-0.626292	2.117451	-1.579473
H	-0.077936	0.526257	-2.046273
H	-1.699294	0.711649	-1.263573
H	-1.699294	0.711649	1.263573
H	-0.077936	0.526257	2.046273
H	-0.626292	2.117451	1.579473
H	-0.663579	-2.227885	0.810688
H	-0.663579	-2.227885	-0.810688
H	-1.991529	-1.786727	0.000000
H	1.065991	1.214885	0.000000
H	2.040220	-1.381119	0.812199
H	2.040220	-1.381119	-0.812199
H	3.065410	-0.419637	0.000000

Imaginary Frequency: 251.45i cm-1

TS(360o), H3N--(CH3)2CHNH3+:

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.531195
H	1.060347	0.000000	-0.268623
N	-3.192441	0.000001	-2.466261
C	-0.673617	1.276932	-0.462401
C	-0.673617	-1.276932	-0.462401
H	0.469287	0.831717	1.913103
H	0.469287	-0.831717	1.913103
H	-0.966262	-0.000000	1.884536
H	-0.156716	2.166681	-0.089654
H	-1.723630	1.299554	-0.160710
H	-0.664391	1.304026	-1.552359
H	-0.664391	-1.304027	-1.552359
H	-0.156717	-2.166681	-0.089653
H	-1.723630	-1.299554	-0.160710
H	-2.862693	-0.000001	-3.430716
H	-3.806573	0.810176	-2.394056
H	-3.806577	-0.810171	-2.394055

Imaginary Frequency: 74.06i cm-1

C5, CH3CHCH2--NH4--NH3+:

C	-1.263204	-1.146911	0.273475
C	-0.269000	-1.802798	0.900268
C	0.650793	-2.787501	0.243471
N	1.044995	1.130784	-0.173370
N	-0.464704	3.365795	-0.855875
H	-0.141714	-1.657502	1.973683
H	1.648719	0.863897	-0.956539
H	0.452153	2.005455	-0.440573
H	0.104309	4.147576	-1.183656
H	-1.135282	3.176633	-1.602045
H	-1.472093	-1.311469	-0.781359
H	-1.951745	-0.506517	0.817388
H	0.428605	0.327742	0.063875
H	0.492054	-3.784147	0.666813
H	0.472078	-2.845737	-0.833390
H	1.703236	-2.539640	0.416990
H	1.638290	1.342912	0.634249
H	-1.012179	3.728001	-0.074002

TS(C3,C5), CH3CHCH2--H--NH3--NH3+:

C	-0.321502	-0.356630	-1.729452
C	-0.636751	-0.398405	-0.346303
N	2.365098	-0.384041	0.109449
N	-1.006169	2.328435	1.182092
H	-0.700667	0.558150	0.204420
C	-0.828182	-1.629838	0.404712
H	-0.539957	0.576337	-2.246569
H	-0.485389	-1.265178	-2.307356

H	0.778736	-0.321700	-1.436434
H	2.724419	-1.309725	0.343797
H	3.073813	0.027220	-0.499210
H	2.417373	0.154122	0.974675
H	-0.962314	2.260818	2.198702
H	-1.924529	2.722574	0.978055
H	-0.338492	3.056628	0.929540
H	-1.919319	-1.649505	0.591092
H	-0.553267	-2.534099	-0.137890
H	-0.364298	-1.577162	1.392652

Imaginary Frequency: 302.88i cm-1

TSb(C3,C5), H3N--(CH3)CHCH2--H--NH3+:

C	1.015731	-0.463379	-0.476902
C	-0.030284	-1.383441	-0.431130
C	1.977917	-0.280003	0.629358
N	-2.420242	-0.197514	0.320929
N	0.108670	1.864976	-0.209322
H	-0.360770	-1.780023	-1.390898
H	0.012378	-2.110545	0.380974
H	-1.025149	-0.692365	-0.091327
H	1.243655	0.022143	-1.420428
H	1.526395	-0.484467	1.602436
H	2.764825	-1.033685	0.471545
H	2.454431	0.698985	0.622843
H	-2.428390	0.364611	1.172680
H	-2.883230	0.343437	-0.410471
H	-3.005677	-1.015612	0.498888
H	-0.111382	2.160329	0.742329
H	-0.676922	2.161532	-0.789016
H	0.890654	2.454358	-0.498753

Imaginary Frequency: 573.80i cm-1

TSc(C3,C5), H3N--(CH3)CHCH2--H--NH3+:

C	0.448628	0.053850	-0.320437
C	-0.357726	-0.846791	0.365664
C	0.623143	1.465820	0.151985
H	0.563152	-0.099194	-1.391653
H	-0.414069	-1.866538	-0.012999
H	-0.385974	-0.764912	1.452687
H	-0.262053	2.048938	-0.131315
H	0.722087	1.511989	1.239031
H	1.485084	1.946650	-0.310929
N	2.513477	-0.536682	-0.090688
H	2.782031	-0.423705	0.887712
H	2.574404	-1.533679	-0.300896
H	3.223111	-0.064724	-0.654491
N	-2.940449	-0.088258	-0.123526
H	-3.232848	0.691510	0.470746
H	-3.155236	0.150716	-1.095026
H	-3.498698	-0.906986	0.131903
H	-1.696462	-0.352763	0.031455

Imaginary Frequency: 1145.90i cm-1

C6, CH3CHCH3+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.439013
H	1.097249	0.000000	1.651608
H	-0.431620	-0.888866	1.898376
H	-0.354458	0.941090	1.870774
C	-0.266240	-1.141628	-0.834602
H	0.220633	0.946065	-0.500874
H	-1.313397	-0.926841	-1.160912
H	0.308325	-1.138914	-1.766040
H	-0.265411	-2.099979	-0.315993

C7, CH3CHCH2--HNH3+:

C	-0.897831	-0.329069	-1.007066
C	-0.993654	-0.303755	0.337743
N	2.215233	-0.337520	-0.440013
H	1.161109	-0.343886	-0.440192

H	2.561036	-0.491336	-1.394777
H	2.568394	-1.083705	0.170743
H	2.557864	0.568443	-0.099221
H	-0.918134	0.588565	-1.591665
H	-0.917827	-1.265058	-1.558938
C	-1.108699	0.942364	1.162290
H	-1.052004	-1.251751	0.874507
H	-0.998932	1.841799	0.550956
H	-2.093907	0.976280	1.637899
H	-0.373121	0.966051	1.972980

TS(C1,C7), CH3CHCH2--H--NH3+:

C	0.758591	1.342997	-0.168647
C	0.799342	0.083986	0.469126
C	1.159837	-1.170944	-0.172365
H	0.480348	0.039009	1.510721
N	-2.118711	-0.151282	-0.035068
H	2.143004	-1.421733	0.270817
H	1.275593	-1.094701	-1.253000
H	0.489250	-1.982895	0.119960
H	0.799706	2.225564	0.467729
H	1.236863	1.427999	-1.142393
H	-0.356039	1.116494	-0.331125
H	-2.423266	-0.733540	0.746539
H	-2.771587	0.634168	-0.040092
H	-2.349520	-0.687622	-0.872361

Imaginary Frequency: 402.00i cm-1

D1, (CH3)3CNH3+:

C	-0.389076	1.406374	-0.516818
C	0.000000	0.000000	-0.086500
C	-1.023412	-1.040143	-0.516816
C	1.412503	-0.366236	-0.516795
N	-0.000014	0.000005	1.450288
H	0.672609	0.683625	1.823875
H	-0.928363	0.240709	1.823861
H	0.255700	-0.924315	1.823877
H	-0.401529	1.451418	-1.608081
H	-1.389297	1.676228	-0.162991
H	0.330220	2.151939	-0.162977
H	2.146308	0.365054	-0.162953
H	1.698527	-1.361948	-0.162951
H	1.457758	-0.377971	-1.608057
H	-2.028743	-0.789994	-0.162989
H	-1.056183	-1.073464	-1.608079
H	-0.757004	-2.041283	-0.162973

D2, H3N--(CH3)3CNH3+:

C	1.454149	0.225878	0.000000
C	0.000000	0.665822	0.000000
C	-0.727075	0.225878	1.259330
C	-0.727075	0.225878	-1.259330
N	0.000000	2.204573	0.000000
N	0.000000	-3.086410	0.000000
H	-0.936321	-3.489724	0.000000
H	0.468162	-3.489724	-0.810878
H	0.468162	-3.489724	0.810878
H	0.479640	2.576203	0.830761
H	0.479640	2.576203	-0.830761
H	-0.959280	2.576203	0.000000
H	1.461801	-0.866187	0.000000
H	1.984201	0.575209	-0.892331
H	1.984201	0.575209	0.892331
H	-0.219319	0.575209	2.164534
H	-1.764882	0.575209	1.272203
H	-0.730900	-0.866187	1.265956
H	-0.219319	0.575209	-2.164534
H	-0.730900	-0.866187	-1.265956
H	-1.764882	0.575209	-1.272203

TS(D2,D2'), H3N--(CH3)3C--NH3+:

C	0.141315	-0.060374	1.477847
C	0.006639	0.005824	0.008187
C	-0.011590	1.324816	-0.659960
C	-0.127401	-1.242550	-0.770149
N	2.648569	-0.034850	-0.080253
N	-2.653003	0.012030	0.031499
H	-3.018757	0.236442	-0.895095
H	-3.055683	-0.897473	0.262981
H	-3.107798	0.673817	0.663141
H	3.063116	0.660320	0.542578
H	3.061530	-0.924101	0.206234
H	3.045571	0.160860	-1.000906
H	-0.874108	-0.182809	1.870424
H	0.714579	-0.938256	1.778648
H	0.570977	0.848740	1.897601
H	0.911796	1.855588	-0.420602
H	-0.134747	1.250144	-1.739906
H	-0.829771	1.911520	-0.232809
H	0.878981	-1.495697	-1.120632
H	-0.492463	-2.067663	-0.157791
H	-0.755962	-1.097984	-1.648139

Imaginary Frequency: 277.96i cm-1

D3, (CH3)3CNH3--NH3+:

C	0.708259	0.526214	-2.034909
C	0.487611	0.156135	-0.574887
N	-1.013027	0.060719	-0.348636
C	1.069239	-1.211761	-0.244693
C	1.005715	1.235377	0.365996
H	-1.468388	0.955074	-0.569255
H	-1.426818	-0.646354	-0.968895
H	-1.263002	-0.198762	0.665138
H	1.780153	0.603132	-2.231633
H	0.299940	-0.234851	-2.707844
H	0.255085	1.493168	-2.276612
H	0.553432	2.208382	0.147672
H	0.811653	0.979682	1.411553
H	2.085969	1.336070	0.238855
H	0.662394	-1.989096	-0.899819
H	2.151492	-1.188065	-0.391050
H	0.875679	-1.486767	0.796045
N	-1.749167	-0.620650	2.304901
H	-1.400801	-1.528351	2.615784
H	-1.441419	0.050299	3.009919
H	-2.764946	-0.669839	2.397238

TS(D2,D3), H3N--(CH3)3CNH3+:

C	1.682920	0.000001	1.270481
C	0.748807	0.000000	0.069940
N	1.648829	-0.000001	-1.177546
C	-0.089390	1.265276	-0.011091
C	-0.089389	-1.265277	-0.011089
N	-3.326195	0.000000	0.003178
H	-0.723563	-1.271493	-0.901314
H	-0.762330	-1.297281	0.846536
H	0.539161	-2.162088	0.006472
H	-0.723564	1.271490	-0.901316
H	-0.762331	1.297280	0.846534
H	0.539159	2.162088	0.006468
H	2.317282	0.892157	1.291410
H	1.082207	0.000002	2.182600
H	2.317283	-0.892153	1.291412
H	1.082767	-0.000002	-2.036618
H	2.254693	0.831174	-1.202009
H	-3.675206	-0.000077	0.960766
H	-3.758194	-0.810277	-0.438964
H	2.254693	-0.831175	-1.202008
H	-3.758180	0.810357	-0.438829

Imaginary Frequency: 64.17i cm-1

"TS(D3,D3'), (CH3)3C(NH3)2+":

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.462496
C	1.248414	0.000000	-0.742732
C	-1.246553	-0.068146	-0.742732
H	-0.029446	1.078057	1.714712
H	-0.893902	-0.456223	1.887409
H	0.917473	-0.406748	1.887409
H	2.138089	0.152392	-0.134488
H	1.232351	-1.027347	-1.174509
H	1.218595	0.659535	-1.614380
H	-1.252780	0.592033	-1.614379
H	-1.174434	-1.093085	-1.174509
H	-2.143220	0.035454	-0.134488
N	0.074186	-2.716102	-2.153600
N	0.090053	-3.297006	1.192406
H	0.082335	-3.014420	2.172521
H	0.090370	-3.308619	-1.325328
H	-0.702475	-3.933417	1.103048
H	0.916138	-3.889208	1.103048
H	-0.728438	-3.010447	-2.709383
H	0.891681	-2.966195	-2.709384

Imaginary Frequency: 103.03i cm-1 AND 86.91i cm-1
i.e. a SECOND-order saddle point

D4, CH2C(CH3)2:

C	-0.000055	0.000771	0.119450
C	-0.000670	0.009385	1.460243
H	0.923114	0.047189	2.029976
H	-0.924978	-0.021095	2.029567
C	-1.273152	-0.051421	-0.679793
C	1.273776	0.042684	-0.679229
H	2.152896	0.079342	-0.030807
H	1.357557	-0.839601	-1.324284
H	1.292537	0.920369	-1.335628
H	-2.152867	-0.079750	-0.031762
H	-1.356342	0.822497	-1.336215
H	-1.291309	-0.937472	-1.324871

D5, (CH3)2CCH2--NH4--NH3+:

C	0.196784	-1.351538	-0.563381
C	-0.220461	-1.491734	0.712448
C	0.747628	-1.596386	1.859185
C	-1.677834	-1.617839	1.063610
N	-0.005599	1.803371	-0.031450
N	0.788512	2.866512	-2.481663
H	1.254650	-1.345966	-0.815388
H	-0.506264	-1.361541	-1.392985
H	-2.321958	-1.501446	0.188402
H	-1.870223	-2.605039	1.496691
H	-1.970439	-0.883850	1.822994
H	0.661887	-2.582642	2.327250
H	0.521881	-0.861804	2.640498
H	1.783016	-1.465139	1.534874
H	0.013711	0.761160	-0.062221
H	-0.956218	2.111439	0.192800
H	0.304379	2.219263	-0.987906
H	1.734234	2.586061	-2.744443
H	0.186468	2.572629	-3.251905
H	0.622580	2.125404	0.710545
H	0.785200	3.887267	-2.498583

TS(D5,D5') (CH3)2CCH3--NH3--NH3+:

C	0.152312	-1.150524	-0.886024
C	0.127881	-1.575591	0.492272
C	1.287939	-1.327280	1.328497
N	0.435380	1.740125	0.469316
N	-0.758889	3.061341	-2.070744
C	-1.112966	-2.079405	1.091879
H	1.256554	-1.809855	2.304565
H	1.169365	-0.221494	1.451704
H	2.240010	-1.470207	0.814297

H	0.050576	-0.044691	-0.687692
H	1.120611	-1.267657	-1.375460
H	-0.684304	-1.495341	-1.491797
H	0.026847	2.171307	-0.374705
H	1.363841	2.153113	0.561624
H	-0.100997	2.111171	1.254149
H	-1.749438	2.919838	-2.263634
H	-0.655624	4.060052	-1.895238
H	-0.277059	2.888638	-2.951933
H	-1.028252	-3.178579	1.008522
H	-1.192866	-1.848403	2.155945
H	-2.005691	-1.781361	0.539903

Imaginary Frequency: 138.71i cm-1

TSb(D3,D5), (CH3)2CCH2--H--NH3--NH3+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.473195
C	1.221025	0.000000	-0.718473
C	-1.294656	-0.025644	-0.697790
H	0.006246	1.065127	1.760116
H	-0.896717	-0.455709	1.891054
H	0.904614	-0.449749	1.885636
H	2.101535	0.287915	-0.142776
H	1.378559	-1.143897	-0.958729
H	1.169706	0.454135	-1.709178
H	-1.223530	0.227210	-1.755031
H	-1.649399	-1.060016	-0.580774
H	-2.022523	0.614984	-0.189443
N	2.032083	-2.664413	-1.635277
N	-0.645250	-3.062290	0.632616
H	-1.398152	-3.150648	1.315631
H	2.495240	-3.264794	-0.953756
H	-0.875681	-3.737112	-0.096527
H	0.178327	-3.440464	1.100060
H	1.337885	-3.241482	-2.108772
H	2.737495	-2.434079	-2.335499

Imaginary Frequency: 77.69i cm-1

TS(D2,D5), H3N--(CH3)2CCH2--H--NH3+:

C	0.286794	0.000028	0.151110
C	-0.459612	-0.000185	-1.019119
C	0.477027	1.272417	0.913957
C	0.477038	-1.272084	0.914415
H	-0.367698	-1.392249	1.606721
H	-0.367711	1.392824	1.606220
H	1.383351	-1.237001	1.518954
H	1.383339	1.237560	1.518508
H	0.507951	2.142672	0.256234
H	0.507970	-2.142576	0.257004
H	-0.479613	0.917783	-1.605754
H	-0.479611	-0.918366	-1.605420
N	2.565911	-0.000119	-0.673059
H	3.359085	-0.000002	-0.030069
H	2.691924	0.814254	-1.274867
H	2.691931	-0.814721	-1.274558
N	-3.066700	-0.000034	-0.174495
H	-3.344362	0.826709	0.358862
H	-3.344343	-0.826554	0.359217
H	-3.602647	-0.000228	-1.045328
H	-1.721527	-0.000087	-0.475029

Imaginary Frequency: 1147.50i cm-1

D6, (CH3)3C+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.462165
H	1.067748	0.000000	1.751820
H	-0.486137	-0.866670	1.907855
H	-0.397353	0.941167	1.858842
C	-0.285655	-1.225847	-0.740892
C	0.324975	1.226888	-0.720980
H	-0.488334	-1.061509	-1.799632

H	0.649420	-1.816121	-0.664909
H	-1.056509	-1.832655	-0.258332
H	0.835077	1.034057	-1.668836
H	-0.667593	1.638810	-0.994661
H	0.837524	1.974313	-0.114318

D7, (CH3)2CCH2--HNH3+:

C	-0.647779	0.000269	-1.204679
C	-0.785046	-0.000002	0.140978
N	2.406502	0.000068	-0.732532
H	1.346578	0.000103	-0.727480
H	2.744848	0.000259	-1.702031
H	2.758380	-0.836949	-0.253540
H	2.758437	0.836862	-0.253191
H	-0.668429	0.927374	-1.773631
H	-0.668492	-0.926602	-1.774011
C	-0.902217	1.276638	0.927333
C	-0.902304	-1.276956	0.926810
H	-0.767590	2.161161	0.299837
H	-1.896366	1.334427	1.382896
H	-0.182256	1.306773	1.752730
H	-0.767738	-2.161232	0.298951
H	-0.182345	-1.307479	1.752194
H	-1.896457	-1.334864	1.382350

TS(D1,D7), (CH3)2CCH2--H--NH3+:

C	-0.820030	0.006746	0.124526
C	-0.374324	-0.766392	1.261764
C	-0.726782	1.463670	0.143945
C	-1.244227	-0.671995	-1.101082
H	-1.356063	1.947858	-0.604513
H	-2.342704	-0.753086	-0.993692
H	-0.853957	-1.687576	-1.183543
H	-0.852896	1.896323	1.136997
H	0.329357	1.618671	-0.154457
H	-1.056912	-0.082682	-2.000691
H	-0.477800	-0.262786	2.222982
H	-0.724777	-1.798882	1.273021
N	2.442679	-0.029917	-0.293506
H	0.714739	-0.772672	0.999887
H	2.602597	0.333081	-1.233855
H	3.038358	0.534199	0.313308
H	2.873484	-0.955204	-0.295823

Imaginary Frequency: 79.00i cm-1