Electronic Supplementary Information

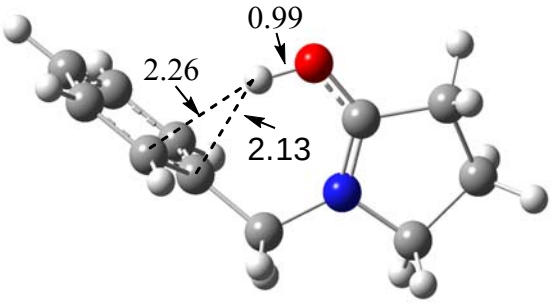
C^{α}–C^{β} and C^{α}–N Bonds Cleavage in the Dissociation of Protonated *N*–benzyllactams: Dissociative Proton Transfer and Intramolecular Proton-Transport Catalysis

Yunfeng Chai, Cheng Guo, Kezhi Jiang, Yuanjiang Pan*, Cuirong Sun*

Department of Chemistry, Zhejiang University, Hangzhou, Zhejiang 310027, China

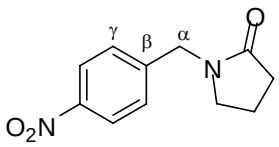
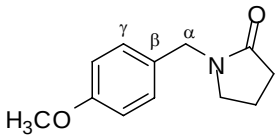
panyuanjiang@zju.edu.cn; suncuirong@zju.edu.cn

Contents



Scheme S1. DFT optimized structure of protonated *N*-benzylbutyrolactam. Chemical bonds are given in Å.

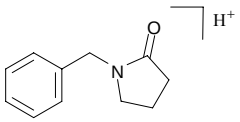
Table S1. Computed relative energies of protonated *N*-(4-methoxybenzyl)butyrolactam and protonated *N*-(4-nitrobenzyl)butyrolactam with different protonation sites. [a]

Compound	Protonation site	Energy (a.u.) [b]
	Carbonyl O	-761.597936
	Amide N	-761.580348
	C^{β}	-761.593833
	C^{γ}	-761.563427
	Substituent	-761.584219
	Carbonyl O	-671.608429
	Amide N	-671.588562
	C^{β}	-671.584537
	C^{γ}	-671.563930
	Substituent	-671.551463

[a] B3LYP/6-31G(d).

[b] Sum of electronic and thermal Energy.

Table S2. The relative energies for 1,2-H shift along the phenyl ring. The calculations were carried out at the B3LYP/6-31++G(d,p) level of theory.



Proton transfer between atoms[a]	Energy (Hartree)[b]	Relative energy (kJ mol^{-1})[c]
$C_{ipso} \leftrightarrow C_{ortho}$	-557.087783	68.4
	-557.085442	74.6
$C_{ortho} \leftrightarrow C_{meta}$	-557.089005	65.2
	-557.084469	77.1
$C_{meta} \leftrightarrow C_{para}$	-557.088685	66.0
	-557.085670	74.0

[a] Two kinds of configurations were considered.

[b] Sum of electronic and thermal Energy.

[c] The relative energy of MH-**2** (-557.113839 Hartree) is zero.

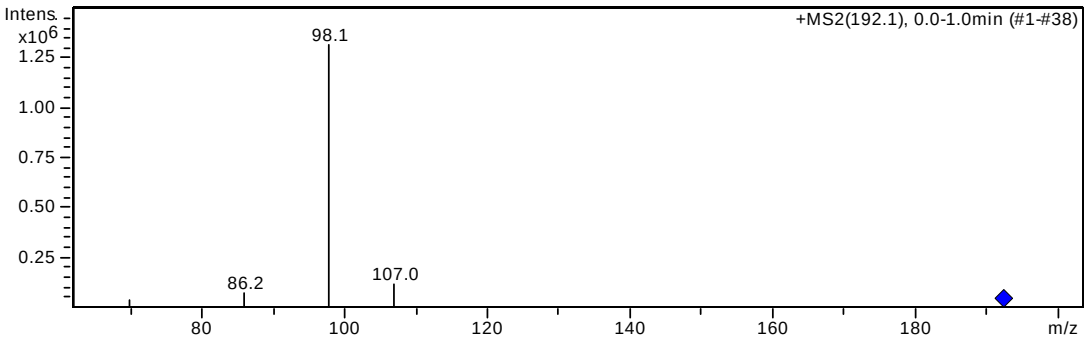


Figure S1. CID mass spectrum of the $[M + H]^+$ ion of Compound **1** (R=*p*-OH).

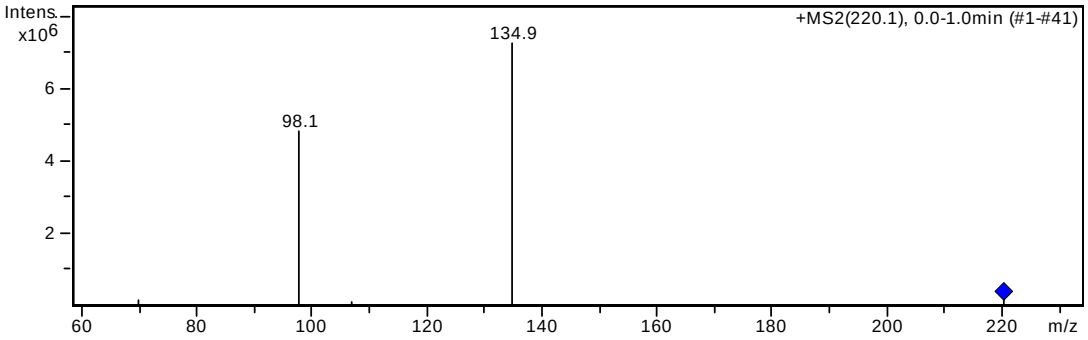


Figure S2. CID mass spectrum of the $[M + H]^+$ ion of Compound **2** (R=*p*-OC_2H_5).

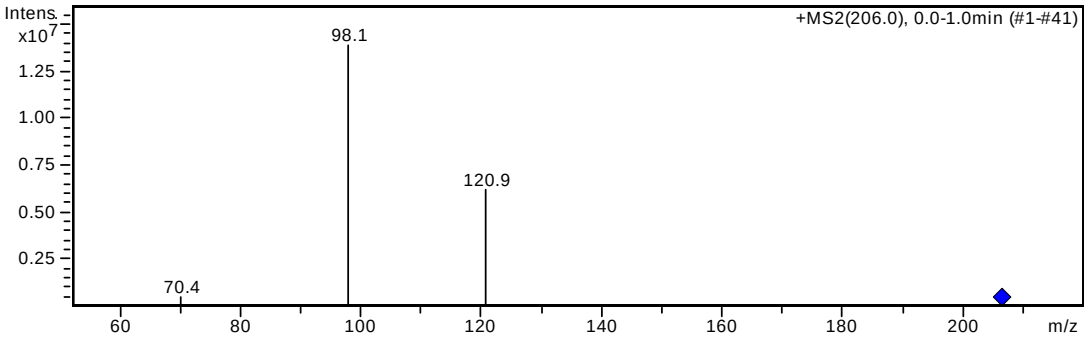


Figure S3. CID mass spectrum of the $[M + H]^+$ ion of Compound **3** (R=*p*-OCH_3).

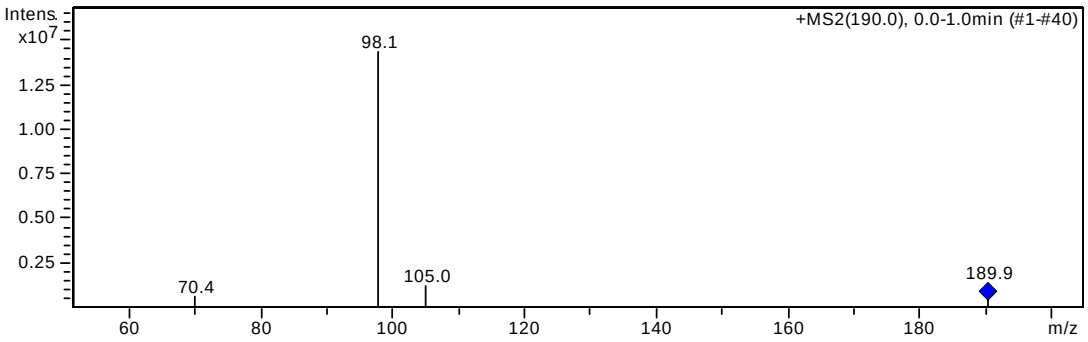


Figure S4. CID mass spectrum of the $[M + H]^+$ ion of Compound **4** (R=*p*-CH_3).

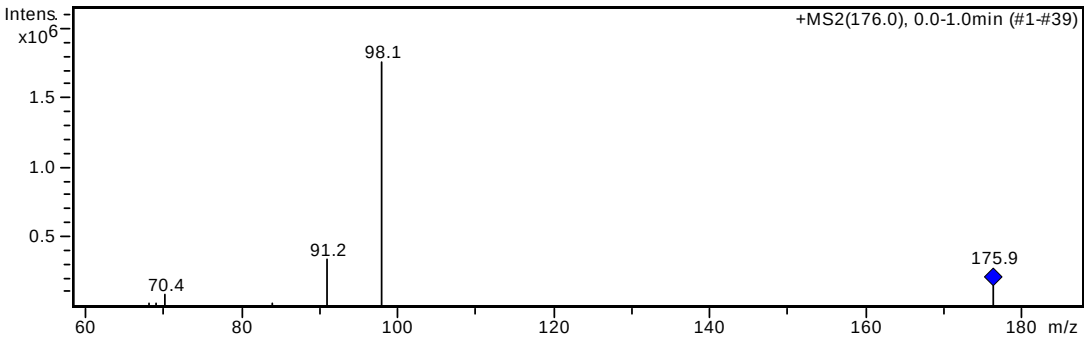


Figure S5. CID mass spectrum of the $[M + H]^+$ ion of Compound **5** (R=H).

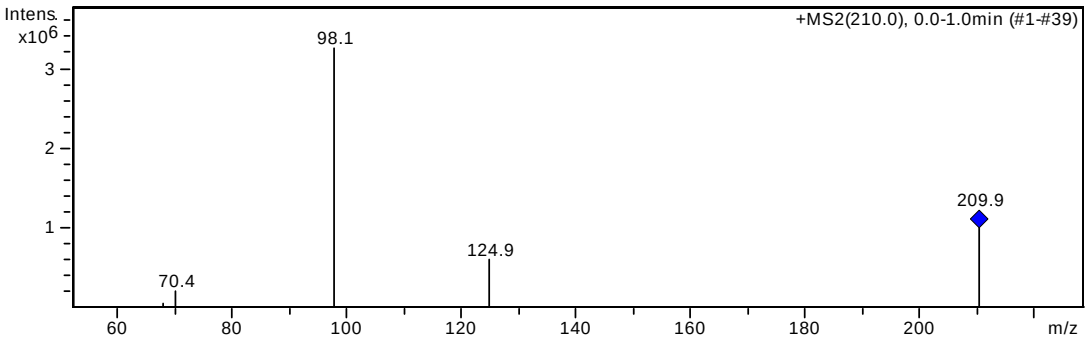


Figure S6. CID mass spectrum of the $[M + H]^+$ ion of Compound **6** (R=*p*-^{35}Cl).

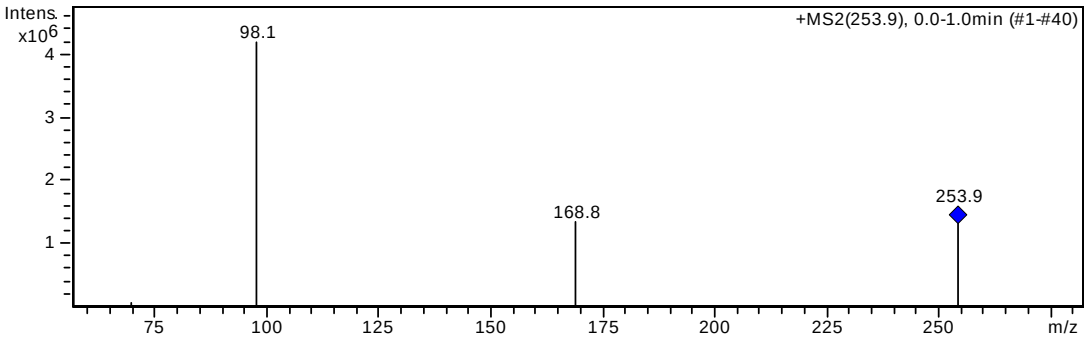


Figure S7. CID mass spectrum of the $[M + H]^+$ ion of Compound **7** (R=*p*-^{79}Br).

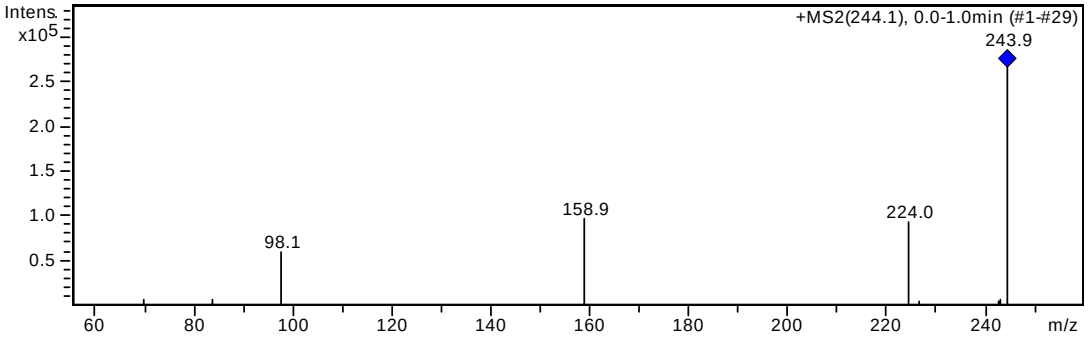


Figure S8. CID mass spectrum of the $[M + H]^+$ ion of Compound **8** (R=*p*-CF_3).

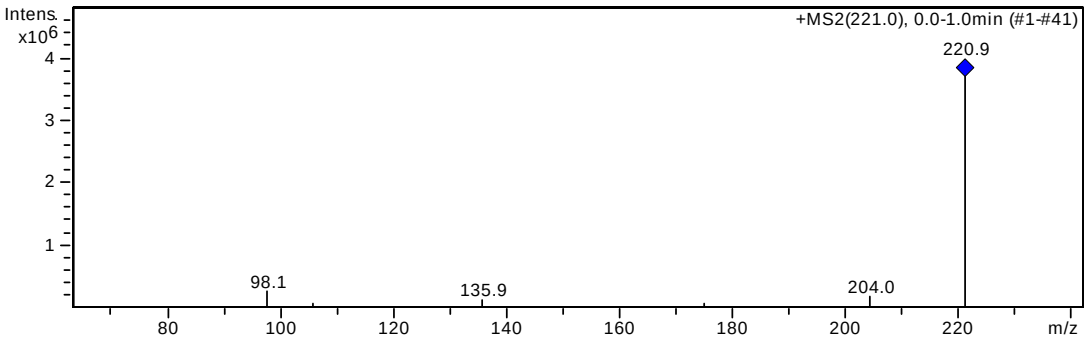


Figure S9. CID mass spectrum of the $[M + H]^+$ ion of Compound **9** (R=*p*-NO_2).

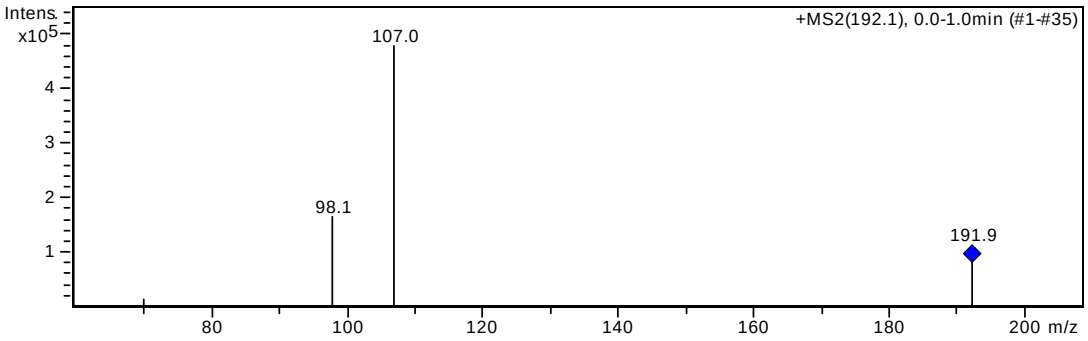


Figure S10. CID mass spectrum of the $[M + H]^+$ ion of Compound **10** (R=*m*-OH).

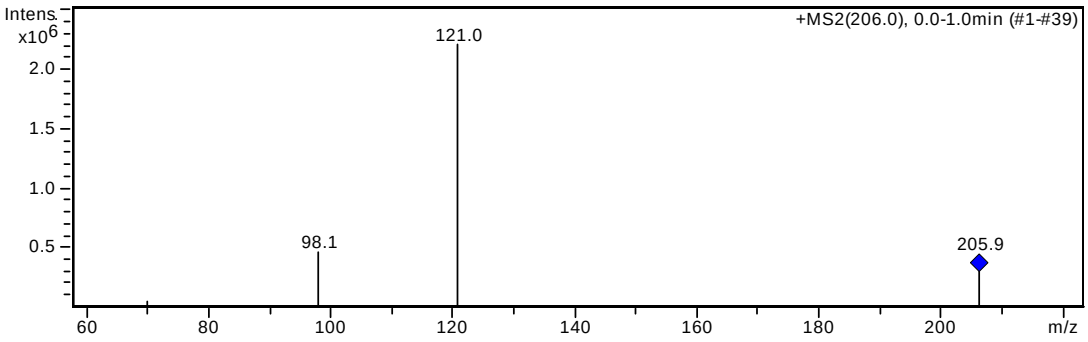


Figure S11. CID mass spectrum of the $[M + H]^+$ ion of Compound **11** (R=*m*-OCH_3).

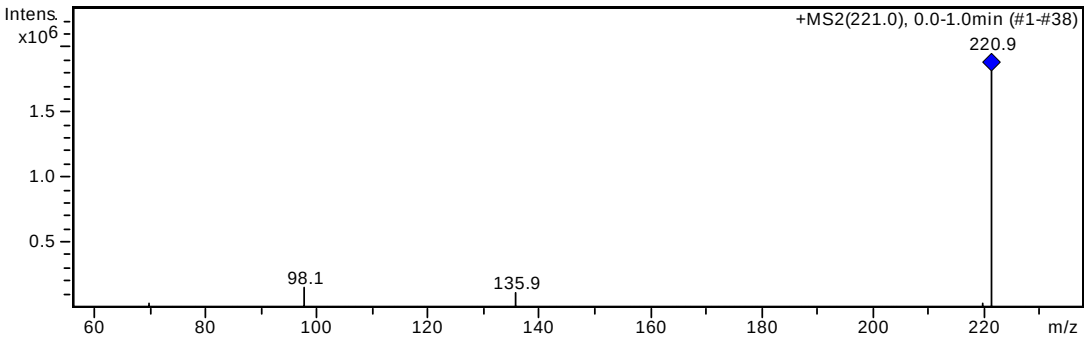


Figure S12. CID mass spectrum of the $[M + H]^+$ ion of Compound **12** (R=*m*-NO_2).

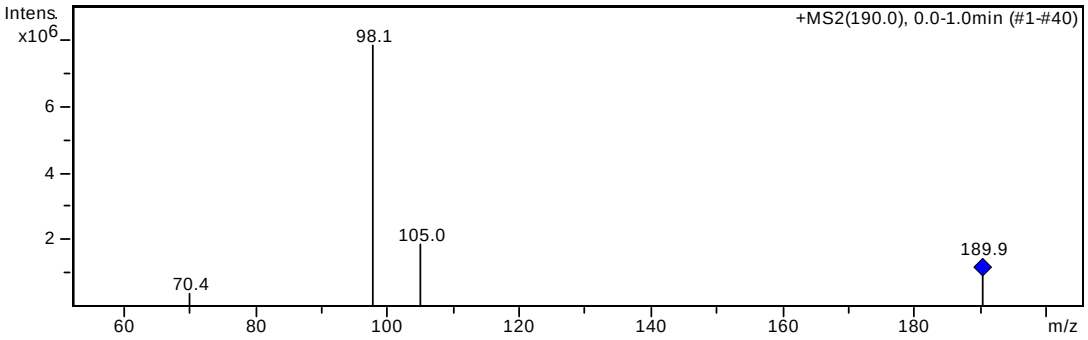


Figure S13. CID mass spectrum of the $[M + H]^+$ ion of Compound **13** (R=*m*-CH_3).

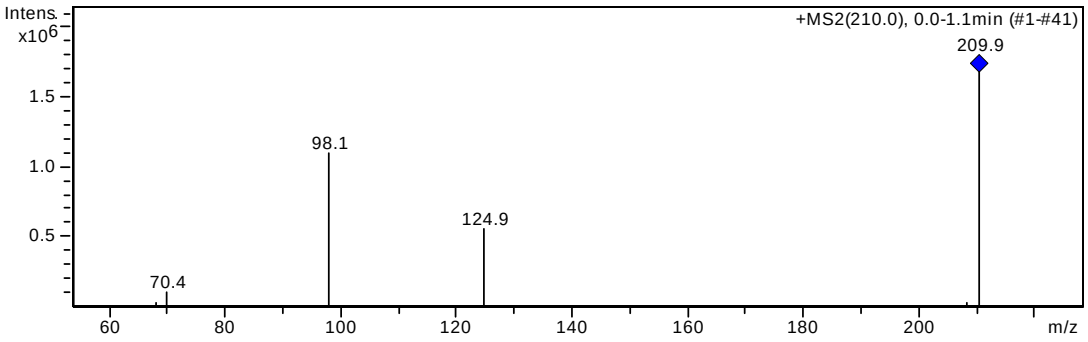


Figure S14. CID mass spectrum of the $[M + H]^+$ ion of Compound **14** (R=*m*-^{35}Cl).

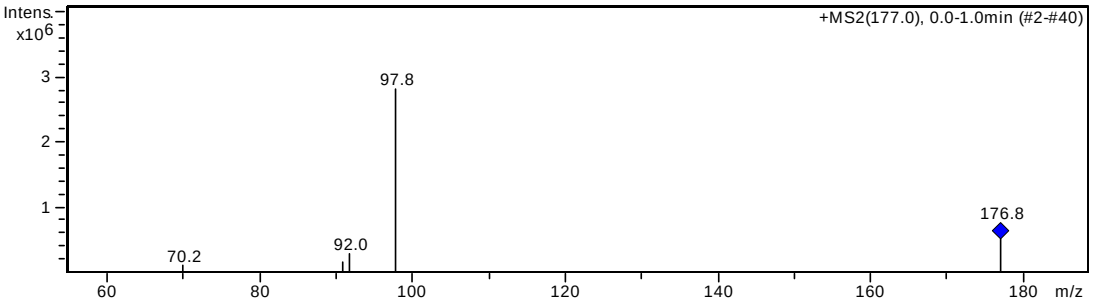


Figure S15. CID mass spectrum of the $[M + D]^+$ ion of Compound **5**.

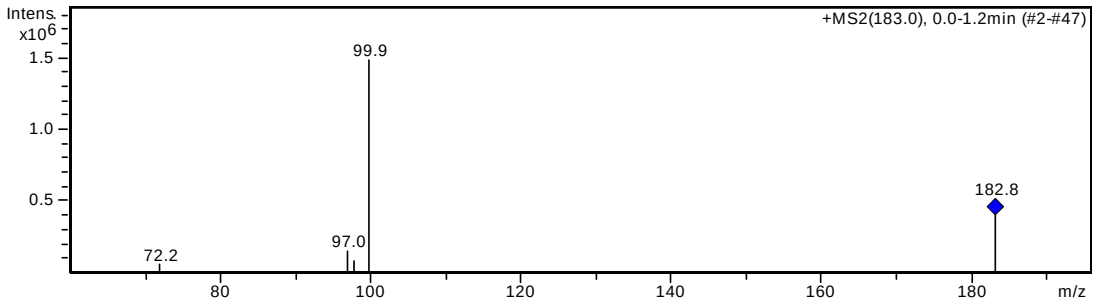


Figure S16. CID mass spectrum of the $[M + H]^+$ ion of Compound **5**-d_7.

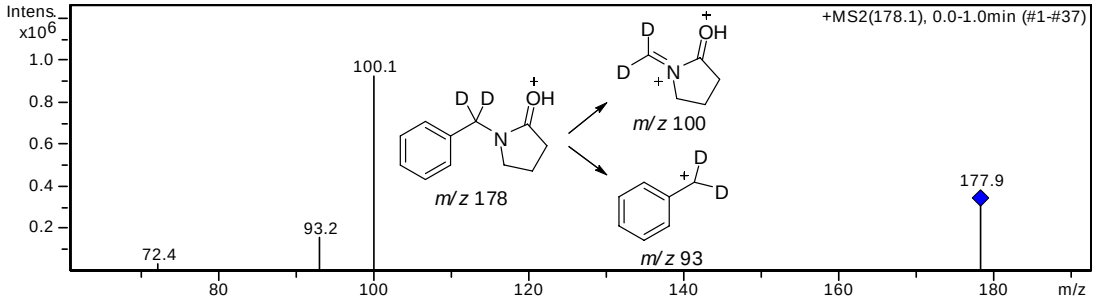


Figure S17. CID mass spectrum of the $[M + H]^+$ ion of Compound **5**-d_2.

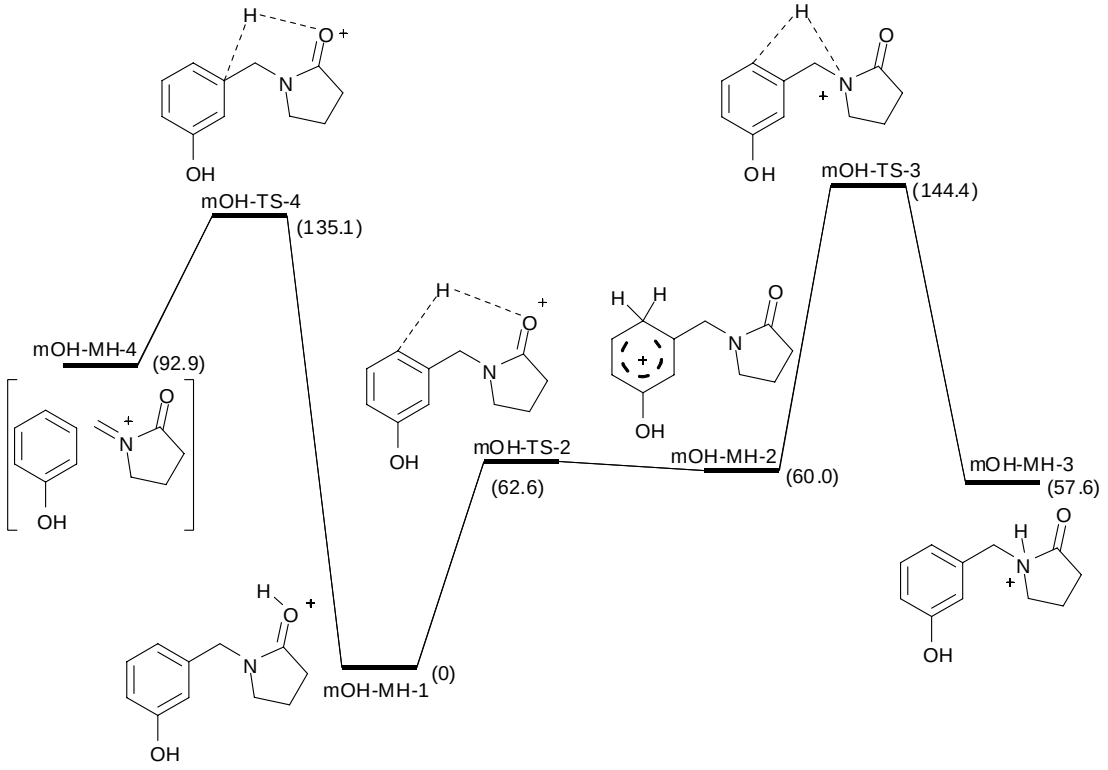
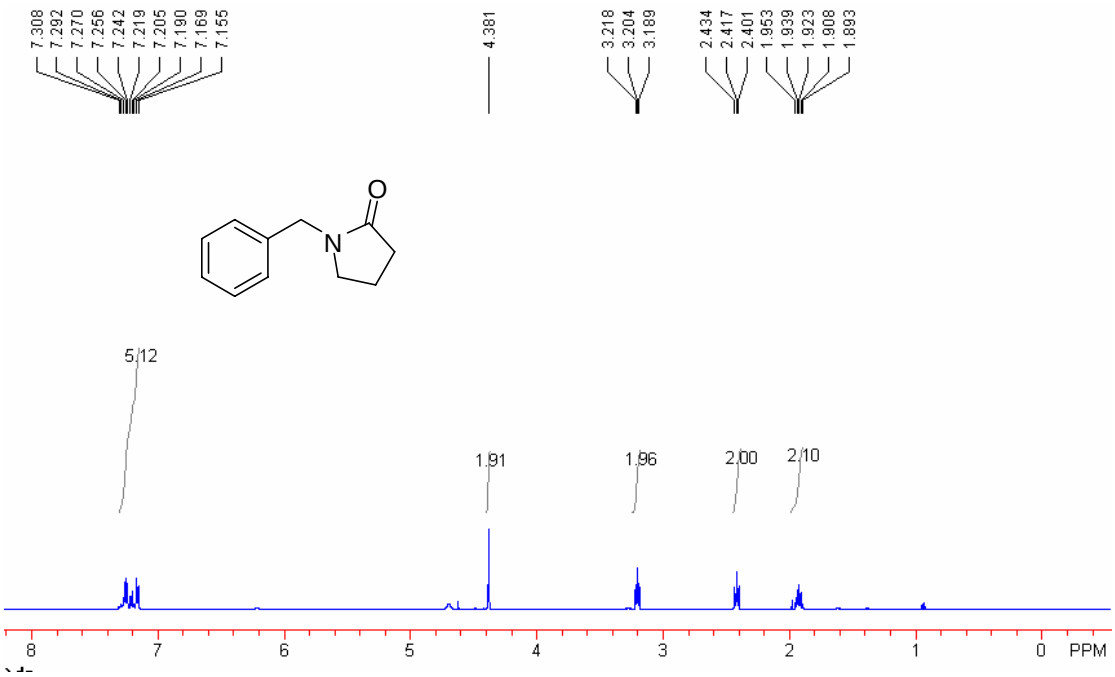
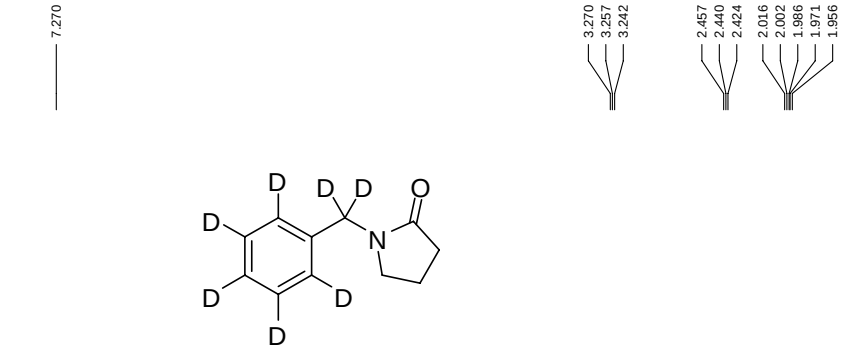
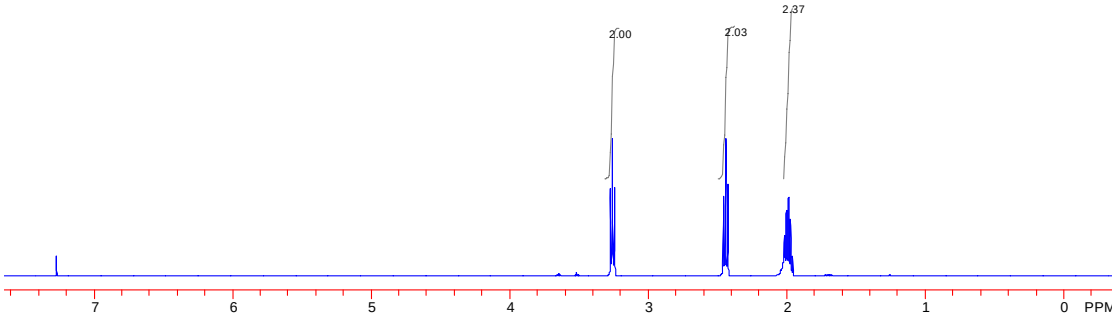
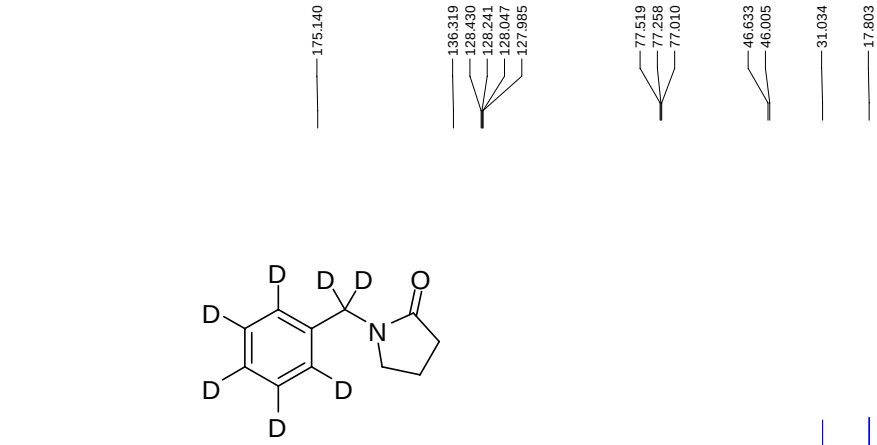


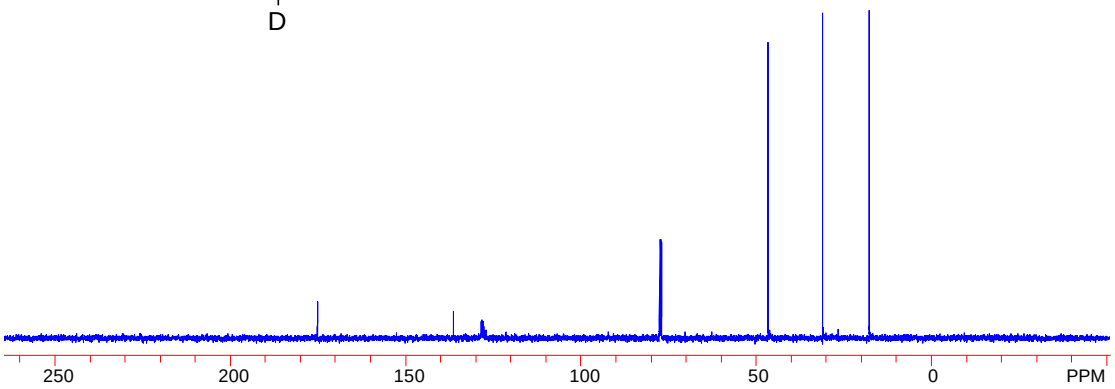
Figure S18. The relative energies of proton transfers in the fragmentation of protonated *N*-(3-hydroxybenzyl)butyrolactam using DFT calculations at the B3LYP/6-31++G(d,p) level. Relative energies are given in kJ mol^{-1}.





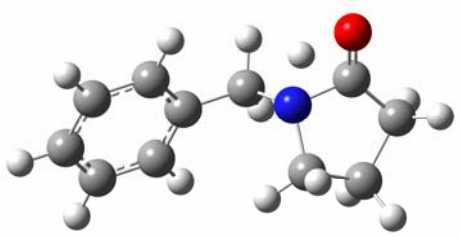






Figures, cartesian coordinates, total energies, zero point energy corrections and the number of imaginary frequencies of all optimized structures discussed in the text at the B3LYP/6-31++G(d,p) level.

TS-1

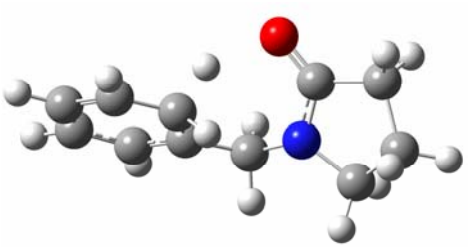


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.560052	-1.623536	0.359565
2	6	0	3.425816	-0.478553	-0.261587
3	6	0	1.338869	-0.917308	1.024294
4	1	0	2.231290	-2.312623	-0.421701
5	1	0	3.124421	-2.202023	1.092817
6	1	0	3.684655	-0.648507	-1.314566
7	1	0	4.363108	-0.269552	0.264446
8	1	0	1.545123	-0.629716	2.058084
9	1	0	0.416034	-1.496228	1.000038
10	6	0	0.196771	0.231446	-0.975243
11	1	0	0.355215	1.135425	-1.570418
12	1	0	0.486814	-0.640031	-1.569921
13	7	0	1.170543	0.345515	0.216922
14	6	0	2.511304	0.677155	-0.127032
15	8	0	2.629307	1.911558	0.016132
16	1	0	1.451714	1.710524	0.460824
17	6	0	-1.222699	0.117762	-0.493483
18	6	0	-1.907497	-1.100732	-0.605873
19	6	0	-1.880776	1.231906	0.050276
20	6	0	-3.232319	-1.206663	-0.173985
21	1	0	-1.416785	-1.963502	-1.050213
22	6	0	-3.200857	1.124015	0.485158
23	6	0	-3.876934	-0.096617	0.375220
24	1	0	-3.758280	-2.150868	-0.272132
25	1	0	-3.706015	1.990926	0.898798
26	1	0	-4.906595	-0.177189	0.708900
27	1	0	-1.369334	2.189040	0.123672

Zero-point correction=	0.227383 (Hartree/Particle)
Thermal correction to Energy=	0.238593
Thermal correction to Enthalpy=	0.239537
Thermal correction to Gibbs Free Energy=	0.188889
Sum of electronic and zero-point Energies=	-557.066128
Sum of electronic and thermal Energies=	-557.054917
Sum of electronic and thermal Enthalpies=	-557.053973
Sum of electronic and thermal Free Energies=	-557.104621

One imaginary vibrational frequency, -1881.62

TS-2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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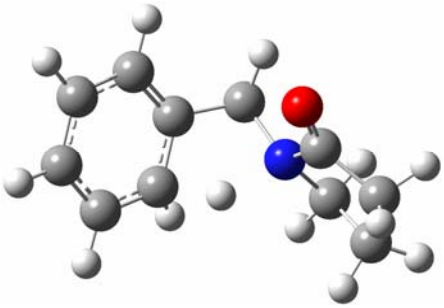
4	1	0	-4.569569	0.409592	0.657206
5	1	0	-3.438667	-0.379501	1.759959
6	1	0	-3.652481	-0.792642	-1.264720
7	1	0	-3.277480	-2.001163	-0.039767
8	1	0	-2.272522	1.699700	1.543779
9	1	0	-2.886565	1.980583	-0.100972
10	6	0	-0.152161	1.291084	-0.330577
11	1	0	-0.174029	1.519689	-1.408335
12	1	0	-0.187232	2.255722	0.187948
13	6	0	1.179799	0.640947	-0.041880
14	6	0	2.358589	1.259176	-0.430873
15	6	0	1.233735	-0.700881	0.526373
16	6	0	3.586821	0.615087	-0.225271
17	1	0	2.341554	2.240083	-0.897139
18	6	0	2.536019	-1.310593	0.745932
19	1	0	0.514032	-0.860646	1.343586
20	6	0	3.685880	-0.670262	0.351770
21	1	0	4.497847	1.124913	-0.527908

22	1	0	2.573750	-2.294718	1.204039
23	1	0	4.658969	-1.129504	0.486279
24	7	0	-1.342744	0.534373	0.030998
25	6	0	-1.661621	-0.663386	-0.555089
26	8	0	-0.850785	-1.364876	-1.176024
27	1	0	0.649966	-1.287350	-0.285322

Zero-point correction= 0.229095 (Hartree/Particle)
Thermal correction to Energy= 0.239721
Thermal correction to Enthalpy= 0.240665
Thermal correction to Gibbs Free Energy= 0.192526
Sum of electronic and zero-point Energies= -557.125791
Sum of electronic and thermal Energies= -557.115165
Sum of electronic and thermal Enthalpies= -557.114220
Sum of electronic and thermal Free Energies= -557.162360

One imaginary vibrational frequency, -40.8945

TS-3



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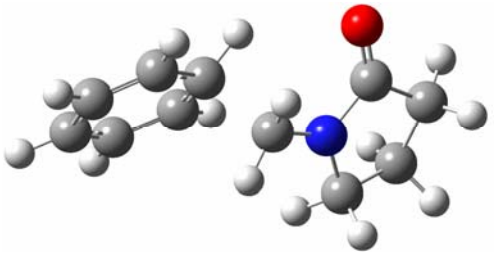
4	1	0	-4.152804	-1.269856	-0.122529
5	1	0	-2.750656	-1.792784	-1.057760
6	1	0	-3.733288	1.076794	-0.642704
7	1	0	-3.009609	0.395966	-2.093862
8	1	0	-1.844956	-1.933234	1.196484
9	1	0	-2.755517	-0.503795	1.729952
10	6	0	-0.130951	0.455600	1.450776
11	1	0	-0.265880	1.530910	1.584365
12	1	0	-0.299570	-0.054868	2.404010
13	6	0	1.225438	0.121832	0.857031

14	6	0	2.254511	1.020939	0.661803
15	6	0	1.226250	-1.147450	0.173760
16	6	0	3.301796	0.684197	-0.214876
17	1	0	2.224765	2.005336	1.118279
18	6	0	2.302589	-1.454359	-0.712723
19	1	0	0.779344	-2.013468	0.678394
20	6	0	3.314551	-0.529357	-0.921179
21	1	0	4.097141	1.404456	-0.383762
22	1	0	2.346316	-2.432782	-1.181728
23	1	0	4.127998	-0.748069	-1.604476
24	7	0	-1.114864	-0.075176	0.455355
25	6	0	-1.633206	0.886049	-0.508868
26	8	0	-1.024365	1.886715	-0.792311
27	1	0	0.002103	-0.813702	-0.219328

Zero-point correction=	0.226837 (Hartree/Particle)
Thermal correction to Energy=	0.237718
Thermal correction to Enthalpy=	0.238662
Thermal correction to Gibbs Free Energy=	0.189487
Sum of electronic and zero-point Energies=	-557.099406
Sum of electronic and thermal Energies=	-557.088525
Sum of electronic and thermal Enthalpies=	-557.087581
Sum of electronic and thermal Free Energies=	-557.136755

One imaginary vibrational frequency, -1311.39

TS-4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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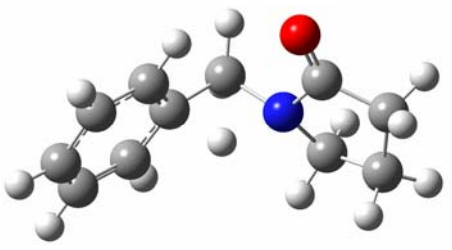
2	6	0	3.403616	0.087162	-0.406050
3	6	0	1.806424	-1.288154	0.849753
4	1	0	2.762606	-1.900907	-1.009633
5	1	0	3.851717	-1.930118	0.375832
6	1	0	3.795979	0.246337	-1.412037
7	1	0	4.140549	0.491940	0.299316

8	1	0	2.082387	-1.359191	1.908082
9	1	0	1.056753	-2.060346	0.643918
10	6	0	0.030379	0.531441	0.985097
11	1	0	-0.434049	-0.068412	1.763302
12	1	0	0.061424	1.596678	1.205126
13	6	0	-1.169033	0.559996	-0.373225
14	6	0	-1.369377	-0.808233	-0.794537
15	6	0	-2.323454	1.265550	0.139436
16	6	0	-2.577170	-1.447526	-0.595306
17	1	0	-0.539882	-1.340795	-1.250907
18	6	0	-3.524245	0.617378	0.342102
19	1	0	-2.216475	2.315604	0.399332
20	6	0	-3.647457	-0.738586	-0.018620
21	1	0	-2.710473	-2.483522	-0.888268
22	1	0	-4.375708	1.146430	0.756790
23	1	0	-4.593930	-1.246844	0.144106
24	7	0	1.260244	0.051210	0.576313
25	6	0	2.111526	0.849842	-0.209494
26	8	0	1.769858	1.944095	-0.617286
27	1	0	-0.516409	1.166837	-1.013263

Zero-point correction= 0.230519 (Hartree/Particle)
Thermal correction to Energy= 0.241739
Thermal correction to Enthalpy= 0.242683
Thermal correction to Gibbs Free Energy= 0.192601
Sum of electronic and zero-point Energies= -557.113931
Sum of electronic and thermal Energies= -557.102711
Sum of electronic and thermal Enthalpies= -557.101767
Sum of electronic and thermal Free Energies= -557.151849

One imaginary vibrational frequency, -101.256

TS-5



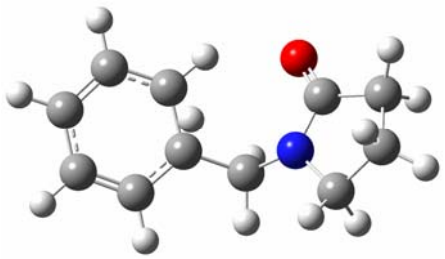
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.024168	-0.986714	-0.968350

2	6	0	-3.165520	0.522201	-0.697115
3	6	0	-2.056690	-1.472344	0.127154
4	1	0	-3.975325	-1.519854	-0.928007
5	1	0	-2.585622	-1.159385	-1.955884
6	1	0	-4.002116	0.745912	-0.022589
7	1	0	-3.302243	1.139280	-1.588302
8	1	0	-1.473902	-2.350304	-0.162163
9	1	0	-2.576428	-1.691779	1.068787
10	6	0	-0.141995	-0.252430	1.421272
11	1	0	-0.312863	0.615902	2.060236
12	1	0	-0.185856	-1.170570	2.009182
13	6	0	1.137880	-0.143947	0.581244
14	6	0	1.643056	1.148560	0.205241
15	6	0	1.958575	-1.296955	0.335082
16	6	0	2.835971	1.251044	-0.496275
17	1	0	1.048602	2.028350	0.433288
18	6	0	3.144946	-1.172024	-0.367431
19	1	0	1.623737	-2.272335	0.677639
20	6	0	3.582592	0.098810	-0.777720
21	1	0	3.199703	2.225047	-0.806122
22	1	0	3.747395	-2.048878	-0.580042
23	1	0	4.520646	0.189522	-1.317473
24	7	0	-1.168099	-0.300662	0.326370
25	6	0	-1.897057	0.909856	0.030624
26	8	0	-1.481626	1.998813	0.352058
27	1	0	0.198433	-0.253114	-0.351962

Zero-point correction= 0.226491 (Hartree/Particle)
Thermal correction to Energy= 0.237555
Thermal correction to Enthalpy= 0.238499
Thermal correction to Gibbs Free Energy= 0.188928
Sum of electronic and zero-point Energies= -557.089560
Sum of electronic and thermal Energies= -557.078497
Sum of electronic and thermal Enthalpies= -557.077552
Sum of electronic and thermal Free Energies= -557.127123

One imaginary vibrational frequency, -1300.16

TS-6



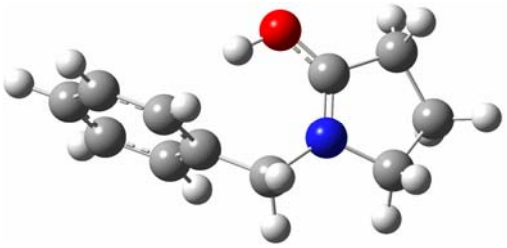
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.328626	-0.674290	-0.972436
2	6	0	-3.296962	0.727260	-0.335430
3	6	0	-2.260240	-1.466525	-0.191358
4	1	0	-4.308107	-1.152225	-0.915702
5	1	0	-3.045933	-0.615419	-2.027964
6	1	0	-4.003968	0.822290	0.498606
7	1	0	-3.503221	1.547092	-1.026515
8	1	0	-1.758400	-2.220506	-0.804489
9	1	0	-2.682678	-1.964270	0.692453
10	6	0	-0.153425	-0.685635	1.056813
11	1	0	-0.214982	-0.095124	1.979664
12	1	0	-0.156231	-1.744340	1.325206
13	6	0	1.186164	-0.356771	0.387236
14	6	0	2.228328	-1.333026	0.265760
15	6	0	1.500027	1.017182	0.028414
16	6	0	3.472622	-0.975730	-0.214575
17	1	0	2.024173	-2.356483	0.564208
18	6	0	2.783919	1.345514	-0.468301
19	1	0	0.936759	0.060399	-0.781894
20	6	0	3.753010	0.362661	-0.579113
21	1	0	4.249616	-1.728040	-0.307418
22	1	0	2.995673	2.375660	-0.733799
23	1	0	4.741156	0.617779	-0.949335
24	7	0	-1.315386	-0.410750	0.224282
25	6	0	-1.900366	0.844331	0.243480
26	8	0	-1.335386	1.842882	0.677789
27	1	0	0.710230	1.755552	0.171755

Zero-point correction= 0.228035 (Hartree/Particle)
Thermal correction to Energy= 0.239217
Thermal correction to Enthalpy= 0.240162
Thermal correction to Gibbs Free Energy= 0.189705
Sum of electronic and zero-point Energies= -557.098966

Sum of electronic and thermal Energies=	-557.087783
Sum of electronic and thermal Enthalpies=	-557.086839
Sum of electronic and thermal Free Energies=	-557.137295

One imaginary vibrational frequency, -717.678

MH-1

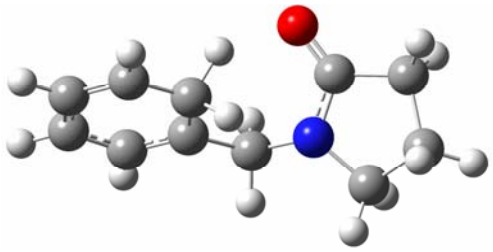


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.607513	-0.143050	0.531640
2	6	0	-2.894236	1.212644	0.342926
3	6	0	-2.713431	-1.148296	-0.220291
4	1	0	-3.650698	-0.400582	1.592874
5	1	0	-4.627305	-0.138520	0.145497
6	1	0	-2.907036	1.863727	1.220841
7	1	0	-3.293761	1.797183	-0.496343
8	1	0	-3.045870	-1.338477	-1.246903
9	1	0	-2.603441	-2.106306	0.292393
10	6	0	-0.197540	-1.211777	-0.777281
11	1	0	-0.319978	-2.236024	-0.414966
12	1	0	-0.266160	-1.238035	-1.870528
13	6	0	1.135001	-0.647831	-0.329603
14	6	0	1.593026	-0.864057	0.981314
15	6	0	1.942230	0.069797	-1.230440
16	6	0	2.826572	-0.355227	1.388024
17	1	0	0.990289	-1.438600	1.680254
18	6	0	3.178907	0.579796	-0.818131
19	1	0	1.617773	0.211242	-2.258941
20	6	0	3.618965	0.369494	0.490261
21	1	0	3.174817	-0.531784	2.400651
22	1	0	3.797639	1.126087	-1.522692
23	1	0	4.580457	0.759437	0.808444
24	7	0	-1.387366	-0.469382	-0.275843
25	6	0	-1.496040	0.809235	-0.002027
26	8	0	-0.547749	1.701591	-0.034480
27	1	0	0.331173	1.319220	-0.262187

Zero-point correction=	0.233513 (Hartree/Particle)
Thermal correction to Energy=	0.244785
Thermal correction to Enthalpy=	0.245729
Thermal correction to Gibbs Free Energy=	0.195194
Sum of electronic and zero-point Energies=	-557.165227
Sum of electronic and thermal Energies=	-557.153955
Sum of electronic and thermal Enthalpies=	-557.153011
Sum of electronic and thermal Free Energies=	-557.203546

No imaginary vibrational frequency

MH-2



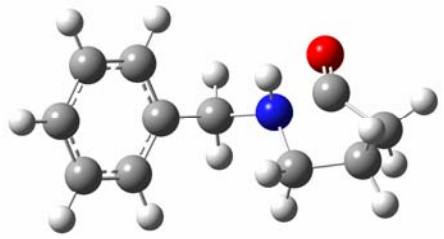
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.495190	0.114398	0.854264
2	6	0	-3.166560	-0.922248	-0.236387
3	6	0	-2.470223	1.242239	0.619500
4	1	0	-4.521278	0.482351	0.803730
5	1	0	-3.344875	-0.321044	1.846803
6	1	0	-3.740812	-0.755617	-1.156879
7	1	0	-3.325979	-1.961876	0.057213
8	1	0	-2.157073	1.735723	1.543474
9	1	0	-2.851139	2.007112	-0.070925
10	6	0	-0.143546	1.237594	-0.444795
11	1	0	-0.161680	1.324155	-1.544531
12	1	0	-0.174361	2.259916	-0.054042
13	6	0	1.186195	0.616066	-0.094935
14	6	0	2.370804	1.262979	-0.411261
15	6	0	1.235803	-0.736418	0.459843
16	6	0	3.598950	0.635670	-0.157596
17	1	0	2.359463	2.254837	-0.853826
18	6	0	2.542665	-1.328495	0.725422
19	1	0	0.516099	-0.874821	1.283901
20	6	0	3.696034	-0.659520	0.400873
21	1	0	4.514114	1.168914	-0.402339

22	1	0	2.576889	-2.320821	1.166010
23	1	0	4.670895	-1.101701	0.574155
24	7	0	-1.332813	0.529185	0.001254
25	6	0	-1.709581	-0.666951	-0.562222
26	8	0	-0.947092	-1.378539	-1.223894
27	1	0	0.674043	-1.344992	-0.326618

Zero-point correction= 0.229584 (Hartree/Particle)
Thermal correction to Energy= 0.241063
Thermal correction to Enthalpy= 0.242007
Thermal correction to Gibbs Free Energy= 0.191236
Sum of electronic and zero-point Energies= -557.125318
Sum of electronic and thermal Energies= -557.113839
Sum of electronic and thermal Enthalpies= -557.112894
Sum of electronic and thermal Free Energies= -557.163666

No imaginary vibrational frequency

MH-3



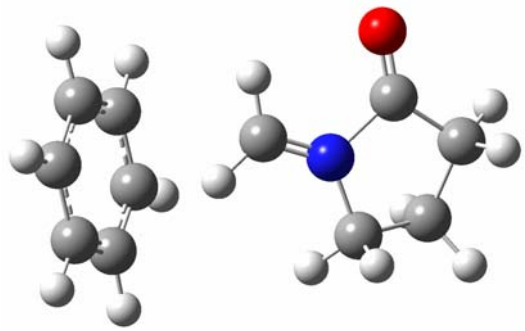
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.749570	-1.527155	-0.769136
2	6	0	-3.559559	-0.375321	-0.153055
3	6	0	-1.345276	-1.368237	-0.169293
4	1	0	-3.166793	-2.507623	-0.533975
5	1	0	-2.715769	-1.436813	-1.859923
6	1	0	-3.978523	-0.642828	0.827288
7	1	0	-4.390231	-0.010026	-0.762802
8	1	0	-0.545873	-1.835566	-0.743765
9	1	0	-1.301808	-1.728483	0.861813
10	6	0	-0.099818	0.659708	0.880177
11	1	0	-0.285328	1.735054	0.928327
12	1	0	-0.352420	0.212030	1.844006
13	6	0	1.300229	0.335995	0.435649
14	6	0	1.935364	1.153178	-0.513965
15	6	0	1.979814	-0.775895	0.954204

16	6	0	3.224225	0.847911	-0.954270
17	1	0	1.437017	2.044566	-0.890589
18	6	0	3.272135	-1.075496	0.517949
19	1	0	1.511496	-1.396534	1.714311
20	6	0	3.891653	-0.267986	-0.439941
21	1	0	3.712390	1.488210	-1.681932
22	1	0	3.796706	-1.930950	0.931334
23	1	0	4.897869	-0.499214	-0.774709
24	7	0	-1.133205	0.124960	-0.118490
25	6	0	-2.578798	0.740986	0.077016
26	8	0	-2.685657	1.888137	0.353060
27	1	0	-0.823438	0.442230	-1.046441

Zero-point correction=	0.233265 (Hartree/Particle)
Thermal correction to Energy=	0.244673
Thermal correction to Enthalpy=	0.245617
Thermal correction to Gibbs Free Energy=	0.194217
Sum of electronic and zero-point Energies=	-557.144215
Sum of electronic and thermal Energies=	-557.132806
Sum of electronic and thermal Enthalpies=	-557.131862
Sum of electronic and thermal Free Energies=	-557.183262

No imaginary vibrational frequency

MH-4



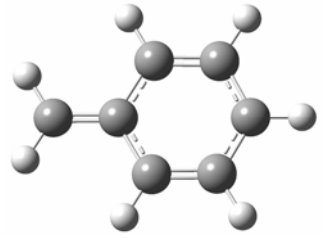
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.967803	-1.452529	0.362879
2	6	0	-3.653641	-0.084177	0.190793
3	6	0	-1.709509	-1.379420	-0.524191
4	1	0	-2.682370	-1.604069	1.407850
5	1	0	-3.610248	-2.282703	0.066946
6	1	0	-4.250677	0.241954	1.045245

7	1	0	-4.310505	-0.061518	-0.690398
8	1	0	-1.927098	-1.640472	-1.565155
9	1	0	-0.871951	-1.982017	-0.169499
10	6	0	-0.203122	0.595114	-0.735319
11	1	0	0.641717	-0.007662	-1.055722
12	1	0	-0.132416	1.677449	-0.655094
13	6	0	2.161277	0.745974	1.243489
14	6	0	1.972996	-0.645311	1.288442
15	6	0	2.872071	1.322305	0.181752
16	6	0	2.489963	-1.455876	0.269283
17	1	0	1.464213	-1.094902	2.136832
18	6	0	3.376065	0.513162	-0.841232
19	1	0	3.046162	2.394156	0.163296
20	6	0	3.184159	-0.875416	-0.798708
21	1	0	2.377091	-2.535042	0.320926
22	1	0	3.937669	0.956703	-1.657832
23	1	0	3.599523	-1.503182	-1.581391
24	7	0	-1.343024	0.056367	-0.486991
25	6	0	-2.539184	0.892678	-0.058589
26	8	0	-2.447060	2.077353	0.014470
27	1	0	1.796901	1.368883	2.055584

Zero-point correction= 0.229172 (Hartree/Particle)
Thermal correction to Energy= 0.241947
Thermal correction to Enthalpy= 0.242891
Thermal correction to Gibbs Free Energy= 0.186130
Sum of electronic and zero-point Energies= -557.128791
Sum of electronic and thermal Energies= -557.116016
Sum of electronic and thermal Enthalpies= -557.115072
Sum of electronic and thermal Free Energies= -557.171833

No imaginary vibrational frequency

Ion **a**, benzyl cation



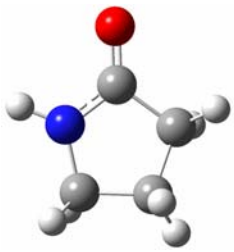
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.122348	-1.236151	0.000008
2	6	0	0.254527	-1.246752	0.000010
3	6	0	0.983938	0.000001	-0.000035
4	6	0	0.254526	1.246753	0.000017
5	6	0	-1.122349	1.236151	0.000003
6	6	0	-1.804095	-0.000001	-0.000019
7	1	0	-1.684838	-2.163383	0.000028
8	1	0	0.807304	-2.181549	0.000016
9	1	0	0.807302	2.181551	0.000026
10	1	0	-1.684840	2.163381	0.000014
11	1	0	-2.890964	-0.000001	0.000037
12	6	0	2.355440	0.000000	-0.000064
13	1	0	2.924095	-0.926896	0.000185
14	1	0	2.924097	0.926895	0.000185

Zero-point correction=	0.117067 (Hartree/Particle)
Thermal correction to Energy=	0.122729
Thermal correction to Enthalpy=	0.123673
Thermal correction to Gibbs Free Energy=	0.087911
Sum of electronic and zero-point Energies=	-270.560288
Sum of electronic and thermal Energies=	-270.554626
Sum of electronic and thermal Enthalpies=	-270.553682
Sum of electronic and thermal Free Energies=	-270.589445

No imaginary vibrational frequency

Butyrolactam



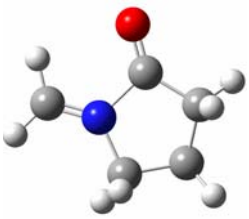
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.415659	0.695307	-0.185759
2	6	0	-0.006231	1.224377	0.136790
3	6	0	-1.329965	-0.817345	0.131049
4	1	0	-2.208805	1.187684	0.382338
5	1	0	-1.631210	0.831704	-1.250509
6	1	0	0.077714	1.580729	1.171053
7	1	0	0.334046	2.031244	-0.515836

8	1	0	-1.953988	-1.420923	-0.535309
9	1	0	-1.633027	-1.029615	1.166764
10	6	0	0.903845	0.001550	-0.006741
11	8	0	2.126108	-0.012129	-0.040239
12	7	0	0.086930	-1.097447	-0.073737
13	1	0	0.485950	-2.025006	-0.032466

Zero-point correction=	0.110889 (Hartree/Particle)
Thermal correction to Energy=	0.116313
Thermal correction to Enthalpy=	0.117257
Thermal correction to Gibbs Free Energy=	0.082053
Sum of electronic and zero-point Energies=	-286.544876
Sum of electronic and thermal Energies=	-286.539453
Sum of electronic and thermal Enthalpies=	-286.538509
Sum of electronic and thermal Free Energies=	-286.573713

No imaginary vibrational frequency

Ion **b**

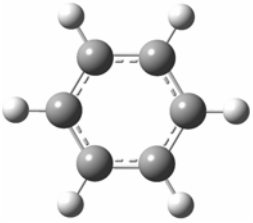


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.768112	-0.238074	-0.277313
2	6	0	1.127337	1.102244	0.128405
3	6	0	0.767818	-1.315913	0.185060
4	1	0	1.896801	-0.285329	-1.362386
5	1	0	2.744812	-0.389042	0.183796
6	1	0	1.418288	1.956118	-0.487935
7	1	0	1.350746	1.366105	1.172333
8	1	0	0.894451	-1.561281	1.245129
9	1	0	0.789649	-2.234668	-0.403147
10	6	0	-1.711328	-1.164606	-0.079153
11	1	0	-1.843855	-2.244088	-0.084488
12	1	0	-2.560561	-0.487829	-0.177169
13	7	0	-0.548867	-0.648763	0.042410
14	6	0	-0.354419	0.890785	0.033590
15	8	0	-1.304173	1.596842	-0.040818

Zero-point correction=	0.127507 (Hartree/Particle)
Thermal correction to Energy=	0.133907
Thermal correction to Enthalpy=	0.134852
Thermal correction to Gibbs Free Energy=	0.097246
Sum of electronic and zero-point Energies=	-324.947434
Sum of electronic and thermal Energies=	-324.941034
Sum of electronic and thermal Enthalpies=	-324.940090
Sum of electronic and thermal Free Energies=	-324.977695

No imaginary vibrational frequency

Benzene

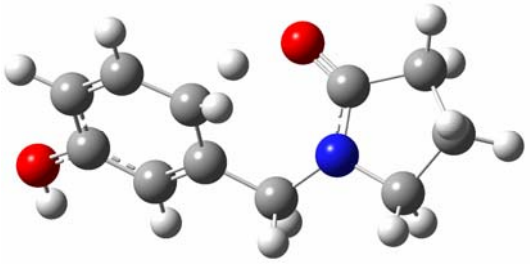


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.276046	0.572296	-0.000011
2	6	0	0.142356	1.391116	0.000015
3	6	0	-1.133666	0.818885	-0.000015
4	6	0	-1.276041	-0.572308	0.000011
5	6	0	-0.142369	-1.391115	-0.000006
6	6	0	1.133674	-0.818875	0.000006
7	1	0	2.267304	1.016993	0.000008
8	1	0	0.253007	2.471912	-0.000012
9	1	0	-2.014290	1.455153	0.000012
10	1	0	-2.267314	-1.016971	-0.000008
11	1	0	-0.252983	-2.471914	0.000004
12	1	0	2.014276	-1.455172	-0.000003

Zero-point correction=	0.100404 (Hartree/Particle)
Thermal correction to Energy=	0.104807
Thermal correction to Enthalpy=	0.105751
Thermal correction to Gibbs Free Energy=	0.072931
Sum of electronic and zero-point Energies=	-232.168035
Sum of electronic and thermal Energies=	-232.163632
Sum of electronic and thermal Enthalpies=	-232.162688
Sum of electronic and thermal Free Energies=	-232.195508

No imaginary vibrational frequency

mOH-TS-2

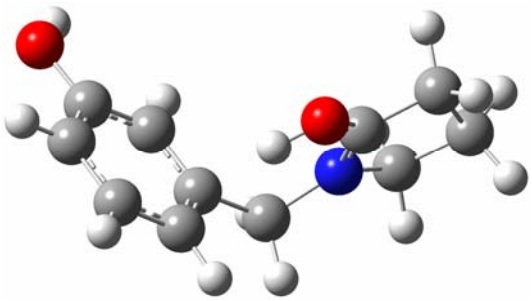


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.043733	-0.132726	0.289920
2	6	0	3.400564	0.831732	-0.721770
3	6	0	2.974215	-1.221325	0.488037
4	1	0	4.990315	-0.550811	-0.056157
5	1	0	4.230223	0.382896	1.236367
6	1	0	3.649857	0.576854	-1.760128
7	1	0	3.654167	1.884077	-0.578678
8	1	0	2.937650	-1.609596	1.509776
9	1	0	3.108377	-2.068379	-0.197992
10	6	0	0.465386	-1.293648	0.301304
11	1	0	0.426941	-2.055406	-0.488850
12	1	0	0.529180	-1.838229	1.253676
13	6	0	-0.829376	-0.511108	0.314186
14	6	0	-1.968300	-1.055824	-0.229855
15	6	0	-0.845002	0.850611	0.817762
16	6	0	-3.181618	-0.320641	-0.211252
17	1	0	-1.952068	-2.042989	-0.685706
18	6	0	-2.115881	1.542898	0.855876
19	1	0	-0.162251	1.063981	1.646585
20	6	0	-3.250349	0.988800	0.327732
21	1	0	-2.148628	2.539935	1.284983
22	1	0	-4.201785	1.508282	0.314019
23	7	0	1.706182	-0.526218	0.165849
24	6	0	1.915032	0.613389	-0.547325
25	8	0	1.025656	1.373801	-0.987050
26	1	0	-0.158772	1.307873	-0.080946
27	8	0	-4.310897	-0.806606	-0.712895
28	1	0	-4.214966	-1.705463	-1.066010

Zero-point correction=	0.232838 (Hartree/Particle)
Thermal correction to Energy=	0.244576
Thermal correction to Enthalpy=	0.245520
Thermal correction to Gibbs Free Energy=	0.194440
Sum of electronic and zero-point Energies=	-632.362104
Sum of electronic and thermal Energies=	-632.350366
Sum of electronic and thermal Enthalpies=	-632.349422
Sum of electronic and thermal Free Energies=	-632.400502

One imaginary vibrational frequency, -394.257

mOH-MH-1



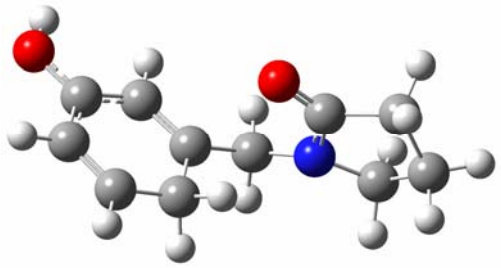
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.946451	0.403687	-0.167900
2	6	0	-3.087879	-0.147324	-1.326073
3	6	0	-2.916457	0.868690	0.880469
4	1	0	-4.602642	1.216767	-0.480279
5	1	0	-4.571326	-0.391146	0.246969
6	1	0	-2.912998	0.585939	-2.124299
7	1	0	-3.486652	-1.047514	-1.800428
8	1	0	-3.197554	0.624055	1.907581
9	1	0	-2.695169	1.940185	0.825543
10	6	0	-0.540839	0.088401	1.484457
11	1	0	-0.574868	1.048726	2.006150
12	1	0	-0.760604	-0.693994	2.218736
13	6	0	0.819400	-0.125565	0.854481
14	6	0	1.512597	0.961394	0.299791
15	6	0	1.388008	-1.408962	0.824554
16	6	0	2.770121	0.763889	-0.285664
17	1	0	1.083818	1.960698	0.336814
18	6	0	2.645444	-1.595152	0.227815
19	1	0	0.882252	-2.246264	1.298488
20	6	0	3.332649	-0.523269	-0.327275

21	1	0	3.092075	-2.584055	0.212511
22	1	0	4.308308	-0.651763	-0.783244
23	7	0	-1.678535	0.119856	0.522771
24	6	0	-1.777290	-0.433679	-0.662947
25	8	0	-0.880268	-1.152120	-1.273436
26	1	0	-0.038687	-1.239961	-0.762065
27	8	0	3.500251	1.764894	-0.831615
28	1	0	3.068105	2.624495	-0.731713

Zero-point correction= 0.237563 (Hartree/Particle)
Thermal correction to Energy= 0.249952
Thermal correction to Enthalpy= 0.250897
Thermal correction to Gibbs Free Energy= 0.197966
Sum of electronic and zero-point Energies= -632.386613
Sum of electronic and thermal Energies= -632.374223
Sum of electronic and thermal Enthalpies= -632.373279
Sum of electronic and thermal Free Energies= -632.426210

No imaginary vibrational frequency

mOH-MH-2



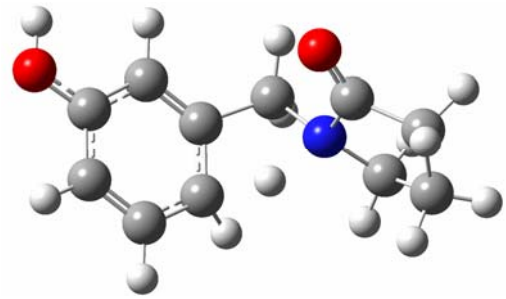
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.968856	0.304323	-0.081007
2	6	0	-3.195870	0.364002	1.251502
3	6	0	-3.079485	-0.564937	-0.996890
4	1	0	-4.972378	-0.111736	0.022704
5	1	0	-4.065355	1.307462	-0.506759
6	1	0	-3.499264	-0.429033	1.946583
7	1	0	-3.283380	1.311653	1.787369
8	1	0	-3.129968	-0.268718	-2.048464
9	1	0	-3.334528	-1.631790	-0.926112
10	6	0	-0.548064	-0.987932	-0.965518
11	1	0	-0.510677	-2.038169	-0.643735
12	1	0	-0.606564	-0.988041	-2.062351

13	6	0	0.735006	-0.295907	-0.567224
14	6	0	1.799999	-1.026323	-0.105205
15	6	0	0.894732	1.161614	-0.847017
16	6	0	3.025355	-0.386446	0.198144
17	1	0	1.698959	-2.091720	0.084380
18	6	0	2.206943	1.757307	-0.489251
19	1	0	0.708566	1.340736	-1.921109
20	6	0	3.225817	1.019654	0.008522
21	1	0	2.330789	2.825206	-0.645359
22	1	0	4.187358	1.443708	0.275233
23	7	0	-1.733901	-0.324620	-0.451343
24	6	0	-1.756137	0.092228	0.857514
25	8	0	-0.737158	0.198687	1.538606
26	1	0	0.094876	1.725470	-0.348116
27	8	0	4.061324	-1.043339	0.680314
28	1	0	3.888884	-1.990969	0.812366

Zero-point correction= 0.235946 (Hartree/Particle)
Thermal correction to Energy= 0.248584
Thermal correction to Enthalpy= 0.249528
Thermal correction to Gibbs Free Energy= 0.196191
Sum of electronic and zero-point Energies= -632.364005
Sum of electronic and thermal Energies= -632.351368
Sum of electronic and thermal Enthalpies= -632.350423
Sum of electronic and thermal Free Energies= -632.403761

No imaginary vibrational frequency

mOH-TS-3



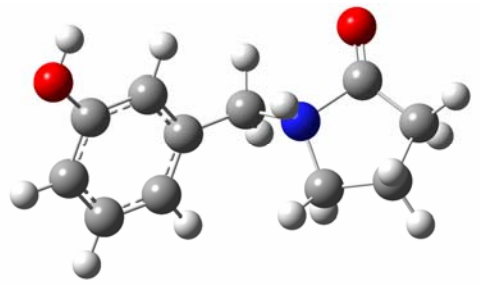
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.545360	0.774193	-0.469277
2	6	0	3.256457	-0.642112	-0.997896
3	6	0	2.675643	0.880749	0.795371

4	1	0	4.600154	0.940800	-0.245020
5	1	0	3.237668	1.528190	-1.200554
6	1	0	3.957403	-1.386046	-0.598088
7	1	0	3.277464	-0.740563	-2.086111
8	1	0	2.390246	1.904730	1.050137
9	1	0	3.161752	0.426438	1.666449
10	6	0	0.459119	-0.288707	1.485564
11	1	0	0.496002	-1.362619	1.677942
12	1	0	0.700465	0.258020	2.401879
13	6	0	-0.867615	0.148212	0.888248
14	6	0	-1.971732	-0.658676	0.768628
15	6	0	-0.746189	1.368125	0.134399
16	6	0	-3.023974	-0.258360	-0.093938
17	1	0	-2.009784	-1.629804	1.255255
18	6	0	-1.818888	1.726527	-0.740653
19	1	0	-0.210119	2.209262	0.587885
20	6	0	-2.926707	0.919231	-0.870583
21	1	0	-1.777394	2.670701	-1.275351
22	1	0	-3.746486	1.170609	-1.534161
23	7	0	1.466072	0.086554	0.437022
24	6	0	1.886481	-0.992120	-0.461417
25	8	0	1.186372	-1.949799	-0.664892
26	1	0	0.491970	0.859168	-0.230867
27	8	0	-4.123308	-0.992540	-0.267554
28	1	0	-4.144082	-1.778417	0.300338

Zero-point correction= 0.231642 (Hartree/Particle)
Thermal correction to Energy= 0.243527
Thermal correction to Enthalpy= 0.244472
Thermal correction to Gibbs Free Energy= 0.193084
Sum of electronic and zero-point Energies= -632.331110
Sum of electronic and thermal Energies= -632.319224
Sum of electronic and thermal Enthalpies= -632.318280
Sum of electronic and thermal Free Energies= -632.369668

One imaginary vibrational frequency, -1481.98

mOH-MH-3



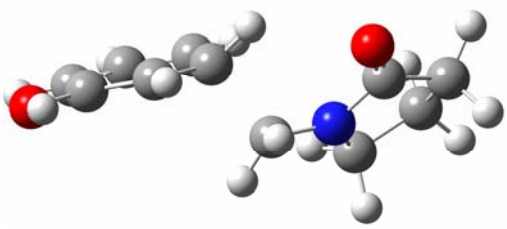
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.135199	1.137109	1.178873
2	6	0	-3.875866	0.068424	0.359352
3	6	0	-1.782049	1.288624	0.469885
4	1	0	-3.669297	2.088148	1.210446
5	1	0	-2.994591	0.803924	2.212529
6	1	0	-4.401968	0.500975	-0.503471
7	1	0	-4.610295	-0.521019	0.914614
8	1	0	-0.985292	1.706242	1.084696
9	1	0	-1.869578	1.875810	-0.448007
10	6	0	-0.434586	-0.286608	-1.103429
11	1	0	-0.531830	-1.331073	-1.407743
12	1	0	-0.801209	0.354221	-1.908211
13	6	0	0.963791	0.062829	-0.673797
14	6	0	1.750473	-0.915425	-0.040972
15	6	0	1.473583	1.348953	-0.880265
16	6	0	3.043157	-0.597015	0.392971
17	1	0	1.375199	-1.930639	0.080316
18	6	0	2.767389	1.656131	-0.441308
19	1	0	0.883734	2.099831	-1.398280
20	6	0	3.547843	0.697983	0.196232
21	1	0	3.171892	2.649171	-0.608582
22	1	0	4.554652	0.921602	0.532082
23	7	0	-1.424241	-0.117898	0.056028
24	6	0	-2.810964	-0.842391	-0.185629
25	8	0	-2.824216	-1.903441	-0.712937
26	1	0	-1.001424	-0.596160	0.862394
27	8	0	3.865695	-1.488612	1.001674
28	1	0	3.472419	-2.371010	1.043652

Zero-point correction= 0.237328 (Hartree/Particle)
Thermal correction to Energy= 0.249887
Thermal correction to Enthalpy= 0.250832
Thermal correction to Gibbs Free Energy= 0.197101

Sum of electronic and zero-point Energies=	-632.364828
Sum of electronic and thermal Energies=	-632.352268
Sum of electronic and thermal Enthalpies=	-632.351324
Sum of electronic and thermal Free Energies=	-632.405055

No imaginary vibrational frequency

mOH-TS-4



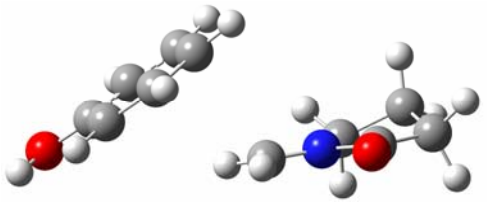
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.536397	1.187357	0.069382
2	6	0	-3.772325	-0.280755	-0.341256
3	6	0	-2.262842	1.161917	0.950285
4	1	0	-3.362912	1.801616	-0.819208
5	1	0	-4.382229	1.619168	0.606324
6	1	0	-4.182320	-0.408521	-1.344751
7	1	0	-4.441936	-0.804054	0.353063
8	1	0	-2.494667	1.141580	2.021325
9	1	0	-1.600895	2.015318	0.765146
10	6	0	-0.320404	-0.486679	0.908665
11	1	0	0.116174	0.109403	1.705797
12	1	0	-0.255033	-1.559821	1.076916
13	6	0	0.820756	-0.347498	-0.476613
14	6	0	0.892439	1.054474	-0.807610
15	6	0	2.045847	-1.006670	-0.075351
16	6	0	2.068307	1.762644	-0.628633
17	1	0	-0.000069	1.554620	-1.170048
18	6	0	3.213618	-0.286659	0.102691
19	1	0	2.022015	-2.077937	0.111479
20	6	0	3.214226	1.104412	-0.168485
21	1	0	2.115089	2.824243	-0.846878
22	1	0	4.141063	1.649686	-0.014319
23	7	0	-1.605087	-0.097851	0.568245
24	6	0	-2.407074	-0.924775	-0.235730
25	8	0	-1.981684	-1.956999	-0.721741
26	1	0	0.190719	-0.957951	-1.137019

27	8	0	4.392453	-0.804108	0.506336
28	1	0	4.347557	-1.760144	0.653616

Zero-point correction= 0.234598 (Hartree/Particle)
Thermal correction to Energy= 0.246911
Thermal correction to Enthalpy= 0.247855
Thermal correction to Gibbs Free Energy= 0.195424
Sum of electronic and zero-point Energies= -632.335061
Sum of electronic and thermal Energies= -632.322748
Sum of electronic and thermal Enthalpies= -632.321804
Sum of electronic and thermal Free Energies= -632.374235

One imaginary vibrational frequency, -90.7612

mOH-MH-4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.370065	-1.457153	0.363392
2	6	0	-4.004146	-0.098315	0.013945
3	6	0	-2.044379	-1.489222	-0.424524
4	1	0	-3.169613	-1.515256	1.437132
5	1	0	-4.008405	-2.300099	0.095994
6	1	0	-4.649698	0.320209	0.788893
7	1	0	-4.596679	-0.146856	-0.910439
8	1	0	-2.179204	-1.872765	-1.441215
9	1	0	-1.247321	-2.050913	0.065874
10	6	0	-0.495492	0.436381	-0.777018
11	1	0	0.334905	-0.208788	-1.038851
12	1	0	-0.419279	1.517430	-0.839738
13	6	0	1.993456	1.528764	0.678808
14	6	0	1.230940	0.596527	1.404313
15	6	0	3.000692	1.102628	-0.183260
16	6	0	1.538922	-0.775027	1.295609
17	1	0	0.489477	0.938282	2.119755
18	6	0	3.280705	-0.271212	-0.303231
19	1	0	3.588426	1.827972	-0.740115
20	6	0	2.545065	-1.212140	0.440900

21	1	0	1.003945	-1.499851	1.903038
22	1	0	2.804024	-2.262278	0.356487
23	7	0	-1.662343	-0.060778	-0.520408
24	6	0	-2.843537	0.823285	-0.244446
25	8	0	-2.731620	2.011935	-0.262996
26	1	0	1.802083	2.591910	0.792090
27	8	0	4.248781	-0.758432	-1.111807
28	1	0	4.753498	-0.048661	-1.534541

Zero-point correction= 0.233535 (Hartree/Particle)
Thermal correction to Energy= 0.247267
Thermal correction to Enthalpy= 0.248211
Thermal correction to Gibbs Free Energy= 0.189848
Sum of electronic and zero-point Energies= -632.352576
Sum of electronic and thermal Energies= -632.338844
Sum of electronic and thermal Enthalpies= -632.337900
Sum of electronic and thermal Free Energies= -632.396263

No imaginary vibrational frequency