Supporting Information for:

The Discrete Existence of Singlet Nitrenium Ions Revisited: Computational Studies of Non-Aryl Nitrenium Ions and their Rearrangements.

Daniel E. Falvey

Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742 (USA)
Falvey@umd.edu

Table S1. Cartesian Coordinates for Structures **1-43.**

1S

****

%chk=NH2-s-CBSAPNO.chk

---

cbs-apno scrf=(smd,solvent=water) geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.141272
2	1	0	0.000000	0.833941	-0.494450
3	1	0	0.000000	-0.833941	-0.494450

1T

%chk=NH2-t-CBSAPNO.chk

---

cbs-apno scrf=check geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.056790
2	1	0	0.000000	1.002306	-0.198765
3	1	0	0.000000	-1.002306	-0.198765

2S

%chk=Methylnitrenium-s-SMDCBS.chk

---

cbs-apno scrf=(smd,solvent=water) geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.756752	-0.110540	0.000046
2	1	0	-1.119494	0.847402	0.000299
3	6	0	0.505058	-0.145573	-0.000019

4	1	0	1.181104	-0.990266	-0.000478
5	1	0	1.101237	0.895822	-0.436939
6	1	0	1.104069	0.894267	0.436908

2T

%chk=Methylnitrenium-t-SMDCBS .chk

---

cbs-apno scrf=(smd,solvent=water) geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.744324	0.100734	0.000016
2	1	0	1.653582	-0.383730	-0.000036
3	6	0	-0.649380	-0.025082	0.000003
4	1	0	-1.090473	0.977223	-0.001156
5	1	0	-0.938412	-0.575020	-0.906464
6	1	0	-0.938687	-0.573120	0.907523

2S-ts

%chk=MethynitreniumTS-s-SMDdft.chk

---

opt=qst3 freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.738407	-0.154009	-0.002689
2	1	0	1.212771	0.764157	0.036006
3	6	0	-0.566621	-0.056972	0.014932
4	1	0	-1.181906	-0.949759	-0.021411
5	1	0	-0.959283	0.819466	0.641500
6	1	0	-0.840701	0.786028	-0.726859

3S

****

%chk=Dimethylnitrenium-s-dft.chk

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.534266
2	6	0	0.000000	1.195069	-0.172710
3	1	0	-1.096422	1.394513	0.041537
4	1	0	0.502245	1.996986	0.379621
5	1	0	0.159085	1.149288	-1.254824
6	6	0	0.000000	-1.195069	-0.172710
7	1	0	1.096422	-1.394513	0.041537
8	1	0	-0.502245	-1.996986	0.379621
9	1	0	-0.159085	-1.149288	-1.254824

3T

****

%chk=DimethylnitreniumC2v-t-CBSAPNO.chk

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.306822
2	6	0	0.000000	1.367164	-0.087966
3	1	0	-0.906908	1.555250	-0.681223
4	1	0	0.000000	1.987210	0.816368
5	1	0	0.906908	1.555250	-0.681223
6	6	0	0.000000	-1.367164	-0.087966
7	1	0	0.906908	-1.555250	-0.681223
8	1	0	0.000000	-1.987210	0.816368
9	1	0	-0.906908	-1.555250	-0.681223

3S-ts

%chk=dimethylnitreniumTS-s-dft.chk

---

opt=(calcfc,tight,qst3) freq=noraman 6-311g(d,p) geom=connectivity m062x int=ultrafine

---

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.024997	-0.516253	-0.032354
2	6	0	1.187721	0.178173	-0.040747
3	1	0	2.049060	-0.384307	-0.407400
4	1	0	1.175710	1.266767	-0.138217
5	6	0	-1.187386	0.164868	0.023041
6	1	0	-1.149719	1.248118	0.152222
7	1	0	-1.543797	-0.091764	-1.009995
8	1	0	-1.907688	-0.375365	0.646608
9	1	0	1.199439	-0.107927	1.089501

4S-iso (did not converge on nitrenium ion)

%chk=Ethylnitrenium-s-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	7	-0.004379586	0.000044844	0.005300497
2	1	0.002093246	-0.000053660	-0.001086154
3	6	0.005476303	0.000045807	0.001228395
4	1	-0.002183877	0.002106748	-0.003372450
5	1	-0.000627052	-0.002180632	-0.003449528
6	6	0.000018756	-0.000071058	0.001311407
7	1	-0.000411697	-0.000152804	-0.000036607
8	1	0.000461589	0.000078584	0.000101655
9	1	-0.000447682	0.000182172	0.000002785

4T

%chk=Ethylnitrenium-t-dft .chk

---

opt=(calcfc,tight) freq=noraman 6-311g(d,p) guess=save geom=connecti
vity um062x int=ultrafine

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.242497	-0.253367	0.000025
2	1	0	1.580644	-1.224134	-0.000089
3	6	0	0.136466	0.576638	-0.000010
4	1	0	0.207596	1.224587	0.890537
5	1	0	0.207617	1.224536	-0.890595
6	6	0	-1.174758	-0.268340	0.000003
7	1	0	-1.238343	-0.880853	0.897113
8	1	0	-1.986916	0.460559	-0.000029
9	1	0	-1.238325	-0.880911	-0.897068

5S-iso (did not converge on nitrenium)

%chk=isopropyl-s-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.625393	0.639080	0.000055
2	1	0	1.103328	1.537095	-0.000791
3	6	0	-0.656401	0.655974	0.000335
4	6	0	1.483881	-0.560950	-0.000009
5	6	0	-1.516627	-0.538773	0.000101
6	1	0	-1.119964	1.640515	-0.000134
7	1	0	2.519452	-0.233730	0.006564
8	1	0	1.281516	-1.152118	0.892083
9	1	0	1.290535	-1.145457	-0.898581
10	1	0	-2.169557	-0.492530	-0.878111
11	1	0	-0.969037	-1.477485	0.005421
12	1	0	-2.179141	-0.487354	0.870601

5T

```
 %chk=isopropyl-t-dft.chk
 ---------------------------------------------------------------------
# opt=rcfc freq=noraman 6-311g(d,p) guess=read geom=connectivity um062
x
 ---------------------------------------------------------------------
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.018821	1.390287	-0.016602
2	1	0	-0.059670	2.015596	-0.830776
3	6	0	0.001671	0.068098	0.387388
4	6	0	1.313156	-0.603222	-0.125093
5	6	0	-1.294895	-0.635576	-0.122171
6	1	0	0.003177	0.078794	1.489703
7	1	0	2.194264	-0.077850	0.238326
8	1	0	1.304082	-1.616841	0.278539
9	1	0	1.313291	-0.646779	-1.213610
10	1	0	-2.188323	-0.138430	0.251152
11	1	0	-1.301109	-0.670474	-1.211268
12	1	0	-1.253561	-1.651828	0.273403

6S-iso (did converge on Nitrenium Ion)

```
 %chk=tertbutyl-s-dft.chk
 ------------------------------------------------------
# opt freq=noraman 6-311g(d,p) geom=connectivity m062x
 ------------------------------------------------------
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.621976	-0.693109	-0.003172
2	1	0	0.540859	-1.706482	0.001422
3	6	0	-0.473339	-0.011972	0.004812
4	6	0	1.986000	-0.145720	0.001250
5	6	0	-1.781846	-0.712920	0.000089
6	6	0	-0.432976	1.476118	0.003754
7	1	0	2.265966	0.133276	1.018080
8	1	0	2.662081	-0.913794	-0.364875

9	1	0	2.035552	0.722119	-0.653121
10	1	0	-2.329863	-0.437012	0.905942
11	1	0	-2.372212	-0.350322	-0.846407
12	1	0	-1.688282	-1.796706	-0.055200
13	1	0	-0.130103	1.825002	-0.990273
14	1	0	-1.416917	1.885105	0.222025
15	1	0	0.292053	1.857543	0.725183

6T

%chk=tertbutyl-t-dft.chk

---

opt freq 6-311g(d,p) geom=connectivity um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.327000	-0.000337	1.396984
2	1	0	1.110414	-0.001140	2.061304
3	6	0	-0.013737	0.000010	0.055014
4	6	0	0.611610	1.291721	-0.566999
5	6	0	0.608535	-1.293204	-0.566918
6	6	0	-1.557058	0.001833	-0.088149
7	1	0	0.177541	2.185084	-0.120660
8	1	0	1.695767	1.298273	-0.457774
9	1	0	0.357921	1.256864	-1.628772
10	1	0	0.172440	-2.185495	-0.120404
11	1	0	0.354809	-1.257892	-1.628666
12	1	0	1.692684	-1.302260	-0.457816
13	1	0	-1.775973	0.002132	-1.156336
14	1	0	-1.986388	-0.890204	0.366238
15	1	0	-1.984313	0.894834	0.366299

7s-iso (did not converge on nitrenium)

%chk=DitBunitrenium-s-dft.chk

---

opt freq=noraman 6-311g(d,p) guess=read geom=connectivity m062x

---

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	0.266528	0.475561	-0.009143
2	6	0	1.381537	-0.182437	0.012491
3	6	0	-1.142457	-0.145958	0.010282
4	6	0	-1.528196	-0.481229	-1.430235
5	1	0	-0.859095	-1.215323	-1.880644
6	1	0	-2.536930	-0.898057	-1.434807
7	1	0	-1.534417	0.412993	-2.057464
8	6	0	-2.123823	0.886167	0.588901
9	1	0	-3.101974	0.408147	0.633915
10	1	0	-1.851350	1.173142	1.606862
11	1	0	-2.238283	1.779146	-0.022123
12	6	0	0.297709	1.949006	-0.132176
13	1	0	-0.427103	2.234825	-0.890774
14	1	0	0.034961	2.418010	0.815118
15	1	0	1.273806	2.283902	-0.460022
16	6	0	2.695795	0.523257	0.180540
17	1	0	3.425096	-0.183183	0.574830
18	1	0	3.065047	0.858987	-0.794847
19	1	0	2.635965	1.380238	0.848201
20	6	0	1.501102	-1.663664	-0.156141
21	1	0	1.555028	-2.147964	0.823738
22	1	0	0.698921	-2.107913	-0.732599
23	1	0	2.449126	-1.858703	-0.659412
24	6	0	-1.199953	-1.364203	0.944774
25	1	0	-0.843380	-2.288015	0.500095
26	1	0	-0.657426	-1.174515	1.873841
27	1	0	-2.243953	-1.530271	1.209482

7T

%chk=DitBunitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.000001	0.000157	0.405912

2	6	0	1.381839	0.000047	0.055235
3	6	0	-1.381854	-0.000063	0.055242
4	6	0	-1.767427	1.436624	-0.359969
5	1	0	-1.238401	1.743881	-1.261873
6	1	0	-2.839473	1.437941	-0.565030
7	1	0	-1.567010	2.143847	0.445292
8	6	0	-2.171216	-0.445332	1.302603
9	1	0	-3.229380	-0.460254	1.037543
10	1	0	-1.874209	-1.445840	1.617625
11	1	0	-2.025752	0.255153	2.125061
12	6	0	1.573505	1.002378	-1.105615
13	1	0	1.003775	0.707667	-1.987587
14	1	0	1.296610	2.012612	-0.803439
15	1	0	2.635084	0.992626	-1.360789
16	6	0	2.171491	0.442115	1.303565
17	1	0	2.025800	-0.260200	2.124419
18	1	0	3.229635	0.457220	1.038444
19	1	0	1.874874	1.442009	1.620895
20	6	0	1.766597	-1.435941	-0.363100
21	1	0	2.838759	-1.437465	-0.567584
22	1	0	1.565363	-2.144881	0.440453
23	1	0	1.237931	-1.740830	-1.266002
24	6	0	-1.572946	-0.999943	-1.107787
25	1	0	-1.003196	-0.703196	-1.989062
26	1	0	-1.295839	-2.010743	-0.807723
27	1	0	-2.634500	-0.989962	-1.363073

8s-iso (did not converge on nitrenium)

%chk=azidinylnitrenium-s-dft.chk

---

opt freq 6-311g(d,p) nosymm geom=connectivity m062x

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.002161674	0.001326153	-0.002433167
2	6	-0.006407238	0.005211826	-0.004242984
3	1	0.000106789	0.000469271	-0.000130697
4	1	0.001611065	0.000639353	0.000803419

5	1	-0.000420079	-0.001182895	0.000515997
6	1	-0.003220871	0.000476859	0.000974039
7	7	0.010492009	-0.006940567	0.004513393

%chk=azidinylnitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.861203	0.273481	0.000000
2	6	0	0.861208	0.273480	0.000000
3	1	0	-1.313844	0.578104	0.944146
4	1	0	-1.313844	0.578104	-0.944146
5	1	0	1.313830	0.578114	0.944165
6	1	0	1.313830	0.578114	-0.944165
7	7	0	0.000000	-0.799172	0.000000

9S-iso (did not converge on nitrenium)

%chk=azetidinylnitrenium-s-dft.chk

---

opt=rcfc freq 6-311g(d,p) nosymm geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.050824	-1.171818	-0.205712
2	6	0	-0.922596	0.051711	0.205443
3	6	0	1.079251	-0.193135	-0.172339
4	1	0	0.028310	-1.971482	0.531978
5	1	0	-0.250691	-1.594145	-1.191365
6	1	0	-1.354535	0.025497	1.203761
7	1	0	-1.634463	0.410873	-0.534969
8	1	0	0.598410	1.784878	0.345714
9	1	0	2.151024	-0.208021	-0.349001
10	7	0	0.356106	0.810549	0.167183

9T

%chk=azetidinylnitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000011	-0.986205	-0.000103
2	6	0	-1.129050	0.107158	-0.000164
3	6	0	1.129047	0.107167	0.000173
4	1	0	-0.000128	-1.566728	0.919674
5	1	0	0.000145	-1.566538	-0.920002
6	1	0	-1.740603	0.198696	0.901730
7	1	0	-1.740326	0.198904	-0.902223
8	1	0	1.740319	0.198722	0.902257
9	1	0	1.740604	0.198931	-0.901693
10	7	0	-0.000008	0.995614	0.000117

10S-iso (does not converge on nitrenium)

%chk=pyrollidinylnitrenium-s-dft.chk

---

opt freq 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.798352	-0.969190	-0.102405
2	6	0	0.041725	1.222143	0.042310
3	6	0	-1.204703	0.427762	-0.094751
4	6	0	-0.721199	-1.022377	0.129001
5	1	0	1.102874	-1.263908	-1.108425
6	1	0	1.383244	-1.526091	0.627521
7	1	0	2.029920	0.851981	0.095417
8	1	0	0.123808	2.303053	0.107410
9	1	0	-1.971250	0.764019	0.605300
10	1	0	-1.600328	0.605220	-1.103085
11	1	0	-0.932160	-1.328777	1.152949
12	1	0	-1.204021	-1.726663	-0.543814

13	7	0	1.083266	0.481592	0.045971

10-T

%chk=pyrollidinylnitrenium-t-dft.chk

---

opt freq 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.243386	-0.485452	-0.122598
2	6	0	1.243571	-0.485143	0.122527
3	6	0	0.740668	0.950682	-0.221175
4	6	0	-0.741039	0.950418	0.221198
5	1	0	-1.594097	-0.588084	-1.159399
6	1	0	-1.988897	-0.910695	0.554081
7	1	0	1.594565	-0.587603	1.159267
8	1	0	1.989093	-0.910070	-0.554329
9	1	0	1.339017	1.698222	0.296187
10	1	0	0.827170	1.098169	-1.297998
11	1	0	-0.827548	1.097948	1.298011
12	1	0	-1.339616	1.697823	-0.296123
13	7	0	0.000204	-1.168392	0.000084

11-iso (did not converge on nitrenium)

%chk=TMPnitrenium-s-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.251243	-0.263783	-0.150925
2	6	0	-1.251512	-0.263930	-0.150857

3	6	0	-1.251242	1.241274	-0.326651
4	6	0	-0.000286	1.862847	0.260173
5	6	0	1.251617	1.241232	-0.324443
6	1	0	-1.313794	1.489063	-1.418912
7	1	0	-2.156146	1.677805	0.170371
8	1	0	-0.000151	2.965869	0.060454
9	1	0	-0.001310	1.721915	1.373100
10	1	0	1.317010	1.490621	-1.416173
11	1	0	2.155651	1.676574	0.175353
12	7	0	-0.000069	-0.885287	-0.737010
13	6	0	-2.494479	-0.863302	-0.834512
14	1	0	-2.506682	-1.922976	-0.686719
15	1	0	-3.377401	-0.433690	-0.409327
16	1	0	-2.462974	-0.649686	-1.882499
17	6	0	2.494034	-0.862404	-0.835559
18	1	0	3.377123	-0.434957	-0.408542
19	1	0	2.505059	-1.922522	-0.690893
20	1	0	2.463418	-0.645657	-1.882929
21	6	0	1.338696	-0.606095	1.348000
22	1	0	1.256936	-1.665094	1.477365
23	1	0	2.277714	-0.270795	1.736227
24	1	0	0.542202	-0.120235	1.871868
25	6	0	-1.338259	-0.604203	1.348573
26	1	0	-2.365546	-0.674475	1.639510
27	1	0	-0.851170	-1.539305	1.530863
28	1	0	-0.858334	0.164747	1.917157

Rotational constants (GHZ): 1.9577184 1.1327178 1.0171450

11T

%chk=TMPnitrenium-t-dft.chk

---

opt freq 6-311g(d,p) geom=connectivity um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.251243	-0.263783	-0.150925
2	6	0	-1.251512	-0.263930	-0.150857
3	6	0	-1.251242	1.241274	-0.326651
4	6	0	-0.000286	1.862847	0.260173

5	6	0	1.251617	1.241232	-0.324443
6	1	0	-1.313794	1.489063	-1.418912
7	1	0	-2.156146	1.677805	0.170371
8	1	0	-0.000151	2.965869	0.060455
9	1	0	-0.001310	1.721915	1.373100
10	1	0	1.317010	1.490621	-1.416173
11	1	0	2.155651	1.676574	0.175354
12	7	0	-0.000069	-0.885287	-0.737010
13	6	0	-2.494479	-0.863302	-0.834512
14	1	0	-2.506681	-1.922976	-0.686719
15	1	0	-3.377401	-0.433691	-0.409328
16	1	0	-2.462974	-0.649686	-1.882499
17	6	0	2.494034	-0.862404	-0.835559
18	1	0	3.377123	-0.434957	-0.408542
19	1	0	2.505059	-1.922522	-0.690893
20	1	0	2.463418	-0.645657	-1.882929
21	6	0	1.338696	-0.606095	1.348000
22	1	0	1.256936	-1.665094	1.477365
23	1	0	2.277714	-0.270796	1.736228
24	1	0	0.542202	-0.120235	1.871868
25	6	0	-1.338259	-0.604204	1.348573
26	1	0	-2.365546	-0.674476	1.639511
27	1	0	-0.851170	-1.539306	1.530862
28	1	0	-0.858334	0.164746	1.917157

12S-iso (did not converge on nitrenuim)

chk=bicyclohex-s-DFT.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.581624	0.127937	-0.020517
2	6	0	0.534508	1.199139	0.036352
3	6	0	-0.618057	-0.729703	-0.390124
4	6	0	0.709991	-1.141902	0.236592
5	1	0	2.053246	0.115383	-1.011368
6	1	0	2.371353	0.303512	0.711244
7	1	0	1.122953	-2.035100	-0.225869

8	1	0	0.606823	-1.325024	1.308222
9	6	0	-1.738674	-0.025346	0.315093
10	1	0	-2.685757	0.080845	-0.199401
11	1	0	-1.756892	0.044351	1.396834
12	1	0	0.656263	2.230374	0.359686
13	1	0	-0.864348	-1.091869	-1.384559
14	7	0	-0.617141	0.728111	-0.288452

12T

%chk=bicyclohex-t-DFT.chk

---

opt=calcfc freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.122669	0.785723	0.118265
2	6	0	-0.382706	1.061802	-0.106841
3	6	0	-0.382689	-1.061785	-0.107059
4	6	0	1.122644	-0.785735	0.118372
5	1	0	1.731577	1.205994	-0.679592
6	1	0	1.430860	1.228421	1.066385
7	1	0	1.731777	-1.206161	-0.679222
8	1	0	1.430522	-1.228257	1.066677
9	6	0	-1.079132	-0.000099	0.802584
10	1	0	-2.162757	-0.000085	0.748398
11	1	0	-0.670444	-0.000200	1.820480
12	1	0	-0.766194	2.060976	-0.281391
13	1	0	-0.765987	-2.060940	-0.282105
14	7	0	-0.623439	0.000117	-1.104508

13S-iso (did not converge on nitrenuim)

****

%chk=bicyclohept-s-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.448521	-0.483098	0.265216
2	6	0	0.698344	-1.115845	0.395639
3	6	0	0.418241	1.081227	-0.100764
4	6	0	-0.947184	0.950728	0.636311
5	1	0	-2.284225	-0.508661	-0.429170
6	1	0	-1.654269	-1.134497	1.112769
7	1	0	-1.641451	1.699505	0.256014
8	1	0	-0.855642	1.086379	1.714277
9	6	0	1.486496	0.129847	0.558740
10	1	0	2.420078	0.163263	-0.016679
11	1	0	1.734563	0.281247	1.611577
12	6	0	0.148076	0.219016	-1.329716
13	1	0	1.015131	0.006056	-1.953740
14	1	0	-0.695257	0.524179	-1.946556
15	1	0	0.614902	-1.918582	1.126599
16	1	0	0.762736	2.100710	-0.251340
17	7	0	-0.221326	-0.998693	-0.539474

13T

%chk=bicyclohept-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.427767	-0.262060	-0.528849
2	6	0	-0.308426	-1.182506	0.055115
3	6	0	0.407231	0.921564	0.533355
4	6	0	-0.932455	1.163283	-0.175028
5	1	0	-1.579182	-0.428341	-1.594130
6	1	0	-2.349154	-0.532382	-0.008751
7	1	0	-0.837023	1.810154	-1.046457
8	1	0	-1.617912	1.646838	0.523856
9	6	0	0.145301	-0.379784	1.319601
10	1	0	1.024079	-0.810827	1.797982
11	1	0	-0.676055	-0.301564	2.032963

12	6	0	1.432963	0.401795	-0.562226
13	1	0	2.448304	0.307819	-0.155818
14	1	0	1.450257	0.965646	-1.499059
15	1	0	-0.523839	-2.245404	0.128890
16	1	0	0.827555	1.763589	1.079822
17	7	0	0.847412	-0.878469	-0.730158

14iso (did not converge on nitrenium)

%chk=gassman-s-dft.chk

opt freq 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.112104	-0.514104	-0.364337
2	6	0	0.193162	-1.410230	0.400273
3	6	0	0.043110	0.822370	-0.057655
4	6	0	1.231348	0.580941	-1.047224
5	1	0	3.074234	-0.162440	-0.001141
6	1	0	2.247959	-1.425433	-0.944973
7	1	0	1.798951	1.507689	-1.137543
8	1	0	0.906198	0.291975	-2.045945
9	6	0	-0.899765	-0.478985	-0.009828
10	6	0	0.788716	0.578119	1.254627
11	1	0	0.182595	0.541037	2.156109
12	1	0	1.651003	1.223714	1.418641
13	1	0	0.305949	-2.427295	0.023578
14	7	0	1.248671	-0.793038	0.888317
15	6	0	-2.100647	-0.312167	0.941880
16	1	0	-2.830039	0.340480	0.460248
17	1	0	-2.575855	-1.278891	1.111220
18	1	0	-1.836247	0.116003	1.907023
19	6	0	-1.417042	-0.963832	-1.374762
20	1	0	-2.122581	-1.786353	-1.248888
21	1	0	-1.944275	-0.136359	-1.856009
22	1	0	-0.623547	-1.291486	-2.048822
23	6	0	-0.682451	2.133233	-0.255974
24	1	0	0.023274	2.965397	-0.217713
25	1	0	-1.173408	2.164853	-1.231615
26	1	0	-1.436110	2.296305	0.515615

14T

%chk=gassman-t-dft.chk

---

opt freq 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.632108	-0.961624	-0.617357
2	6	0	0.600653	-1.236835	0.519083
3	6	0	0.037704	0.849193	-0.226139
4	6	0	1.228255	0.445379	-1.116731
5	1	0	2.655529	-1.022157	-0.250499
6	1	0	1.501886	-1.739603	-1.371115
7	1	0	2.041757	1.168776	-1.054343
8	1	0	0.904961	0.416728	-2.158692
9	6	0	-0.718883	-0.504647	0.001982
10	6	0	0.693065	1.069241	1.227876
11	1	0	-0.019169	1.508406	1.934829
12	1	0	1.615591	1.657505	1.213348
13	1	0	0.515623	-2.258972	0.883329
14	7	0	0.937732	-0.287541	1.519165
15	6	0	-1.826895	-0.471231	1.051378
16	1	0	-2.641185	0.167385	0.701487
17	1	0	-2.237547	-1.473190	1.189258
18	1	0	-1.511527	-0.110159	2.031059
19	6	0	-1.259770	-1.148828	-1.271244
20	1	0	-1.602597	-2.164077	-1.062054
21	1	0	-2.129737	-0.579742	-1.609774
22	1	0	-0.546330	-1.190141	-2.092130
23	6	0	-0.757700	2.052745	-0.668716
24	1	0	-0.118834	2.932891	-0.767839
25	1	0	-1.198335	1.854610	-1.650127
26	1	0	-1.565433	2.284169	0.028320

15S

%chk=cyclopropylnitrenium-s-CBSAPNO.chk

---

cbs-apno geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.440073	0.000119	-0.362793
2	1	0	-2.377766	0.000087	0.056624
3	6	0	-0.522748	-0.000172	0.506086
4	6	0	0.992649	-0.696166	-0.127720
5	6	0	0.992716	0.696228	-0.127489
6	1	0	-0.563354	-0.000407	1.595014
7	1	0	0.735847	-1.245712	-1.028841
8	1	0	1.387108	-1.254796	0.719709
9	1	0	1.387112	1.254551	0.720172
10	1	0	0.735865	1.246109	-1.028393

15T

%chk=cyclopropylnitrenium-t-CBSAPNO.chk

---

cbs-apno geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.503663	-0.087752	-0.191351
2	1	0	-2.207811	0.602673	-0.466463
3	6	0	-0.354007	-0.081910	0.483216
4	6	0	0.934537	-0.691060	-0.200547
5	6	0	0.890026	0.771055	-0.088693
6	1	0	-0.441634	-0.203933	1.565421
7	1	0	0.748481	-1.140604	-1.171661
8	1	0	1.533016	-1.265164	0.501051
9	1	0	1.415043	1.274587	0.719047
10	1	0	0.655213	1.358201	-0.971789

16S

%chk=methylcyclopropylnitrenium-s-dft.chk

---

opt freq 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.797981	-0.000442	-0.398086
2	6	0	0.127607	0.002748	0.470077
3	6	0	1.565690	-0.699838	-0.112924
4	6	0	1.566427	0.698054	-0.115688
5	1	0	0.019815	0.005377	1.553970
6	1	0	1.352822	-1.247584	-1.022003
7	1	0	1.967196	-1.252664	0.730843
8	1	0	1.970187	1.253560	0.725219
9	1	0	1.355259	1.242168	-1.027341
10	6	0	-2.172251	-0.000252	0.025173
11	1	0	-2.644312	-0.874093	-0.436666
12	1	0	-2.312981	0.004243	1.107339
13	1	0	-2.646949	0.867818	-0.444589

16T

%chk=methylcyclopropylnitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) nosymm geom=connectivity um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.506713	0.004889	-0.182699
2	6	0	-0.336322	0.079256	0.465333
3	6	0	0.858477	-0.767016	-0.065143
4	6	0	0.903927	0.682041	-0.282551
5	1	0	-0.415221	0.207613	1.544812
6	1	0	0.620924	-1.407291	-0.905046
7	1	0	1.445583	-1.209215	0.729598
8	1	0	1.508220	1.306899	0.364203
9	1	0	0.700942	1.065004	-1.274802
10	6	0	-2.570874	0.773745	-0.714572
11	1	0	-2.171804	1.500331	-1.433116
12	1	0	-3.293994	0.112889	-1.193909
13	1	0	-3.053315	1.310958	0.114504

16S-ts (ring expansion)

%chk=methylcyclopropylnitreniumringTS-s-dft.chk

---

opt=(calcfc,qst2) freq=noraman 6-311g(d,p) geom=connectivity m062x

---

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.660617	-0.013314	-0.445852
2	6	0	0.244146	-0.646810	0.245136
3	6	0	1.656189	-0.380930	-0.205730
4	6	0	1.049523	0.905239	0.183344
5	1	0	1.839912	-0.503283	-1.266455
6	1	0	2.394495	-0.804409	0.465774
7	1	0	1.048779	1.230697	1.219697
8	1	0	0.813318	1.643674	-0.571795
9	1	0	0.041072	-1.107662	1.215750
10	6	0	-2.015950	0.034534	0.055324
11	1	0	-2.614026	-0.525570	-0.672298
12	1	0	-2.135673	-0.379284	1.058811
13	1	0	-2.367004	1.066836	0.003035

17S

%chk=tbutylcyclopropylnitrenium-s-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.245422	0.000192	-0.404066
2	6	0	-1.193590	-0.001115	0.446261
3	6	0	-2.604687	0.700389	-0.173651
4	6	0	-2.604987	-0.699718	-0.175075

5	1	0	-1.124247	-0.002325	1.530812
6	1	0	-2.371574	1.246587	-1.077930
7	1	0	-3.039489	1.251918	0.653503
8	1	0	-3.040528	-1.252654	0.650747
9	1	0	-2.372486	-1.244107	-1.080602
10	6	0	1.153822	-0.000008	-0.003873
11	6	0	1.397113	-0.002315	1.499963
12	1	0	0.985635	-0.895718	1.977406
13	1	0	2.471658	-0.001756	1.684455
14	1	0	0.984166	0.888796	1.980408
15	6	0	1.744858	-1.257528	-0.675486
16	1	0	1.560356	-1.246923	-1.749392
17	1	0	2.821790	-1.257892	-0.499158
18	1	0	1.322404	-2.166472	-0.243912
19	6	0	1.743976	1.260057	-0.671510
20	1	0	2.820850	1.260836	-0.494827
21	1	0	1.559824	1.252491	-1.745498
22	1	0	1.320565	2.167309	-0.237330

17T

%chk=tbutylcyclopropylnitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.172851	-0.510634	-0.085088
2	6	0	1.387046	-0.377999	0.482985
3	6	0	2.640053	-0.590171	-0.404200
4	6	0	2.321300	0.781679	0.012865
5	1	0	1.446693	-0.715378	1.517367
6	1	0	2.431740	-0.878343	-1.426351
7	1	0	3.433418	-1.129805	0.096210
8	1	0	2.870581	1.236420	0.828072
9	1	0	1.889584	1.455569	-0.715463
10	6	0	-1.172415	-0.004019	-0.040229
11	6	0	-1.612082	-0.126431	1.439207
12	1	0	-2.638279	0.241932	1.497241
13	1	0	-1.594558	-1.165415	1.769434

14	1	0	-0.983721	0.484654	2.088844
15	6	0	-2.051050	-0.860560	-0.957014
16	1	0	-3.074090	-0.487255	-0.899516
17	1	0	-1.714464	-0.792574	-1.991927
18	1	0	-2.041751	-1.904516	-0.642734
19	6	0	-1.140823	1.469245	-0.489550
20	1	0	-0.519691	2.071638	0.174965
21	1	0	-0.784067	1.558640	-1.516591
22	1	0	-2.163529	1.848408	-0.448324

18S

%chk=cyclobutylnitrenium-s-dft.chk

---

opt=rcfc freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.211224	0.847023	0.184785
2	6	0	-1.109424	-0.299557	0.328473
3	6	0	0.135907	-0.237300	-0.536516
4	6	0	1.783543	-0.423755	0.152747
5	1	0	1.504758	1.593349	-0.542443
6	1	0	0.757228	1.209835	1.099718
7	1	0	-1.007126	-0.788355	1.303854
8	1	0	-0.011350	0.223219	-1.513444
9	1	0	0.432621	-1.279468	-0.780804
10	1	0	2.464797	-0.709831	-0.641907
11	1	0	1.696756	-1.094677	1.001975
12	7	0	-2.143964	0.202185	-0.164346
13	1	0	-2.957435	0.112162	0.446542

18T

%chk=cyclobutylnitrenium-t-dft.chk

---

opt=calcfc freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.420184	-1.111475	-0.086601
2	6	0	0.616565	0.000231	0.446870
3	6	0	-0.420052	1.111452	-0.086702
4	6	0	-1.485197	-0.000034	-0.067592
5	1	0	-0.148638	-1.433469	-1.090715
6	1	0	-0.512557	-1.957066	0.590279
7	1	0	0.655259	-0.000164	1.543207
8	1	0	-0.148474	1.433205	-1.090879
9	1	0	-0.512971	1.957174	0.589942
10	1	0	-2.166618	-0.000069	-0.915980
11	1	0	-2.042297	-0.000001	0.868194
12	7	0	1.834887	0.000014	-0.101315
13	1	0	2.285295	-0.000757	-1.020696

19S

%chk=Vinylnitrenium-s-CBSAPNO.chk

---

cbs-apno geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.088691	-0.363713	-0.000180
2	6	0	-0.092268	0.477668	-0.000032
3	6	0	1.173144	-0.181899	0.000212
4	1	0	-0.164676	1.565666	-0.000075
5	1	0	2.120277	0.362348	0.000368
6	1	0	1.178780	-1.274344	0.000232
7	1	0	-1.998798	0.117710	-0.000346

19T

%chk=Vinylnitrenium-t-CBSAPNO.chk

---

cbs-apno geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.155415	-0.255016	-0.000210
2	6	0	-0.056132	0.410093	-0.000026
3	6	0	1.224295	-0.189860	0.000227
4	1	0	-0.174816	1.504559	-0.000111
5	1	0	2.100089	0.449208	0.000359
6	1	0	1.329005	-1.270279	0.000305
7	1	0	-2.175350	-0.219777	-0.000290

20S

%chk=Vinylmethylnitrenium-s-dft .chk

---

opt freq 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.406884	-0.424363	0.000384
2	6	0	-1.736061	0.044366	-0.000215
3	1	0	-2.233403	-0.442041	-0.856701
4	1	0	-2.234778	-0.441356	0.855646
5	1	0	-1.866759	1.127058	-0.000693
6	6	0	0.580281	0.441705	0.000338
7	6	0	1.838061	-0.151287	-0.000182
8	1	0	0.438117	1.521961	0.000433
9	1	0	2.754927	0.433165	-0.001228
10	1	0	1.896392	-1.236949	0.000211

20T

%chk=Vinylmethylnitrenium-t-dft .chk

---

opt freq 6-311g(d,p) geom=connectivity um062x

1	7	0	-0.453850	-0.141876	-0.000314
2	6	0	-1.865812	-0.080899	-0.000038
3	1	0	-2.254021	-0.553626	-0.905080
4	1	0	-2.253560	-0.565840	0.898917
5	1	0	-2.147222	0.983752	0.008409

6	6	0	0.694054	0.439595	-0.000174
7	6	0	1.905835	-0.254189	0.000094
8	1	0	0.668598	1.535706	-0.000158
9	1	0	2.832502	0.301964	0.000553
10	1	0	1.926191	-1.335869	0.000268

20S-ts

%chk=VinylmethylnitreniumTS-s-dft .chk

---

opt=qst2 freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.024997	-0.516253	-0.032354
2	6	0	1.187721	0.178173	-0.040747
3	1	0	2.049060	-0.384307	-0.407400
4	1	0	1.175710	1.266767	-0.138217
5	6	0	-1.187386	0.164868	0.023041
6	1	0	-1.149719	1.248118	0.152222
7	1	0	-1.543797	-0.091764	-1.009995
8	1	0	-1.907688	-0.375365	0.646608
9	1	0	1.199439	-0.107927	1.089501

21S

****

%chk=Vinyltbutylnitrenium-s-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.570921	-0.447829	-0.154597
2	6	0	0.749070	0.015315	-0.064808
3	6	0	-1.608957	0.369043	-0.008277
4	6	0	-2.828326	-0.260202	-0.119137
5	1	0	-1.520164	1.442353	0.137636
6	1	0	-3.765601	0.287856	-0.083797
7	1	0	-2.848502	-1.336182	-0.265180
8	6	0	0.992973	1.517683	-0.125044
9	1	0	0.521081	2.055751	0.699340
10	1	0	2.065402	1.703743	-0.065417
11	1	0	0.636797	1.927884	-1.073680
12	6	0	1.629348	-0.789614	-1.035452
13	1	0	2.677662	-0.615635	-0.791585
14	1	0	1.411058	-1.854606	-0.966144
15	1	0	1.446367	-0.452978	-2.057142
16	6	0	1.052325	-0.536522	1.414312
17	1	0	0.915553	-1.613629	1.466753
18	1	0	2.103600	-0.278026	1.560519
19	1	0	0.434597	-0.025946	2.151306

21T

%chk=Vinyltbutylnitrenium-t-dft .chk

---

opt freq 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.593297	-0.185245	-0.000263
2	6	0	0.834012	-0.046113	0.000141
3	6	0	-1.751210	0.381849	-0.000327
4	6	0	-2.951226	-0.330121	-0.000546
5	1	0	-1.745920	1.477392	-0.000245
6	1	0	-3.888262	0.207821	-0.000621
7	1	0	-2.952937	-1.411657	-0.000651
8	6	0	1.084449	1.488373	0.000292
9	1	0	0.675253	1.955059	0.897155
10	1	0	2.168129	1.618779	0.000537
11	1	0	0.675642	1.955161	-0.896695
12	6	0	1.390374	-0.696259	-1.273270
13	1	0	2.471548	-0.551906	-1.282205

14	1	0	1.184651	-1.766826	-1.281643
15	1	0	0.967557	-0.237960	-2.167825
16	6	0	1.389655	-0.696390	1.273803
17	1	0	1.183815	-1.766936	1.282014
18	1	0	2.470841	-0.552152	1.283292
19	1	0	0.966436	-0.238091	2.168168

21S-ts

%chk=VinyltbutylnitreniumTS-s-dft.chk

opt=qst3 freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.477859	-0.393696	-0.287418
2	6	0	0.787120	0.068673	-0.146262
3	6	0	-1.576121	0.393715	-0.033218
4	6	0	-2.766991	-0.177722	-0.297309
5	1	0	-1.477797	1.426122	0.287028
6	1	0	-3.691040	0.383741	-0.220697
7	1	0	-2.807773	-1.212435	-0.619713
8	6	0	0.571817	-0.789445	1.365330
9	6	0	1.829916	-0.712586	-0.915787
10	1	0	-0.167289	-0.333608	2.015254
11	1	0	1.587826	-0.532770	1.681470
12	1	0	0.451765	-1.857735	1.229503
13	1	0	1.526115	-1.749900	-1.049199
14	1	0	2.798288	-0.662497	-0.417206
15	1	0	1.931215	-0.250614	-1.901228
16	6	0	1.094750	1.526696	0.114392
17	1	0	0.525979	1.945276	0.944650
18	1	0	2.156574	1.644871	0.328620
19	1	0	0.868202	2.099437	-0.789432

22S

%chk=phenylnitrenium.chk

ccsd=(t,saveamplitudes)/cc-pvtz guess=save geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.096175	2.292100	0.000000
2	6	0	0.000000	1.012322	0.000000
3	6	0	-1.261421	0.271627	0.000000
4	6	0	1.261443	0.270716	0.000000
5	6	0	-1.252345	-1.093271	0.000000
6	1	0	-2.171811	0.861434	0.000000
7	6	0	1.239398	-1.088516	0.000000
8	1	0	2.192700	0.828585	0.000000
9	6	0	-0.011104	-1.758105	0.000000
10	1	0	-2.171313	-1.664786	0.000000
11	1	0	2.153742	-1.667703	0.000000
12	1	0	-0.008005	-2.844472	0.000000
13	1	0	0.822084	2.753593	0.000000

22T

%chk=phenylnitrenium-t-ccsd .chk

# uccsd=(t,readamplitudes,saveamplitudes)/cc-pvtz guess=(read,save) ge
om=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.030205	2.300272	0.000000
2	6	0	0.016144	0.981733	0.000000
3	6	0	-0.014507	0.273341	1.250860
4	6	0	-0.014507	0.273341	-1.250860
5	6	0	-0.014507	-1.093549	1.229393
6	1	0	-0.026874	0.838412	2.174171
7	6	0	-0.014507	-1.093549	-1.229393
8	1	0	-0.026874	0.838412	-2.174171
9	6	0	-0.014876	-1.784264	0.000000
10	1	0	-0.020961	-1.648860	2.158733
11	1	0	-0.020961	-1.648860	-2.158733
12	1	0	-0.022647	-2.867592	0.000000

13	1	0	0.670312	3.044267	0.000000

23S

%chk=phenylmethylnitrenium-s-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.733504	-0.637694	-0.000048
2	6	0	0.495967	-0.240249	-0.000343
3	6	0	-0.474169	-1.319160	-0.000240
4	6	0	0.021904	1.132466	-0.000399
5	6	0	-1.817549	-1.049809	0.000109
6	1	0	-0.075775	-2.327520	-0.000349
7	6	0	-1.319540	1.373678	0.000004
8	1	0	0.723974	1.955544	-0.000748
9	6	0	-2.229574	0.289605	0.000330
10	1	0	-2.550029	-1.846233	0.000269
11	1	0	-1.700761	2.386626	0.000045
12	1	0	-3.292772	0.509732	0.000755
13	6	0	2.852429	0.240792	0.000351
14	1	0	3.464881	-0.044755	0.865597
15	1	0	3.465704	-0.045026	-0.864221
16	1	0	2.653442	1.311548	0.000120

23T

%chk=phenylmethylnitrenium-t-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.736750	0.398863	0.019455
2	6	0	-0.444736	0.198796	0.009419
3	6	0	0.061579	-1.145907	0.009049

4	6	0	0.450272	1.316849	0.003212
5	6	0	1.419090	-1.333312	-0.000738
6	1	0	-0.631839	-1.977272	0.014334
7	6	0	1.800661	1.081060	-0.005674
8	1	0	0.039563	2.318002	0.005208
9	6	0	2.293540	-0.233468	-0.007816
10	1	0	1.817349	-2.340201	-0.002757
11	1	0	2.489369	1.916071	-0.011197
12	1	0	3.362834	-0.403673	-0.014718
13	6	0	-3.042056	-0.139582	-0.019053
14	1	0	-3.167739	-0.849983	0.806274
15	1	0	-3.752778	0.681465	0.128481
16	1	0	-3.229613	-0.603070	-0.992208

23S-ts

%chk=phenylmethylnitreniumTS-s-dft .chk

---

opt=(calcfc,qst2) freq 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.812320	-0.558323	-0.120688
2	6	0	-0.476315	-0.204687	-0.037431
3	6	0	0.411502	-1.295215	-0.021038
4	6	0	-0.000096	1.122954	-0.034149
5	6	0	1.774684	-1.063416	0.022539
6	1	0	0.002064	-2.298057	-0.045106
7	6	0	1.360094	1.337078	-0.000922
8	1	0	-0.672777	1.970682	-0.080679
9	6	0	2.242689	0.247792	0.034039
10	1	0	2.468954	-1.893069	0.039244
11	1	0	1.749556	2.346752	-0.009354
12	1	0	3.309966	0.433983	0.060755
13	6	0	-2.834724	0.294381	0.022714
14	1	0	-3.824384	-0.114844	-0.170737
15	1	0	-2.502499	-0.537750	0.965047
16	1	0	-2.711644	1.367241	0.171132

24S

%chk=phenyltertbutylnitrenium-s-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.674256	0.685375	-0.000278
2	6	0	0.559302	0.255996	-0.000216
3	6	0	1.522076	1.341813	-0.000155
4	6	0	1.063810	-1.105977	-0.000105
5	6	0	2.871321	1.099419	0.000050
6	1	0	1.110845	2.344432	-0.000255
7	6	0	2.413223	-1.320605	-0.000010
8	1	0	0.388920	-1.945590	-0.000173
9	6	0	3.308567	-0.229901	0.000073
10	1	0	3.586373	1.911432	0.000158
11	1	0	2.805923	-2.329171	0.000008
12	1	0	4.374636	-0.433930	0.000184
13	6	0	-1.919594	-0.014843	-0.000002
14	6	0	-2.646773	0.543530	-1.256276
15	6	0	-1.956184	-1.539351	-0.000111
16	6	0	-2.645952	0.543313	1.256815
17	1	0	-2.668454	1.631817	-1.238246
18	1	0	-2.151486	0.204499	-2.167209
19	1	0	-3.667963	0.158964	-1.243355
20	1	0	-1.495702	-1.961517	0.895988
21	1	0	-3.001340	-1.852088	-0.000043
22	1	0	-1.495837	-1.961350	-0.896358
23	1	0	-3.667105	0.158632	1.244557
24	1	0	-2.149998	0.204283	2.167393
25	1	0	-2.667791	1.631601	1.238914

24T

%chk=phenylterbutylnitrenium-t-dft .chk

---

opt freq 6-311g(d,p) geom=connectivity um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.699645	-0.000217	-0.584361
2	6	0	-0.597078	-0.000120	-0.318045
3	6	0	-1.297921	1.241876	-0.212990
4	6	0	-1.298117	-1.242006	-0.213004
5	6	0	-2.648024	1.222123	0.034882
6	1	0	-0.749551	2.168222	-0.327550
7	6	0	-2.648218	-1.222038	0.034865
8	1	0	-0.749886	-2.168433	-0.327573
9	6	0	-3.326648	0.000095	0.159804
10	1	0	-3.190822	2.153942	0.129503
11	1	0	-3.191160	-2.153774	0.129473
12	1	0	-4.392922	0.000183	0.349782
13	6	0	2.007709	-0.000017	0.027997
14	6	0	2.085714	1.270481	0.898938
15	6	0	2.085950	-1.270182	0.899392
16	6	0	3.070453	-0.000112	-1.070325
17	1	0	2.010386	2.170023	0.286533
18	1	0	1.305650	1.273929	1.662265
19	1	0	3.059516	1.270976	1.392235
20	1	0	2.011163	-2.169953	0.287261
21	1	0	3.059593	-1.270107	1.393004
22	1	0	1.305665	-1.273692	1.662494
23	1	0	4.056116	0.000089	-0.603129
24	1	0	2.983004	-0.888717	-1.696248
25	1	0	2.982809	0.888228	-1.696598

25S

%chk=methoxynitrenium-s-CBSAPNO.chk

---

cbs-apno geom=connectivity

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.184813	0.142662	0.000000
2	1	0	1.059481	1.224940	-0.000002
3	1	0	1.638736	-0.262045	0.905373
4	1	0	1.638738	-0.262049	-0.905370
5	8	0	-0.197065	-0.460140	0.000000
6	7	0	-1.125820	0.338750	0.000000
7	1	0	-1.988577	-0.246946	0.000000

25T

%chk=methoxynitrenium-t-CBSAPNO.chk

cbs-apno geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.210728	0.177064	-0.011264
2	1	0	1.344526	0.547424	1.004729
3	1	0	1.854763	-0.663392	-0.256770
4	1	0	1.186476	0.955758	-0.773241
5	8	0	-0.176686	-0.480925	-0.023685
6	7	0	-1.194193	0.218782	0.129909
7	1	0	-1.877292	0.413754	-0.627017

26S

%chk=Methoxymethylnitrenium-s-dft .chk

opt freq=noraman 6-311g(d,p) nosymm geom=connectivity m062x

1	7	0	-0.327972	0.689743	-0.405877
2	6	0	1.052347	0.660282	-0.047154
3	1	0	1.302023	-0.408200	0.030445
4	1	0	1.585162	1.003677	-0.946258
5	1	0	1.286217	1.233021	0.848023
6	8	0	-0.997821	1.360772	0.364573

7	6	0	-2.447956	1.450483	0.071751
8	1	0	-2.929872	1.054500	0.963333
9	1	0	-2.636651	2.515950	-0.042847
10	1	0	-2.639805	0.870252	-0.827050

26T

%chk=Methoxymethylnitrenium-t-dft .chk

---

opt freq=noraman 6-311g(d,p) nosymm geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.285026	0.629212	0.612435
2	6	0	1.022188	0.603571	-0.035370
3	1	0	1.450894	-0.377775	0.153100
4	1	0	0.879472	0.788012	-1.104564
5	1	0	1.620654	1.393578	0.433067
6	8	0	-1.091935	1.577013	0.662266
7	6	0	-2.394906	1.462026	-0.076231
8	1	0	-2.961451	0.679698	0.423463
9	1	0	-2.834112	2.445045	0.053736
10	1	0	-2.160106	1.230097	-1.112963

26S-ts

%chk=MethoxymethylnitreniumTS-s-dft.chk

---

opt=(calcfc,ts) freq=noraman 6-311g(d,p) geom=connectivity m062x

---

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.533230	-0.405965	-0.126174
2	6	0	1.761591	0.096601	-0.013444
3	1	0	1.144991	-0.676738	0.933912
4	1	0	2.566567	-0.608329	-0.209213
5	1	0	1.920093	1.165075	0.140378
6	8	0	-0.412338	0.475697	-0.000152
7	6	0	-1.748283	-0.120868	0.010647

8	1	0	-1.925154	-0.557629	0.992117
9	1	0	-2.411262	0.719160	-0.170965
10	1	0	-1.808983	-0.859754	-0.785011

27S

%chk=Methoxytbutylnitrenium-s-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.497620	-0.530246	0.011895
2	6	0	0.826203	0.029036	0.001182
3	8	0	-1.393311	0.312393	-0.000605
4	6	0	-2.773607	-0.209620	0.004708
5	1	0	-3.234543	0.226209	0.888162
6	1	0	-3.223160	0.176795	-0.907210
7	1	0	-2.718808	-1.294455	0.034680
8	6	0	0.885818	1.543921	-0.009897
9	1	0	1.933290	1.846072	-0.016475
10	1	0	0.405338	1.958294	-0.897975
11	1	0	0.413205	1.969830	0.877056
12	6	0	1.454845	-0.619958	-1.265394
13	1	0	2.512499	-0.351368	-1.251524
14	1	0	1.362297	-1.705356	-1.248306
15	1	0	0.999111	-0.221496	-2.171949
16	6	0	1.477450	-0.604677	1.262051
17	1	0	1.382689	-1.690056	1.259648
18	1	0	2.535212	-0.338687	1.227508
19	1	0	1.038444	-0.195422	2.172059

27T

%chk=Methoxytbutylnitrenium-t-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.449054	0.216056	-0.688137
2	6	0	-0.888691	-0.050489	0.023035
3	8	0	1.494858	0.633796	-0.141857
4	6	0	2.657791	-0.294841	-0.056622
5	1	0	2.960082	-0.519697	-1.076752
6	1	0	3.403851	0.283452	0.477041
7	1	0	2.333068	-1.176163	0.492869
8	6	0	-0.586249	-1.081005	1.106309
9	1	0	-1.529168	-1.292452	1.616560
10	1	0	-0.220326	-2.017875	0.682994
11	1	0	0.117849	-0.695539	1.845976
12	6	0	-1.834109	-0.558341	-1.050166
13	1	0	-2.804818	-0.734655	-0.583555
14	1	0	-1.964395	0.178298	-1.843186
15	1	0	-1.484074	-1.498331	-1.477735
16	6	0	-1.292974	1.315658	0.583132
17	1	0	-1.427895	2.048581	-0.212106
18	1	0	-2.252892	1.171670	1.086241
19	1	0	-0.568137	1.684058	1.309335

27S-ts

%chk=MethoxytbutylnitreniumTS-s-dft .chk

---

opt=(calcfc,qst2) freq=noraman 6-311g(d,p) geom=connectivity m062x

---

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.353764	0.341148	0.403938
2	6	0	0.879001	-0.129527	0.121350
3	8	0	-1.313665	-0.493595	0.072083
4	6	0	-2.625576	0.086046	0.282946
5	1	0	-2.819911	0.828574	-0.491413
6	1	0	-3.312573	-0.750026	0.194410
7	1	0	-2.665495	0.529460	1.275523

8	6	0	1.071845	-1.500226	-0.449650
9	1	0	2.090511	-1.613228	-0.818136
10	1	0	0.913578	-2.218819	0.360718
11	1	0	0.351210	-1.724790	-1.234307
12	6	0	2.003148	0.526144	0.873071
13	1	0	2.880293	0.635511	0.234302
14	1	0	1.706558	1.489284	1.285694
15	1	0	2.267655	-0.140011	1.698748
16	6	0	0.390100	1.126716	-1.122989
17	1	0	0.507852	2.136325	-0.750059
18	1	0	1.265180	0.786854	-1.686682
19	1	0	-0.510305	0.946675	-1.701390

28S

%chk=formylnitrenium-s-CBSAPNO.chk

---

cbs-apno geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.919958	-0.108549	-0.142081
2	1	0	-1.338840	-0.428368	0.748605
3	6	0	0.217572	0.610204	0.026492
4	8	0	0.736118	-0.513707	0.001551
5	1	0	0.584169	1.636640	0.074605

28T

%chk=formylnitrenium-t-CBSAPNO.chk

---

cbs-apno geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.137591	-0.201955	-0.121642
2	1	0	-1.828306	-0.191652	0.641985
3	6	0	0.073607	0.359687	0.007773

4	8	0	1.150631	-0.253190	0.022131
5	1	0	0.144750	1.472740	-0.014175

29S

%chk=acetylnitrenium-s-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.090780	-0.007807	0.004905
2	8	0	-0.813820	0.846759	0.013606
3	6	0	1.532151	-0.072958	0.019164
4	1	0	1.956555	0.895144	0.282914
5	1	0	1.861479	-0.878239	0.681617
6	1	0	1.827115	-0.351911	-1.004997
7	7	0	-1.059372	-0.704537	-0.138946
8	1	0	-1.456570	-1.022721	0.759826

29T

%chk=acetylnitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.128714	0.073360	0.011534
2	8	0	-0.368459	1.277400	0.001596
3	6	0	1.339156	-0.350859	0.017497
4	1	0	1.975024	0.514239	0.197230
5	1	0	1.455328	-1.111169	0.793602
6	1	0	1.512012	-0.780479	-0.974456
7	7	0	-1.078391	-0.870361	-0.123645
8	1	0	-1.708610	-1.084273	0.662193

30S-iso (does not converge on nitrenium ion)

%chk=Acetylmethylnitrenium-s-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.029009	-0.328225	-0.184834
2	6	0	-2.150744	-0.668308	-0.267696
3	1	0	-3.177215	-0.971012	-0.353868
4	1	0	-3.437456	2.203845	1.013386
5	1	0	-3.282127	1.717540	1.463418
6	6	0	1.153127	0.333508	-0.023677
7	8	0	1.089528	1.411418	-0.290482
8	6	0	1.565636	-1.002657	0.333895
9	1	0	1.060029	-1.269786	1.263102
10	1	0	1.262548	-1.671244	-0.473936
11	1	0	2.652956	-0.978371	0.450461

30T

%chk=Acetylmethylnitrenium-t-dft .chk

---

opt freq 6-311g(d,p) geom=connectivity um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.694976	-0.612331	-0.000046
2	6	0	-2.035363	-0.204405	-0.000018
3	1	0	-2.662961	-1.103284	-0.000100
4	1	0	-2.241624	0.399870	0.897787
5	1	0	-2.241616	0.400033	-0.897715
6	6	0	0.628690	0.207662	-0.000018
7	8	0	0.373035	1.348802	0.000089
8	6	0	1.846622	-0.620623	-0.000017
9	1	0	1.832684	-1.261296	0.886080
10	1	0	1.832720	-1.261276	-0.886130
11	1	0	2.721656	0.026043	0.000011

31S

%chk=FormylVinylnitrenium-s-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.063699	0.623086	0.103771
2	6	0	0.851545	-0.369970	-0.157096
3	6	0	2.207643	-0.043805	0.080497
4	1	0	0.533116	-1.313224	-0.601234
5	1	0	3.027442	-0.642526	-0.314773
6	1	0	2.426910	0.868670	0.632212
7	6	0	-1.356351	0.423170	-0.180222
8	8	0	-1.850809	-0.575668	0.220481
9	1	0	-1.843916	1.274459	-0.665523

31T

%chk=FormylVinylnitrenium-t-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.012293	-0.092277	-0.000006
2	6	0	1.197008	0.427659	0.000012
3	6	0	2.355536	-0.358072	0.000010
4	1	0	1.256595	1.522911	-0.000018
5	1	0	3.323524	0.124998	-0.000041
6	1	0	2.287986	-1.438785	-0.000030
7	6	0	-1.409710	0.326797	-0.000004
8	8	0	-2.299037	-0.421707	0.000002
9	1	0	-1.418862	1.432168	-0.000006

32S

%chk=Acetylmethoxynitrenium-s-dft .chk

---

opt=calcfc freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.318662	-0.585708	-0.058215
2	6	0	-1.133873	0.212384	-0.007451
3	8	0	-1.061477	1.372965	-0.010164
4	6	0	-2.211203	-0.796496	0.022394
5	1	0	-2.158136	-1.405067	-0.884942
6	1	0	-2.062751	-1.462607	0.876795
7	1	0	-3.172216	-0.291527	0.089619
8	8	0	1.185531	0.244345	0.033638
9	6	0	2.601075	-0.219805	0.006500
10	1	0	3.032815	0.304450	-0.844377
11	1	0	3.014053	0.141547	0.946537
12	1	0	2.587178	-1.301826	-0.092572

32T

%chk=Acetylmethoxynitrenium-t-dft .chk

---

opt freq 6-311g(d,p) scrf=(smd,solvent=water) geom=connectivity um06
2x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.301421	-0.894144	-0.158823
2	6	0	1.153306	0.329804	-0.021980
3	8	0	0.763894	1.385437	-0.180159
4	6	0	2.273365	-0.558584	0.244922
5	1	0	2.040735	-1.137668	1.140227
6	1	0	2.373371	-1.231037	-0.609737
7	1	0	3.157396	0.064803	0.378046
8	8	0	-1.369526	-0.387343	-0.557764
9	6	0	-2.288916	0.177622	0.463725
10	1	0	-1.748477	0.972080	0.974556
11	1	0	-3.125958	0.548303	-0.116455

12	1	0	-2.568589	-0.635276	1.128509

33S-iso (does not converge on nitrenium)

%chk=betalactnitrenium-s-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.376306	-0.086623	0.000094
2	6	0	0.461566	1.107496	0.000005
3	1	0	2.454058	-0.217205	-0.000168
4	1	0	0.567599	-2.023808	-0.000126
5	1	0	0.499815	1.730694	0.896362
6	1	0	0.500274	1.729824	-0.896913
7	7	0	0.478493	-1.004486	0.000022
8	6	0	-0.660489	0.058078	0.000070
9	8	0	-1.804437	-0.082726	-0.000041

33T-iso2 (does not converge on nitrenium ion)

%chk=betalactnitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.366745	0.189544	0.325448
2	6	0	0.109174	0.946326	-0.218739
3	1	0	1.329918	0.123494	1.419814
4	1	0	2.242421	0.784201	0.037221
5	1	0	-0.076420	1.903855	0.283962
6	1	0	0.180175	1.108353	-1.302570
7	7	0	1.391941	-1.108890	-0.263364
8	6	0	-1.072215	0.140663	-0.029392
9	8	0	-1.980238	-0.477109	0.117652

34S-iso (does not converge on nitrenium)

%chk=gamlactnitrenium-s-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.216941	-0.868085	-0.000187
2	6	0	-0.082938	1.236008	-0.000173
3	6	0	-1.475456	0.595660	0.000062
4	1	0	-1.977133	-1.644834	-0.001859
5	1	0	0.434188	-2.086318	-0.000448
6	1	0	0.108465	1.852019	0.880060
7	1	0	0.108350	1.852398	-0.880102
8	1	0	-2.082204	0.848151	0.875834
9	1	0	-2.083863	0.849008	-0.874191
10	6	0	0.899428	0.089279	0.000045
11	8	0	2.065939	0.006555	-0.000173
12	7	0	0.031447	-1.148577	0.000516

34T-iso2 (does not converge on nitrenium)

%chk=gamlactnitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.685174	-0.443906	-0.084840
2	6	0	0.309647	1.110518	-0.341550
3	6	0	-1.028397	0.863252	0.402078
4	1	0	-2.102653	-0.324610	-1.095779
5	1	0	-2.503758	-0.732788	0.587032
6	1	0	0.779838	2.060762	-0.057475
7	1	0	0.188404	1.090126	-1.432845
8	1	0	-0.846420	0.825417	1.476405
9	1	0	-1.663479	1.724386	0.194164

10	6	0	1.312722	0.105628	-0.049861
11	8	0	2.176992	-0.550985	0.185229
12	7	0	-0.674380	-1.435480	-0.101186

35S-iso (does not converge on nitrenium)

%chk=succinimidyl-s-dft.chk

---

opt=tight freq=noraman 6-311g(d,p) nosymm geom=connectivity m062x in t=ultrafine

---

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000880	0.667916	-1.872030
2	6	0	-0.000326	-0.664193	-1.873924
3	1	0	-0.926621	1.233630	-1.917612
4	1	0	0.924335	1.234400	-1.918702
5	1	0	-0.925597	-1.230543	-1.921124
6	1	0	0.925362	-1.229767	-1.922216
7	6	0	0.000248	1.157205	1.044981
8	8	0	-0.000384	2.246957	0.778433
9	7	0	0.001008	-0.002987	1.513264
10	6	0	0.001264	-1.161822	1.041636
11	8	0	0.001592	-2.250796	0.771925

35T

%chk=succinimidyl-t-dft.chk

---

opt=(calcfc,tight) freq=noraman 6-311g(d,p) nosymm geom=connectivity m062x int=ultrafine

---

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000665	0.771153	-1.228671
2	6	0	0.000002	-0.769245	-1.230909
3	1	0	-0.890675	1.210642	-1.681391
4	1	0	0.888650	1.211379	-1.682050

5	1	0	-0.889734	-1.208167	-1.684715
6	1	0	0.889580	-1.207396	-1.685759
7	6	0	-0.000146	1.054681	0.280410
8	8	0	-0.000653	2.242461	0.639739
9	7	0	0.000832	-0.002410	1.087463
10	6	0	0.000985	-1.057141	0.277325
11	8	0	0.001824	-2.245956	0.633189

36S

%chk=allylnitrenium-s-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.422591	0.201683	0.187286
2	6	0	0.379098	-0.425562	-0.406361
3	1	0	2.390032	0.253203	-0.303623
4	1	0	1.338916	0.628761	1.182813
5	1	0	0.418121	-0.871837	-1.391311
6	6	0	-0.958004	0.655600	-0.169800
7	1	0	-1.276274	0.791065	-1.200536
8	1	0	-0.900747	1.533893	0.471253
9	7	0	-0.894261	-0.608832	0.320438
10	1	0	-0.772328	-0.663584	1.331592

36T

%chk=allylnitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.581962	-0.271426	0.198082
2	6	0	0.563337	0.373169	-0.410438

3	1	0	2.548054	-0.359700	-0.287200
4	1	0	1.485743	-0.684034	1.198251
5	1	0	0.633381	0.716150	-1.437454
6	6	0	-0.749670	0.581865	0.283967
7	1	0	-1.333173	1.438991	-0.066247
8	1	0	-0.695109	0.613326	1.379669
9	7	0	-1.422126	-0.624672	-0.090223
10	1	0	-1.057794	-1.453677	-0.585121

37S-iso (does not converge on nitrenium)

%chk=homoallylnitrenium-s-dft.chk

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.002137	-0.967542	-0.002512
2	6	0	-1.048839	-0.022293	0.483047
3	1	0	0.135612	-1.815949	0.672748
4	1	0	-0.216013	-1.351388	-1.001929
5	1	0	-1.004882	0.259587	1.531736
6	6	0	-2.034264	0.409502	-0.294789
7	1	0	-2.809787	1.058035	0.093994
8	1	0	-2.113767	0.114437	-1.336471
9	6	0	1.591240	0.923162	-0.029299
10	1	0	2.613967	1.273896	-0.118697
11	1	0	0.765567	1.614922	0.109893
12	7	0	1.347708	-0.321789	-0.094009
13	1	0	2.133704	-0.957986	-0.231896

37T

%chk=homoallylnitrenium-t-dft.chk

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.639231	0.838311	-0.054970
2	6	0	1.205390	-0.452900	0.232055
3	1	0	2.644184	1.161675	0.197817
4	1	0	0.949178	1.542235	-0.519345
5	1	0	1.741424	-1.020161	0.992103
6	6	0	0.030477	-1.038279	-0.391779
7	1	0	-0.034796	-2.111813	-0.230663
8	1	0	-0.052805	-0.789526	-1.451471
9	6	0	-1.258746	-0.335579	0.273583
10	1	0	-2.097686	-0.931911	-0.115850
11	1	0	-1.237954	-0.462943	1.363067
12	7	0	-1.341556	1.016026	-0.114758
13	1	0	-2.218762	1.430941	0.214318

38S-iso (does not converge on nitrenium)

%chk=pentenylnitrenium-s-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.432780	-0.695820	-0.280155
2	1	0	-2.278181	-1.233924	0.144369
3	1	0	-1.526956	-0.717892	-1.368266
4	6	0	-1.388519	0.741450	0.221038
5	1	0	-2.072604	1.435281	-0.262696
6	1	0	-1.505416	0.795634	1.303462
7	7	0	0.040430	1.151525	-0.081366
8	1	0	0.377450	1.882582	0.549237
9	6	0	-0.077246	-1.258988	0.166352
10	1	0	0.250703	-2.111620	-0.426231
11	1	0	-0.118645	-1.571660	1.213873
12	6	0	0.874530	-0.101140	0.022388
13	6	0	2.188723	-0.025768	-0.035239
14	1	0	0.103381	1.520986	-1.034732
15	1	0	2.720324	0.913240	-0.139177
16	1	0	2.778691	-0.931708	0.023415

38T-iso2 (does not converge on nitrenium)

%chk=pentenylnitrenium-t-dft.chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.495170	-0.677093	-0.129188
2	1	0	-2.252032	-1.169194	0.477574
3	1	0	-1.771095	-0.788650	-1.179723
4	6	0	-1.371824	0.810980	0.218011
5	1	0	-2.030134	1.503526	-0.315450
6	1	0	-1.513906	0.999324	1.296538
7	7	0	0.008139	1.109733	-0.069060
8	1	0	0.394820	2.055192	-0.051850
9	6	0	-0.080177	-1.209706	0.123426
10	1	0	0.133227	-2.134176	-0.409241
11	1	0	0.093823	-1.375974	1.190036
12	6	0	0.831116	-0.070349	-0.359956
13	6	0	2.212476	0.010891	0.181000
14	1	0	0.869548	-0.077275	-1.469485
15	1	0	2.987494	0.544473	-0.350169
16	1	0	2.452759	-0.513721	1.095436

39S-iso (does not converge on nitrenium)

%chk=fluoromethylnitrenium-s-dft .chk

---

opt freq=noraman 6-311g(d,p) nosymm geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.231119	0.959227	-0.379027
2	1	0	-0.432231	1.651550	-0.027727

3	6	0	1.147274	0.488271	0.372597
4	1	0	1.872165	-0.249085	0.035151
5	1	0	0.143608	0.653427	-1.346272
6	9	0	1.237902	0.884020	1.575425

39T

%chk=fluoromethylnitrenium-t-dft .chk

---

opt freq=noraman 6-311g(d,p) nosymm geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.288427	0.718761	-0.088634
2	1	0	-1.098622	1.330792	0.112256
3	6	0	1.147123	0.575573	-0.008710
4	1	0	1.370332	-0.499069	0.025396
5	1	0	1.560236	1.047796	-0.915200
6	9	0	1.509194	1.213558	1.105040

40S-iso (does not converge on nitrenium)

%chk=trifluoromethylnitrenium-s-dft .chk

---

opt freq=noraman 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.651912	-0.639298	0.000007
2	1	0	-0.763547	-1.657622	-0.000214
3	6	0	0.464787	0.000566	-0.000049
4	9	0	-1.772726	0.064495	0.000027
5	9	0	1.549755	-0.633614	0.000036
6	9	0	0.504995	1.250154	-0.000012

40T

%chk=trifluoromethylnitrenium-t-dft .chk

---

opt=(calcall,tight) freq=noraman 6-311g(d,p) geom=connectivity m062x int=ultrafine

---

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.393434	0.015257	0.443884
2	1	0	2.401303	-0.014764	0.186361
3	6	0	-0.120974	-0.000265	-0.014812
4	9	0	-0.334504	-1.219296	-0.361433
5	9	0	-0.791948	0.380841	1.005658
6	9	0	-0.143493	0.828406	-1.000300

41S-iso (does not converge on nitrenium)

%chk=phosphonyl-s-dft.chk

---

opt=calcfc freq=noraman 6-311g(d,p) geom=connectivity m062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.331897	-0.285224	-0.000004
2	1	0	-2.163080	0.304408	-0.000045
3	15	0	0.132922	0.312933	0.000003
4	8	0	1.366488	-0.427588	-0.000006
5	1	0	0.063786	1.709880	0.000022
6	1	0	-1.503159	-1.291009	0.000050

41T

%chk=phosophonyl-t-dft.chk

---

opt=calcfc freq 6-311g(d,p) geom=connectivity um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.387323	-0.280880	-0.000223

2	1	0	-1.504385	-1.310357	0.000715
3	15	0	0.182735	0.469399	0.000057
4	8	0	1.017536	-0.787353	-0.000017
5	1	0	0.166681	1.267100	1.152575
6	1	0	0.167657	1.267250	-1.152445

42S-iso (does not converge on nitrenium)

%chk=silyl-s-dft.chk

---

opt freq 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.057910	-0.000046	-0.000169
2	1	0	-1.624489	-0.843174	0.001238
3	14	0	0.581315	-0.000014	0.000074
4	1	0	1.258139	-1.292326	-0.000859
5	1	0	1.257288	1.292779	0.000297
6	1	0	-1.623986	0.843246	-0.000533

42T

%chk=silyl-t-dft.chk

---

opt=calcfc freq=noraman 6-311g(d,p) geom=connectivity um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.255168	0.000142	-0.000453
2	1	0	-2.284532	-0.000477	0.001438
3	14	0	0.607566	-0.000020	0.000090
4	1	0	0.854770	1.301883	0.634081
5	1	0	0.854249	-1.200292	0.810240
6	1	0	0.855773	-0.101830	-1.443846

43S

%chk=sulfonyl-s-dft.chk

---

opt freq 6-311g(d,p) geom=connectivity rm062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.087795	0.717400	-0.264364
2	1	0	1.762678	0.990905	0.469599
3	16	0	-0.281035	0.000986	0.271034
4	8	0	-1.531951	0.079836	-0.367859
5	8	0	0.962558	-0.814855	-0.204613
6	1	0	-0.325538	-0.148332	1.624181

43T

%chk=sulfonyl-t-dft.chk

---

opt=(calcall,tight) freq=noraman 6-311g(d,p) geom=connectivity int=u
ltrafine um062x

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.439645	0.485408	-0.162641
2	1	0	1.580065	1.464485	-0.471532
3	16	0	-0.098032	0.072408	0.237920
4	8	0	-1.273859	0.681031	-0.273135
5	8	0	0.013123	-1.443686	-0.201484
6	1	0	-0.003174	0.080369	1.600248
