

Supporting Information

Density functional theory–based investigation of HCN and NH₃ formation mechanisms during phenylalanine pyrolysis

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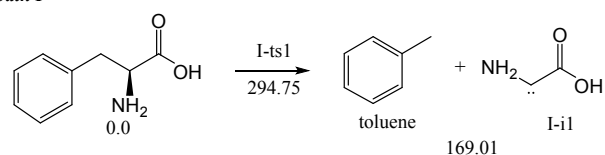
E-mail address: guoshuaidq@126.com (S. Guo)

Possible NH₃ and HCN formation paths (S1-S3)

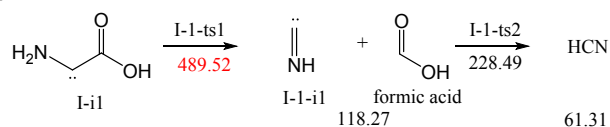
S1: Possible pyrolytic paths affording NH₃ and HCN via 1,2-hydrogen migration reactions of Phe

As shown in Fig. S1, hydrogen transfer from C2 to C3 is accompanied by C2–C3 bond scission, with five paths of subsequent HCN generation available. Among them, paths I-3, I-4, and I-5 are preferred, featuring overall energy barriers of 369.28, 405.28, and 395.68 kJ/mol, respectively. Hence, only these three paths are discussed in detail herein.

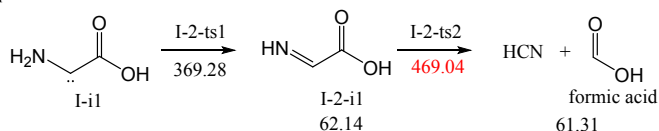
path I



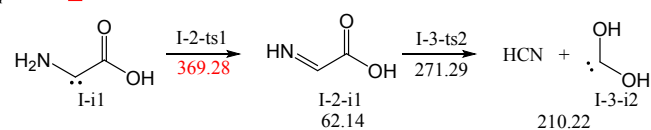
path I-1 $\Delta G = 489.52$



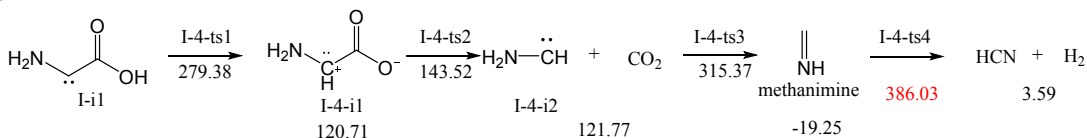
path I-2 $\Delta G = 469.04$



path I-3 $\Delta G = 369.28$



path I-4 $\Delta G = 405.28$



path I-5 $\Delta G = 395.68$

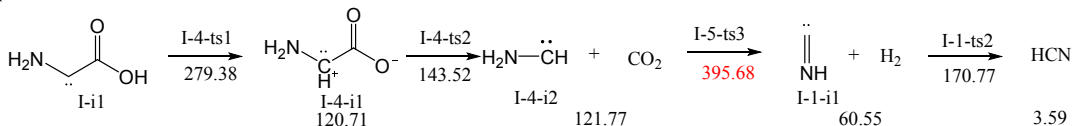


Fig. S1. Five HCN generation paths featuring hydrogen transfer from C2 to C3 as the initial step. Numbers refer to energies in kJ/mol.

In Path I-3, I-1-i1 isomerizes into I-2-i1 via a three-membered ring transition state, I-2-ts1. Then, I-2-i1 decomposes to form HCN and I-3-i2. The rate-determining step of Path I-3 corresponds to isomerization, and the overall energy barrier equals 369.28 kJ/mol.

In path I-4, decarboxylation occurs through transition states I-4-ts1 and I-4-ts2. The energy barrier of the first-step transfer of the carboxyl proton to C2 is 110.37 kJ/mol, while that of C1–C2 bond cleavage to form CO₂ and carbene I-4-i2 (via I-4-ts2) is 143.52 kJ/mol. Apparently, the above decarboxylation is much easier to achieve than the first step of path I-3. I-4-i2 subsequently undergoes 1,2-hydrogen migration to afford methylamine.

In path I-5, decarboxylation is also achieved via I-4-ts1 and I-4-ts2, and is followed by the decomposition of I-4-i2 to form I-1-i1 and H₂. Finally, I-1-i1 affords HCN through a three-membered ring transition state, I-1-ts2. The overall energy barrier for this path equals 395.68 kJ/mol.

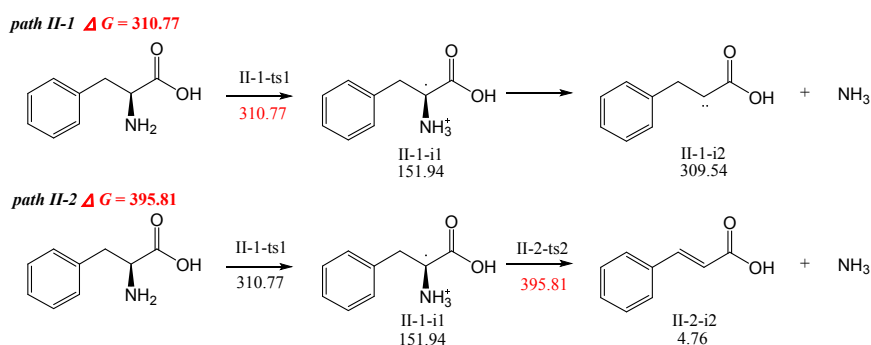


Fig. S2. NH₃ generation paths featuring hydrogen transfer from C2 to N4. Numbers refer to energies in kJ/mol.

Fig. S2 illustrates the two paths of NH_3 formation imitated by proton transfer from C2 to N4 (energy barrier = 310.77 kJ/mol). In path II-1, II-1-i1 directly decomposes to form II-1-i2 and NH_3 without a transition state, while path II-2 features hydrogen transfer from C3 to N4 through transition state II-2-ts2 (energy barrier = 243.87 kJ/mol).

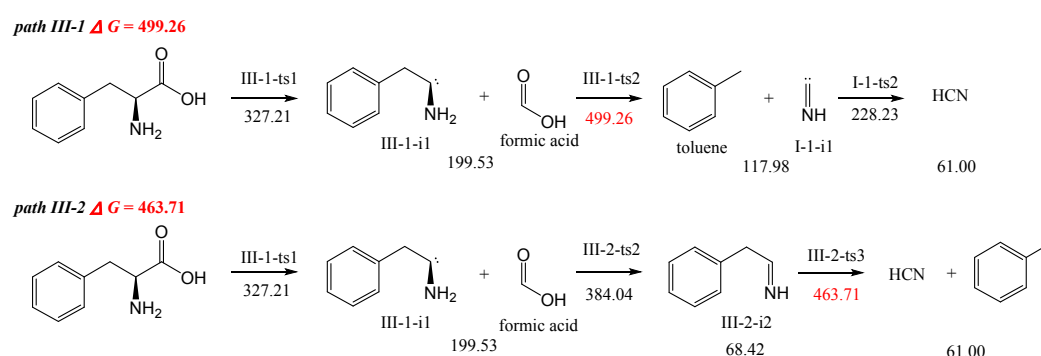


Fig. S3. HCN generation paths III-1 and III-2. Numbers refer to energies in kJ/mol.

Fig. S3 depicts HCN formation paths III-1 and III-2, both of which are initiated by 1,2-hydrogen migration followed by rearrangement to afford carbene III-1-i1 and formic acid. III-1-i1 directly fragments to toluene and I-1-i1, and I-1-i1 isomerizes to HCN. In path III-2, the above carbene isomerizes to 2-phenylethan-1-imine, which decomposes to HCN and toluene. The overall energy barrier of path III-2 (463.71 kJ/mol) is lower than that of path III-1, suggesting that the former route is feasible.

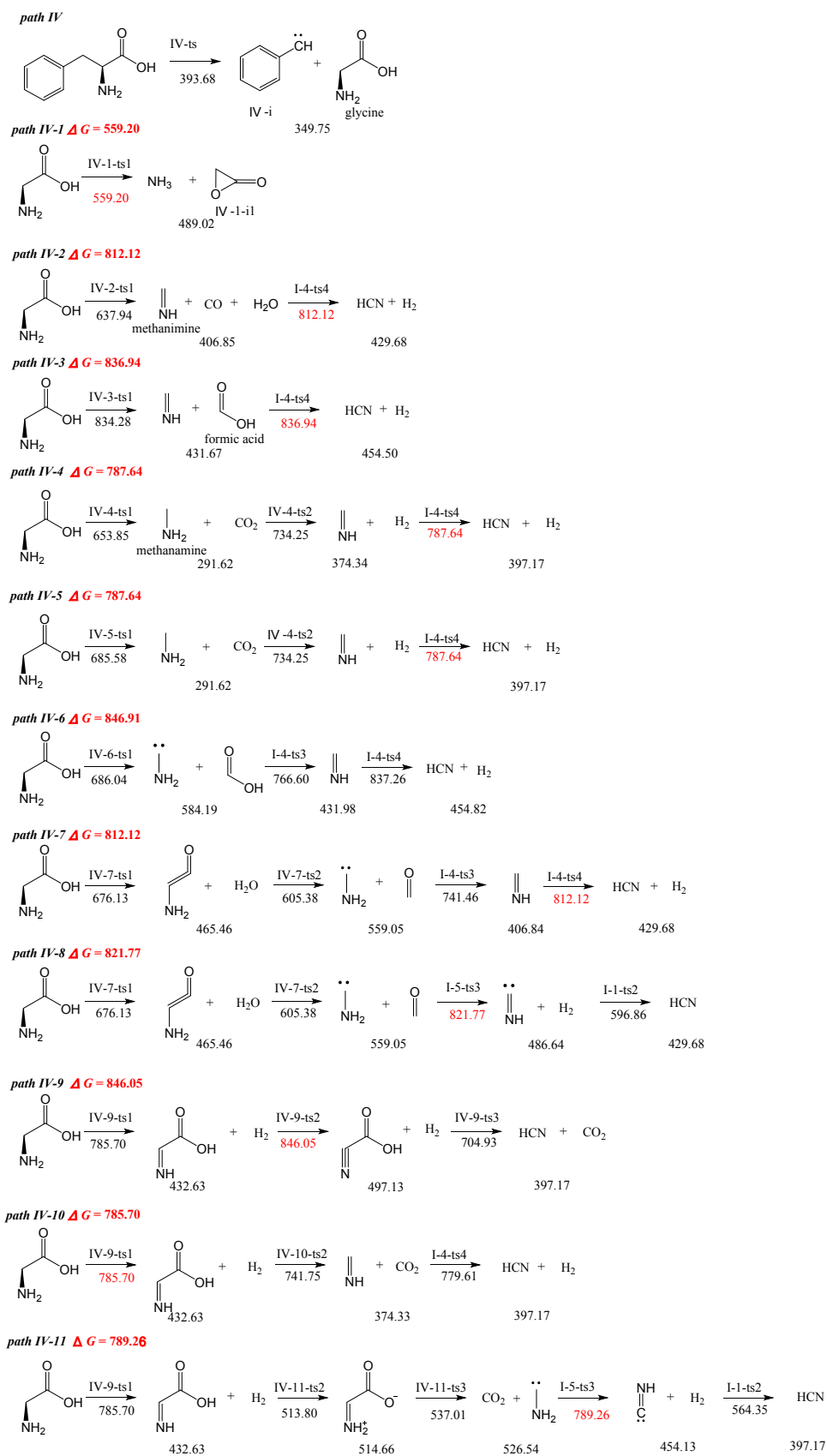


Fig. S4. Phe decomposition paths starting from the transfer of hydrogen from C3 to

C2 to form IV-i and glycine. Numbers refer to energies in kJ/mol.

Fig. S4 presents the 11 paths of Phe decomposition starting from the transfer of hydrogen from C3 to C2 to form IV-i and glycine. Among them, path IV-1 affords NH_3 , and the other 10 paths generate HCN. For path IV-1, the energy barrier of the rate-determining step (209.45 kJ/mol) is much smaller than that of other paths, while the lowest energy barrier of continuous glycine decomposition is lowest for IV-1-ts1. Thus, one can conclude that this series of paths is more likely to generate NH_3 than HCN.

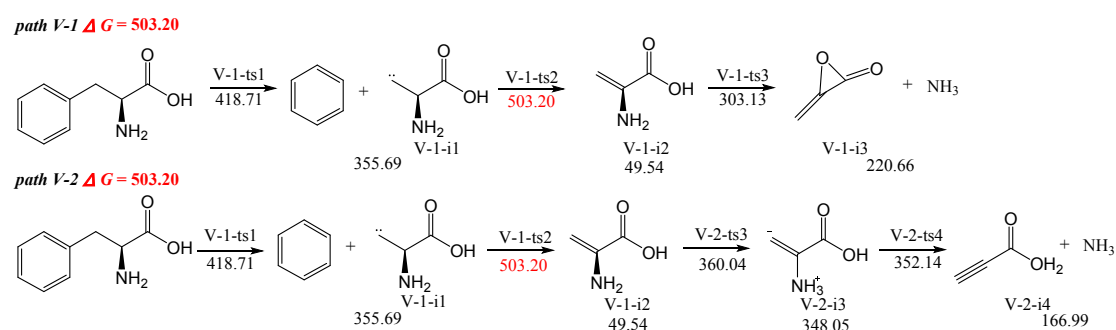


Fig. S5. Phe decomposition paths starting from the transfer of hydrogen from C3 to C7 to form benzene rings and V-1-i1. Numbers refer to energies in kJ/mol.

Fig. S5 shows Phe decomposition paths starting from the transfer of hydrogen from C3 to C7 to form benzene rings and V-1-i1 (an unstable carbene), with the corresponding energy barrier equaling 418.71 kJ/mol. Subsequently, the hydrogen atom on C2 is transferred to C3 to afford dehydroalanine featuring a double C2–C3 bond. The total Gibbs free energy of dehydroalanine and benzene (49.54 kJ/mol) is much lower than that of benzene and V-1-i1, i.e., dehydroalanine is more stable than V-1-i1. Next, dehydroalanine decomposes to generate NH_3 in two ways. In path V-1, the carboxyl hydrogen is transferred to the amino group, which is directly deaminated

to form NH_3 (energy barrier = 253.59 kJ/mol). In path V-2, hydrogen is transferred from C3 to N4 to afford a positively charged $-\text{NH}_3^+$ group and negatively charged C3 (no chemical bond cleavage occurs). Subsequently, the C2–N4 bond in V-2-i3 is broken, and the C2–C3 bond changes from a double bond to a triple one to generate NH_3 and propiolic acid.

For these two paths, the energy barriers of the rate-determining step are the same, but the energy barrier of V-1-ts3 is lower than that of V-2-ts3. So, path V-1 is preferred.

S2: Possible pyrolytic paths affording NH_3 and HCN via 1,3-hydrogen migration reactions of Phe

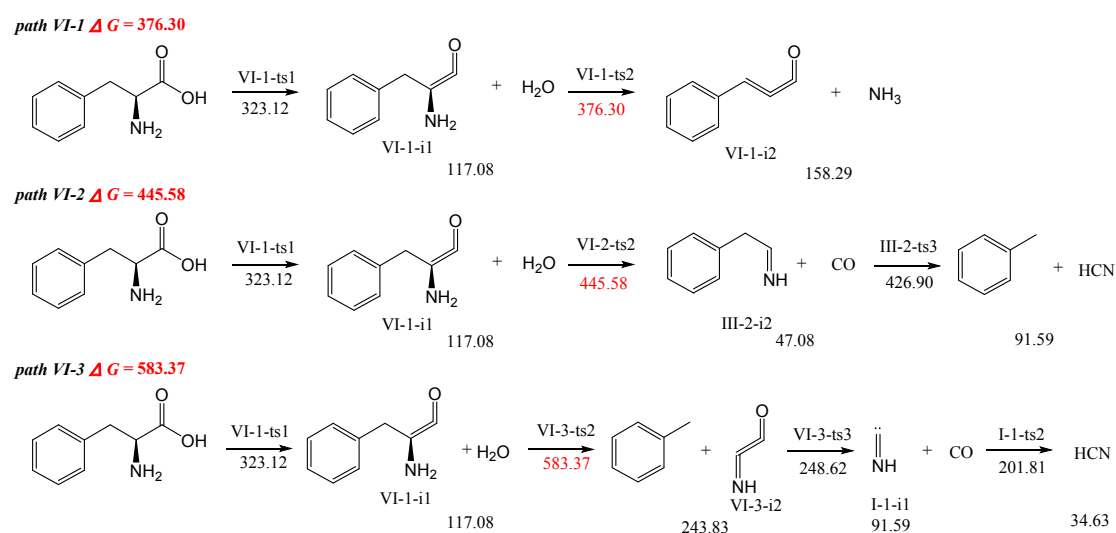


Fig. S6. Phe decomposition paths starting from a 1,2-dehydration reaction between OH and C2-H. Numbers refer to energies in kJ/mol.

Fig. S6 shows paths starting from the 1,2-dehydration of Phe between OH and C2-H via a four-membered ring transition state, I-3-ts2 (energy barrier = 323.12 kJ/mol).

The thus produced intermediate VI-1-i1 subsequently decomposes in one of the three

possible ways.

In path VI-1, VI-1-i1 decomposes through transition state VI-1-ts2 to generate VI-1-i2 (energy barrier = 259.22 kJ/mol). In this process, hydrogen on C3 is transferred to N4, the C3–C2 bond changes from a single bond to a double one, and the C2–N4 bond is broken to generate NH₃. In path VI-2, VI-1-i1 undergoes decarbonylation to form 2-phenylethan-1-imine, which decomposes into toluene and HCN. In path VI-3, VI-1-i1 undergoes 1,2-hydrogen migration, the C2–C3 bond is cleaved to form toluene and VI-3-i2, and intermediate VI-3-i2 decomposes into CO and I-1-i1. Finally, I-1-i1 isomerizes to HCN. The lowest overall energy barrier of 376.3 kJ/mol is observed for path VI-1, which is therefore the most preferred one among the above three paths.

The direct decarboxylation of Phe can be achieved by elimination of CO₂ from the –COOH group attached to C2 and H transfer to the same (Fig. S7). This reaction is slightly exothermic and has a free Gibbs energy of activation equaling 304.85 kJ/mol (VII-ts). The thus produced phenethylamine can further decompose to afford NH₃ or HCN via six possible paths, among which only one (VII-1) affords NH₃ (and styrene) with an energy barrier of 256.46 kJ/mol. The structure of transition state VII-1-ts1 suggests that hydrogen on C3 is transferred to N4, the C2–N4 bond is broken, and the C2–C3 bond changes from a single bond to a double one. In the paths of phenethylamine decomposition to HCN, C2–C3 cleavage (paths VII-5 and VII-6) is the easiest way to generate toluene and I-4-i2 (energy barrier = 291.39 kJ/mol). Then, HCN can be generated from I-4-i2 in two ways, as shown in Fig. S1.

The overall energy barrier for HCN formation is between 395 and 426 kJ/mol, being

much higher than the energy barrier for NH_3 generation. So, phenethylamine decomposition preferentially affords NH_3 .

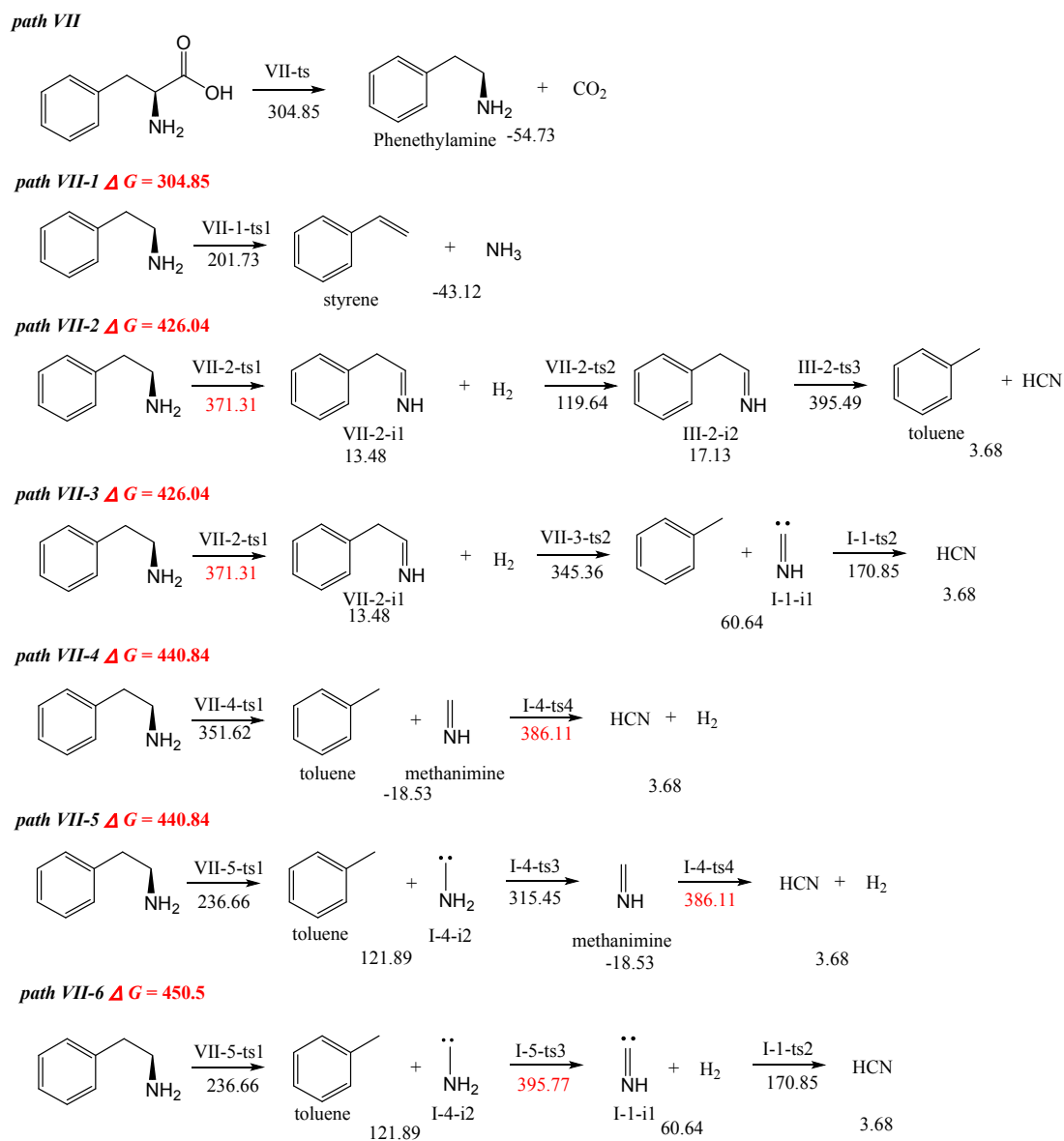


Fig. S7. Phe decomposition paths starting from direct decarboxylation. Numbers refer to energies in kJ/mol.

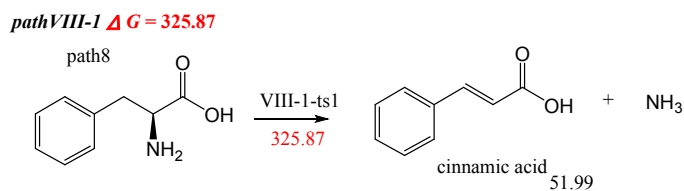


Fig. S8. Direct production of NH_3 from Phe via 1,3-hydrogen migration between $-\text{NH}_2$ and C3. Numbers refer to energies in kJ/mol.

As shown in Fig. S8, NH_3 and cinnamic acid can be directly produced from Phe via 1,3-hydrogen migration between $-\text{NH}_2$ and C3 via a four-membered ring transition state, VIII-1-ts1 (energy barrier = 325.87 kJ/mol).

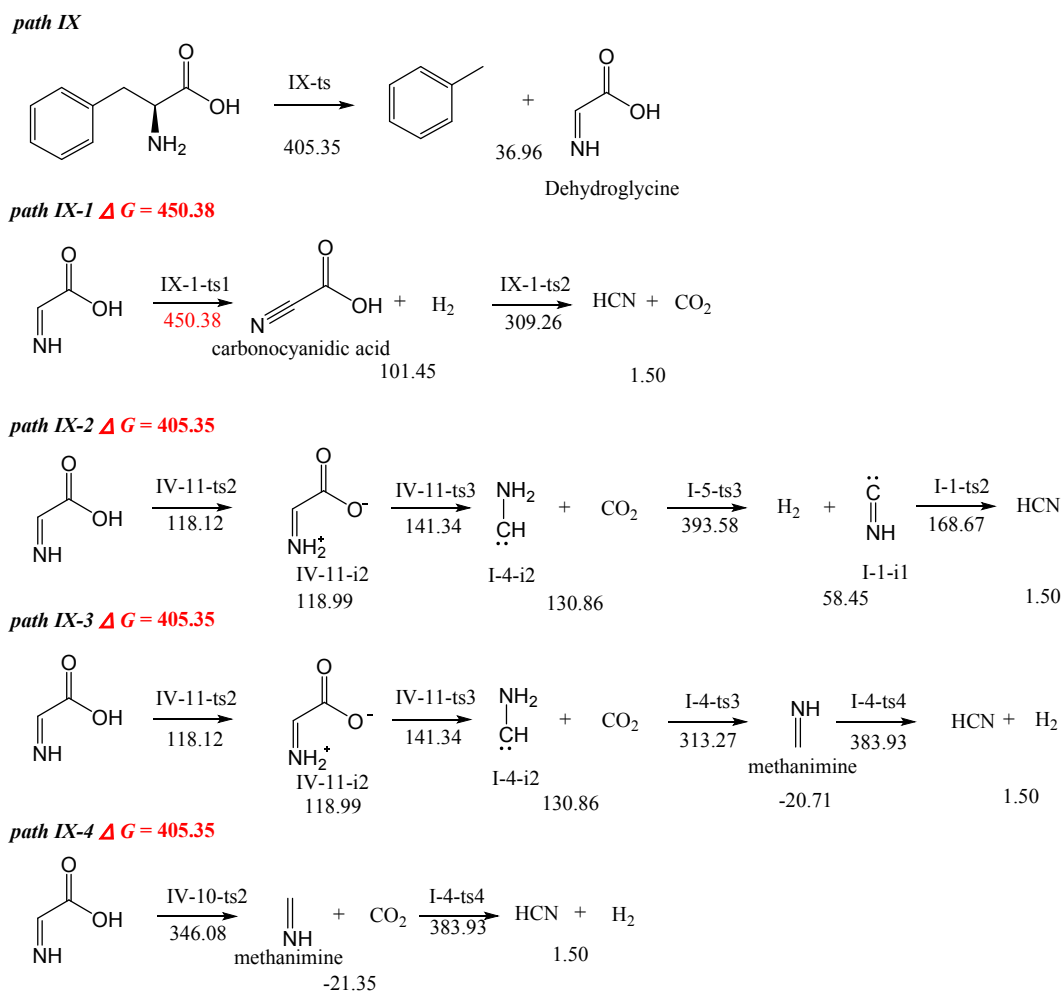


Fig. S9. Phe decomposition paths involving the initial formation of dehydroglycine.

Numbers refer to energies in kJ/mol.

As shown in Fig. S9, transfer of H on N4 to C3 affords toluene and dehydroglycine, which can subsequently afford HCN via four paths, e.g., via the formation of a zwitterion (paths IX-2 and IX-3; energy barrier = 81.16 kJ/mol). Although the electron energy of IV-11-i2 is lower than that of dehydroglycine, the free energy of the former is higher than that of dehydroglycine. Subsequently, IV-11-i2 further decomposes into I-4-i2 and CO₂ (energy barrier = 22.35 kJ/mol), and I-4-i2 affords HCN via two paths.

S3: Possible pyrolytic paths affording NH₃ and HCN via 1,4-hydrogen migration reactions of Phe

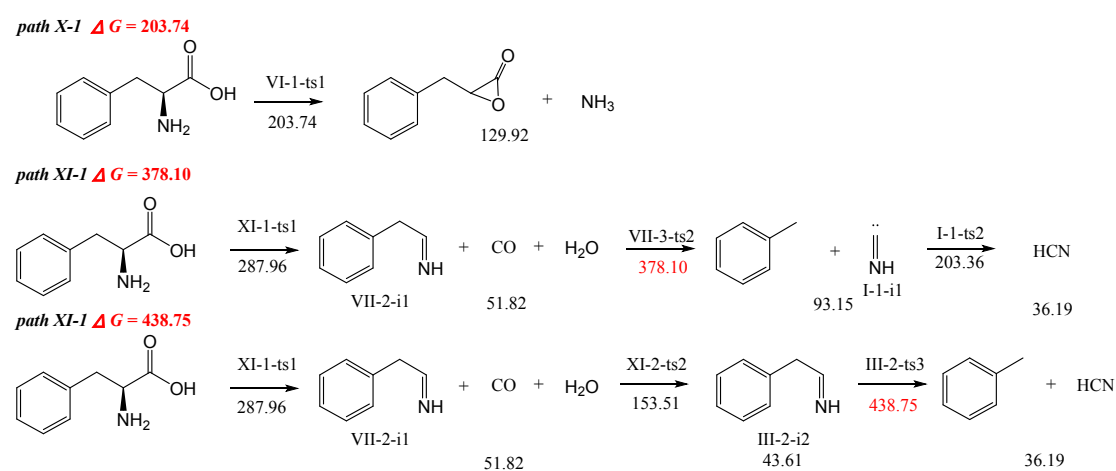


Fig. S10. Phe decomposition paths involving 1,4-hydrogen migration. Numbers refer to energies in kJ/mol.

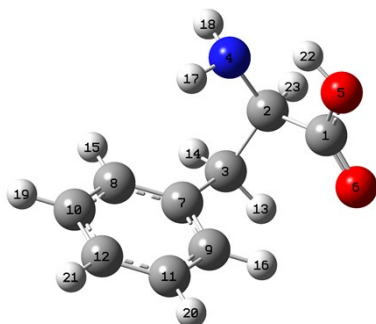
Only three paths feature 1,4-hydrogen transfer as the initial step to generate NH₃ or HCN (Fig. S10). In path X-1, the carboxyl hydrogen is transferred to the amino group,

and the C2–N4 bond is cleaved to generate NH₃. In paths XI-1 and XI-2, hydrogen on N4 is first transferred to O5, which is followed by decomposition into CO, H₂O, and VII-2-i2. Then, VII-2-i2 undergoes the reactions described in path VII to generate HCN.

Cartesian coordinates (X, Y, Z) and vibrational frequencies (cm⁻¹)

S4: Geometries at the M06-2X/6-311G(d,p) level. X, Y, Z Cartesian coordinates in Angstrom (Å) and vibrational frequencies of transient states

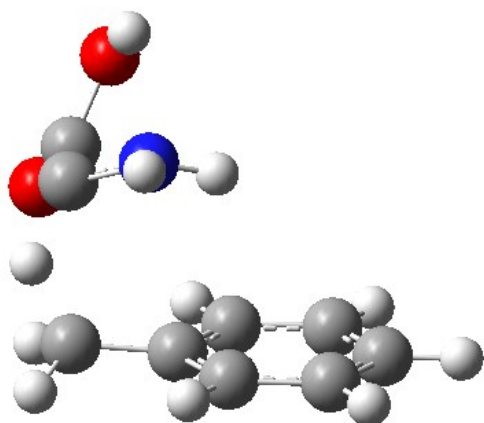
Phenylalanine (Phe)



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6	1.660270	0.822124	-0.352643
6	-0.779967	0.245635	-0.694505
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6	-1.017327	-1.108543	-0.441846
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6	-2.176179	-1.510576	0.211826
6	-3.113930	-0.569319	0.625117
1	0.802177	-0.014527	-2.125503
1	0.344844	1.668673	-1.831717
1	-1.565569	2.234346	-0.486650
1	-0.286137	-1.842400	-0.761496
1	0.436592	1.501328	1.147999
1	1.533335	2.617312	0.658553
1	-3.619021	1.518921	0.686359

1	-2.348345	-2.564172	0.396800
1	-4.016985	-0.886446	1.132546
6	2.161264	-0.567976	0.083096
8	2.600322	-0.615582	1.336853
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1	2.515855	1.268013	-0.870758

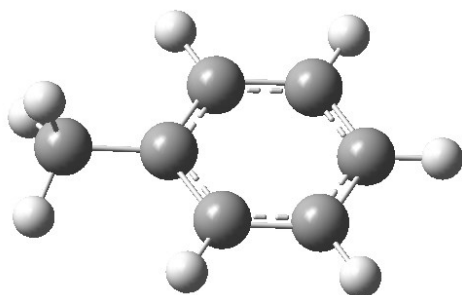
I -ts



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6	1.835239	1.150938	0.157607
6	0.873505	-0.974816	0.756983
6	2.856714	0.498601	-0.526506
6	1.890441	-1.622806	0.070255
6	2.888730	-0.889897	-0.570761
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1	-0.037050	2.124403	1.819026
1	1.817707	2.235563	0.196903
1	0.092751	-1.542617	1.251356
1	-0.203292	0.320896	-1.617415
1	-0.639035	1.951041	-1.819686
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1	1.909455	-2.705690	0.039069
1	3.685326	-1.400458	-1.098015
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8	-2.726416	-0.954848	-1.081657
8	-2.417125	-0.761343	1.104196

1	-2.561186	-0.419026	-1.865873	
1	-1.270706	1.591016	0.685616	
Vibrational		frequencies		(cm ⁻¹)
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241.21	294.99	373.52		
384.76	412.58	417.50		
515.26	534.46	563.28		
589.29	631.85	647.65		
677.52	720.51	731.40		
763.07	789.88	831.26		
844.87	879.68	922.12		
949.62	1007.21	1016.32		
1024.17	1028.04	1061.89		
1082.20	1122.39	1171.65		
1178.73	1202.48	1206.92		
1265.18	1309.31	1334.00		
1348.80	1359.25	1419.21		
1480.72	1496.22	1539.28		
1648.74	1671.85	1674.48		
1845.29	2086.24	3113.27		
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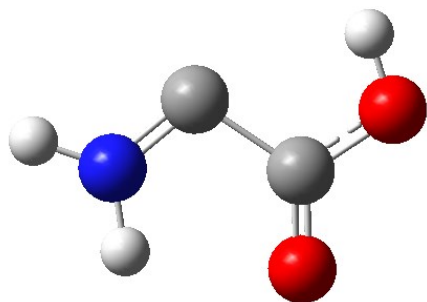
Toluene



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6	1.195798	-1.201028	0.002089
6	1.195895	1.200973	0.002088
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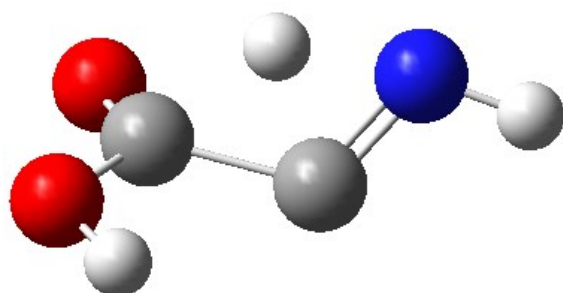
1	-2.817326	-0.883780	-0.488724
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1	1.732339	-2.142612	0.001939
1	1.732497	2.142522	0.001944
1	2.979764	-0.000084	0.013846
1	-2.787317	-0.001234	1.038151

I -i1



Atomic Number	X	Y	Z
7	-1.768136	0.089074	0.000161
6	-0.719691	0.846994	-0.000314
1	-1.684205	-0.934713	0.000509
1	-2.697467	0.487518	0.000091
6	0.495063	-0.110712	-0.000072
8	1.650911	0.548332	0.000170
8	0.433733	-1.308773	-0.000102
1	1.429238	1.489507	0.000043

I -1-ts1



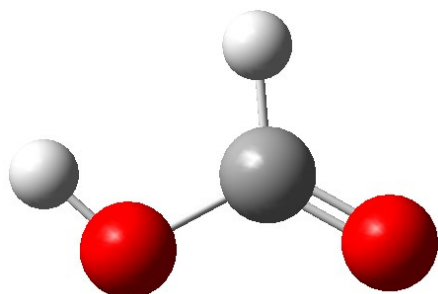
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8	-1.352365	-0.933623	0.120634
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Vibrational frequencies (cm⁻¹)

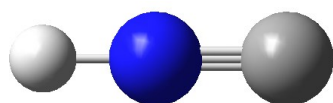
-1713.06	115.65	298.58
356.54	435.76	504.59
560.12	615.02	779.17
898.66	1151.85	1278.02
1308.07	1575.93	1857.20
2186.41	3430.36	3854.26

Formic acid



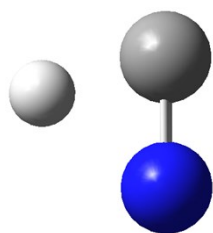
Atomic Number	X	Y	Z
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I -1-i1



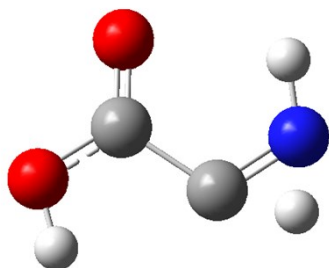
Atomic Number	X	Y	Z
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I -1-ts2



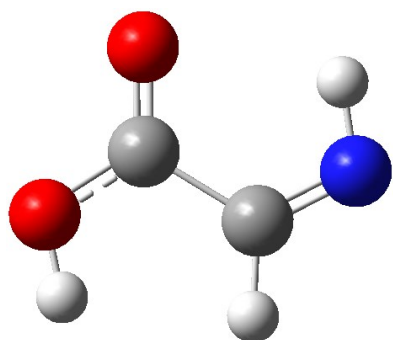
Atomic Number	X	Y	Z
7	0.081140	-0.567789	0.000000
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Vibrational frequencies (cm ⁻¹)			
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I -2-ts1



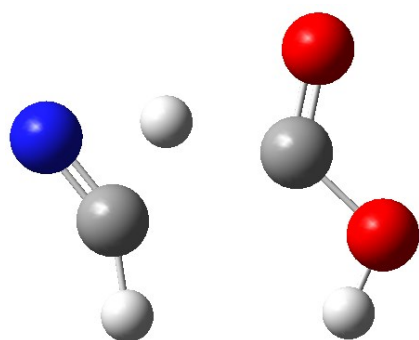
Atomic Number	X	Y	Z
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1	1.839152	-1.165975	0.456546
6	-0.508625	0.116612	-0.016118
8	-1.637782	-0.582368	0.039476
8	-0.466316	1.309839	-0.002861
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Vibrational frequencies (cm ⁻¹)			
-1873.31	119.19	299.92	
370.16	500.17	612.15	
641.44	702.31	859.24	
1026.42	1229.96	1302.47	
1381.15	1585.01	1916.95	
2489.96	3210.72	3828.29	

I -2-i1



Atomic Number	X	Y	Z
7	1.941591	-0.084743	0.000219
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6	-0.478818	0.139827	-0.000090
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I -2-ts2



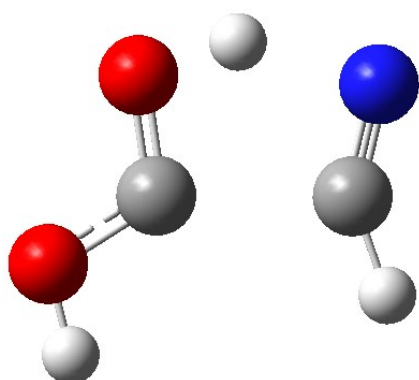
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7	-2.158871	0.294628	0.000193
6	-1.410216	-0.639494	0.000192
1	-0.804318	0.474085	0.000044
1	-1.245529	-1.715019	0.000263
6	0.664975	0.125657	-0.000078
8	1.639416	-0.802470	-0.000098
8	0.908396	1.295415	-0.000194
1	1.250892	-1.681995	-0.000002

Vibrational frequencies (cm⁻¹)

-2121.74	60.53	105.83
261.63	330.10	506.77
511.43	632.73	691.83
761.73	1027.68	1201.71

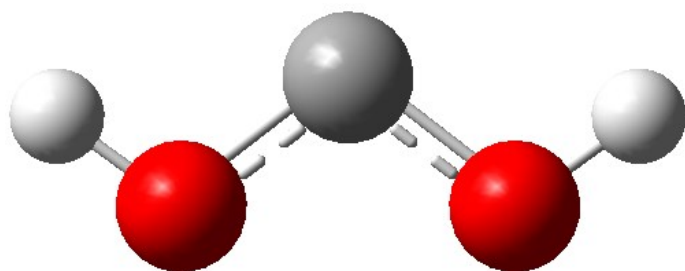
1292.48	1745.15	1932.22
2160.83	3143.68	3895.19

I -3-ts2



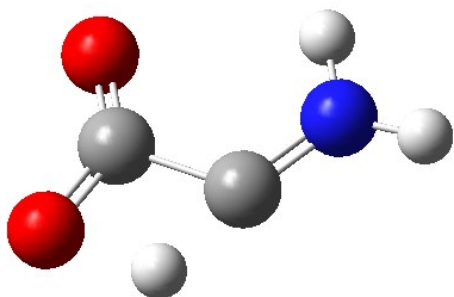
Atomic Number	X	Y	Z
7	-1.947352	0.180857	-0.000001
6	-1.289651	-0.802917	0.000000
1	-0.740690	1.095746	0.000000
1	-1.267042	-1.879714	0.000002
6	0.599578	-0.089555	0.000000
8	1.885811	-0.359674	0.000000
8	0.337124	1.133177	0.000000
1	1.996154	-1.315226	0.000000
Vibrational frequencies (cm ⁻¹)			
-455.52	235.45	350.17	
388.28	597.14	646.74	
670.06	822.84	1009.58	
1218.95	1227.54	1268.42	
1382.23	1663.94	1978.09	
2230.14	3309.23	3887.66	

I -3-i2



Atomic Number	X	Y	Z
1	-1.823757	0.314577	-0.000000
6	-0.000000	0.556636	-0.000000
8	1.045135	-0.248171	0.000000
8	-1.045120	-0.247947	0.000000
1	1.823638	0.314554	-0.000000

I -4-ts1

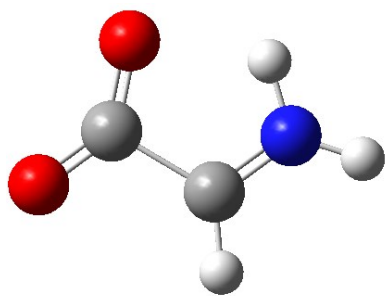


Atomic Number	X	Y	Z
7	1.794683	0.015351	0.032964
6	0.698875	-0.634305	-0.082992
1	1.723240	1.037651	0.091316
1	2.711340	-0.414236	0.060954
6	-0.619251	0.137451	-0.023194
8	-1.418330	-0.864935	0.048318
8	-0.735330	1.339950	-0.010412
1	-0.245826	-1.549868	-0.049153

Vibrational frequencies (cm⁻¹)

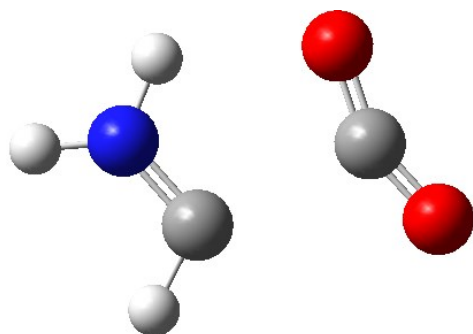
-1642.88	33.42	236.62
542.84	673.57	686.97
830.29	883.54	905.29
1123.24	1265.18	1355.89
1550.80	1701.69	1871.24
2148.19	3400.40	3624.73

I -4-i1



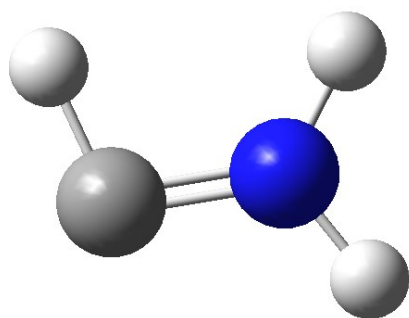
Atomic Number	X	Y	Z
7	1.717491	0.008530	0.000016
6	0.688873	-0.742800	-0.000026
1	1.430155	1.009473	-0.000057
1	2.681851	-0.300573	0.000046
6	-0.688452	0.072101	-0.000011
8	-1.667925	-0.648609	0.000012
8	-0.447310	1.283756	0.000003
1	0.784909	-1.825589	0.000000

I -4-ts2



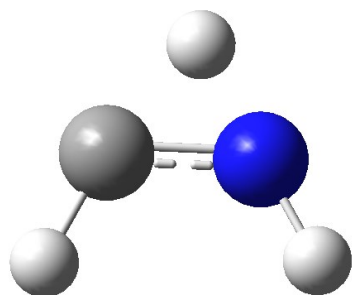
Vibrational	frequencies		(cm ⁻¹)
-206.14	715.37	1521.92	
106.13	883.66	1685.17	
248.36	1045.97	2274.57	
386.37	1156.34	3061.90	
392.12	1337.10	3445.31	
624.02	1379.56	3564.27	

I -4-i2



Atomic Number	X	Y	Z
7	0.525578	0.024110	0.000006
6	-0.765974	-0.191655	-0.000008
1	1.161077	-0.764149	0.000020
1	0.988594	0.931577	0.000005
1	-1.232877	0.813733	-0.000022

I -4-ts3

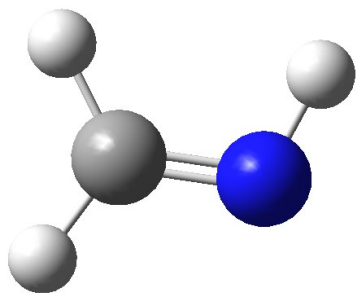


Atomic Number	X	Y	Z
7	0.614012	0.026287	-0.064369
6	-0.709043	0.083721	-0.051818
1	-1.243712	-0.856479	0.176531
1	1.099277	-0.840266	0.217207
1	0.100611	1.010414	0.367750

Vibrational frequencies (cm⁻¹)

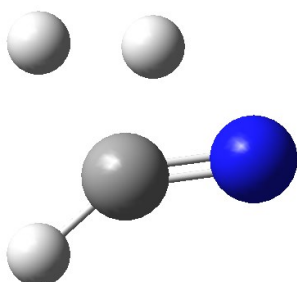
-1968.19	477.43	1143.72
1189.16	1396.50	1509.61
2544.59	2955.45	3278.64

I -4-i3



Atomic Number	X	Y	Z
7	0.665705	-0.154487	0.000036
6	-0.583338	0.028682	-0.000101
1	1.154590	0.743029	-0.000048
1	-1.073508	1.007597	0.000235
1	-1.240987	-0.841310	0.000172

I -4-ts4

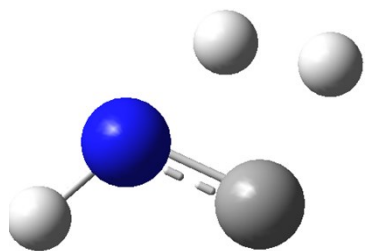


Atomic Number	X	Y	Z
7	0.867103	-0.430525	-0.002261
6	-0.290706	-0.066927	0.001720
1	0.461593	0.920926	-0.004769
1	-0.491713	1.410537	-0.001537
1	-1.335971	-0.383056	0.007000

Vibrational frequencies (cm⁻¹)

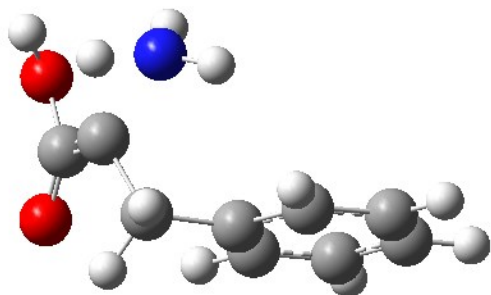
-2457.95	505.85	907.81
915.67	1323.64	1650.47
1895.55	2371.18	3110.74

I -5-ts3



Atomic Number	X	Y	Z
7	-0.591100	0.157020	-0.000008
6	0.616656	-0.357831	0.000007
1	-1.327913	-0.547897	-0.000021
1	0.399344	0.966110	0.000011
1	1.366333	0.629630	0.000022
Vibrational frequencies (cm ⁻¹)			
-1810.47	74.04	1003.67	
1180.33	1341.79	1526.54	
2183.78	2330.92	3466.46	

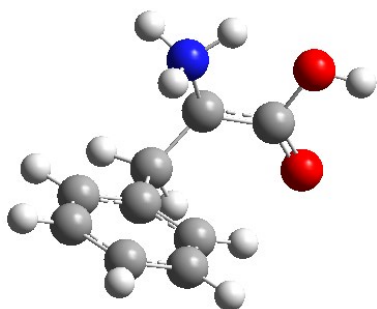
II -1-ts1



Atomic Number	X	Y	Z
7	-1.160632	1.512255	-1.040753
6	-0.411677	0.760730	1.297242
6	-1.557654	0.793921	0.317874
6	0.865765	0.245947	0.667776
6	1.936635	1.104203	0.418645
6	0.961111	-1.086804	0.252273
6	3.084658	0.647916	-0.227713
6	2.105834	-1.543104	-0.386875
6	3.170376	-0.677110	-0.631781
1	-0.731003	0.101467	2.107126
1	-0.231856	1.746880	1.735802
1	1.881418	2.136095	0.754719
1	0.130496	-1.757592	0.444938
1	-1.349561	0.933636	-1.854333
1	-0.204700	1.854509	-1.001379
1	3.909697	1.327135	-0.407776
1	2.171633	-2.580415	-0.693536
1	4.062010	-1.037905	-1.130260
6	-2.306785	-0.421829	0.093813
8	-3.080734	-0.442933	-1.057632
8	-2.314566	-1.384214	0.815991
1	-3.470806	0.424819	-1.199140
1	-1.970089	1.939543	-0.345279
Vibrational frequencies (cm ⁻¹)			
-1644.93	41.66	67.35	
87.98	122.77	181.53	
207.50	239.46	279.95	
363.70	372.51	416.74	
419.91	483.47	538.54	
565.93	630.94	635.48	
718.77	728.72	766.57	
784.20	836.99	878.42	

887.17	924.07	951.62
983.35	1010.74	1018.08
1029.23	1037.70	1063.28
1106.98	1127.80	1176.64
1189.47	1207.69	1221.17
1232.45	1306.80	1341.71
1363.44	1369.53	1454.81
1479.05	1495.79	1538.19
1560.93	1656.39	1677.76
1838.20	2468.57	3065.16
3127.76	3175.40	3199.05
3206.37	3214.15	3225.97
3487.87	3613.77	3884.33

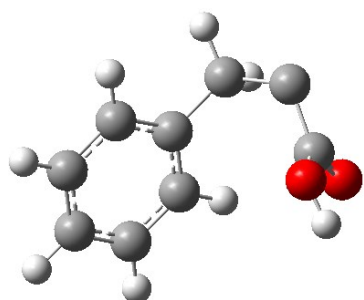
II -1-i1



Atomic Number	X	Y	Z
7	1.179616	-1.452587	-1.006782
6	0.387952	-0.787056	1.268472
6	1.503710	-0.773432	0.271078
6	-0.902247	-0.260489	0.665888
6	-1.992104	-1.092559	0.415844
6	-0.970948	1.077690	0.258322
6	-3.136873	-0.602872	-0.214571
6	-2.111314	1.568575	-0.360858
6	-3.198934	0.728204	-0.601316
1	0.711680	-0.139252	2.085831
1	0.210987	-1.781931	1.696357
1	-1.953197	-2.130059	0.735856
1	-0.115117	1.720691	0.443445
1	1.876555	-1.139735	-1.692107
1	0.239898	-1.201179	-1.352670
1	-3.977656	-1.262208	-0.396608
1	-2.157787	2.610235	-0.656486

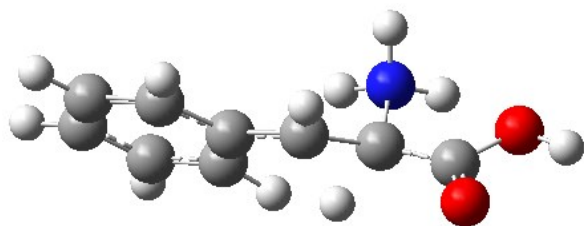
1	-4.087961	1.114086	-1.085563
6	2.346506	0.333542	0.121255
8	3.007036	0.337050	-1.117280
8	2.574071	1.235609	0.911799
1	3.570465	1.117404	-1.092706
1	1.221476	-2.470838	-0.938701

II -1-i2



Atomic Number	X	Y	Z
6	0.725764	1.455843	-0.739388
6	2.006119	1.166015	-0.103401
6	-0.516187	0.652630	-0.424142
6	-1.526283	1.236277	0.336644
6	-0.661911	-0.666659	-0.856190
6	-2.666283	0.512970	0.669314
6	-1.803255	-1.387432	-0.525882
6	-2.806917	-0.800694	0.238015
1	1.128628	1.172529	-1.746717
1	0.529638	2.526863	-0.816328
1	-1.418400	2.262229	0.672383
1	0.119836	-1.129123	-1.448885
1	-3.444124	0.977178	1.263715
1	-1.910696	-2.408409	-0.872070
1	-3.696323	-1.364376	0.492725
6	2.203264	-0.230551	0.244824
8	2.010159	-0.494810	1.541513
8	2.582417	-1.034988	-0.573727
1	2.224965	-1.428897	1.674121

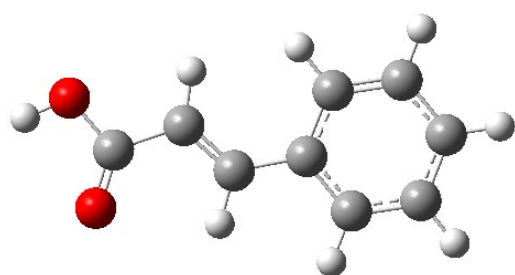
II -2-ts2



Atomic Number	X	Y	Z
7	-1.258030	-1.306868	0.854781
6	-0.337891	0.913805	0.098520
6	-1.417760	-0.105268	-0.072118
6	1.028041	0.466731	-0.024522
6	1.402050	-0.774901	-0.599711
6	2.084105	1.259183	0.484950
6	2.733158	-1.178431	-0.662498
6	3.399610	0.842829	0.424906
6	3.746238	-0.386812	-0.142720
1	-0.553606	1.838780	0.622222
1	-0.837449	0.316776	-1.058000
1	0.652601	-1.391417	-1.093519
1	1.841596	2.217363	0.931799
1	-1.991477	-2.003480	0.711068
1	-1.268209	-0.991999	1.832411
1	2.973754	-2.126249	-1.132138
1	4.174871	1.485964	0.827139
1	4.778840	-0.708344	-0.182420
6	-2.803398	0.273192	-0.240825
8	-3.651574	-0.659911	0.318675
8	-3.235670	1.248555	-0.797305
1	-4.544333	-0.355000	0.115914
1	-0.327345	-1.705448	0.675205
Vibrational frequencies (cm ⁻¹)			
-1575.40	63.17	81.82	
84.58	152.72	207.42	
224.43	234.13	309.22	
346.93	388.03	423.34	
489.00	528.77	543.90	
570.61	576.38	631.94	
656.82	719.54	741.77	
764.80	780.27	845.17	
855.05	887.73	941.40	
982.85	997.56	1002.10	
1010.99	1053.49	1070.40	

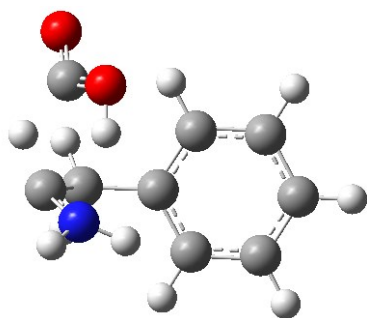
1104.85	1117.38	1173.79
1205.56	1217.48	1261.62
1317.01	1344.41	1364.76
1385.68	1404.40	1455.49
1490.89	1530.41	1613.88
1621.34	1650.68	1673.27
1861.58	2351.27	3143.33
3179.09	3188.33	3196.72
3205.52	3229.59	3349.36
3407.51	3519.47	3856.88

II -2-i2



Atomic Number	Z	Y	Z
6	-0.572637	-0.460089	-0.000095
6	-1.568500	0.429438	0.000031
6	0.866103	-0.181011	-0.000062
6	1.387398	1.119136	-0.000168
6	1.756154	-1.259293	0.000091
6	2.757063	1.328274	-0.000104
6	3.129601	-1.050589	0.000160
6	3.633142	0.244277	0.000066
1	-0.859957	-1.509345	-0.000209
1	-1.421710	1.501807	0.000184
1	0.717974	1.970924	-0.000319
1	1.360668	-2.269162	0.000163
1	3.146946	2.338979	-0.000190
1	3.804732	-1.897608	0.000287
1	4.703381	0.411972	0.000117
6	-2.965332	-0.052876	-0.000006
8	-3.839854	0.972909	0.000268
8	-3.318441	-1.202168	-0.000236
1	-4.723636	0.582906	0.000230

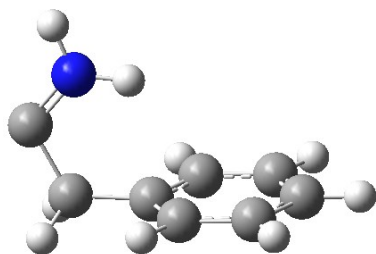
III-1-ts1



Atomic Number	X	Z	Y
7	-1.056406	1.723924	-1.034745
6	-0.484415	1.043491	1.242706
6	-1.522712	1.480257	0.223007
6	0.745956	0.357747	0.685923
6	1.854846	1.108278	0.289233
6	0.775393	-1.027159	0.503853
6	2.965755	0.495125	-0.284573
6	1.885401	-1.641487	-0.062592
6	2.981812	-0.882644	-0.462518
1	-0.977645	0.415024	1.985918
1	-0.179588	1.962476	1.757263
1	1.852681	2.183013	0.447990
1	-0.073777	-1.626488	0.815718
1	-0.071411	1.595048	-1.251466
1	-1.542969	2.404773	-1.598602
1	3.819066	1.092945	-0.582446
1	1.895519	-2.717489	-0.189085
1	3.845842	-1.364679	-0.903675
6	-2.354839	-0.626712	-0.046866
8	-2.086607	-0.893344	-1.317694
8	-2.664148	-1.422165	0.779564
1	-1.739885	-0.068757	-1.704906
1	-2.510128	0.739351	0.242502
Vibrational frequencies (cm ⁻¹)			
-1187.22	46.62		72.93
98.31	113.83		135.66
190.55	273.16		320.86
383.23	417.20		450.58
487.74	505.16		547.75
594.05	608.89		633.36
659.29	724.75		732.36
772.06	774.10		847.43
885.96	927.30		946.67

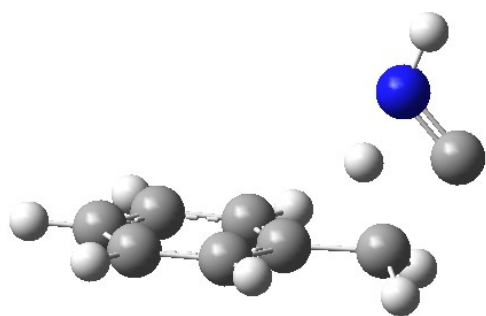
962.62	1011.11	1018.65
1032.82	1064.00	1113.09
1124.85	1178.29	1186.48
1209.46	1217.90	1232.24
1313.89	1335.53	1349.10
1362.66	1375.52	1413.97
1464.66	1495.48	1539.57
1648.86	1658.08	1678.08
1912.16	2096.24	3052.02
3132.46	3179.29	3199.09
3206.74	3216.66	3226.83
3506.00	3643.82	3658.35

III-1-i1



Atomic Number	X	Y	Z
7	2.211773	-0.000164	1.254201
6	1.620382	0.000420	-1.027982
6	2.706001	-0.000357	0.044290
6	0.177325	0.000202	-0.590376
6	-0.491553	1.199261	-0.332461
6	-0.491271	-1.199052	-0.332837
6	-1.797268	1.201786	0.146480
6	-1.796989	-1.202019	0.146127
6	-2.454916	-0.000231	0.385507
1	1.835513	-0.867204	-1.660438
1	1.835866	0.868812	-1.659271
1	0.018395	2.139473	-0.517552
1	0.018760	-2.139118	-0.518408
1	1.214073	0.000478	1.485376
1	2.842417	-0.000574	2.043541
1	-2.302469	2.142751	0.330245
1	-2.302045	-2.143139	0.329479
1	-3.473193	-0.000391	0.755131

III-1-ts2



Atomic	Number	X	Y
7	2.526911	-0.000300	1.214321
6	1.504058	0.000313	-1.048348
6	3.027944	0.000006	0.025868
6	0.067157	0.000141	-0.570031
6	-0.590952	1.203348	-0.296926
6	-0.590847	-1.203226	-0.297307
6	-1.890682	1.202894	0.191938
6	-1.890577	-1.203028	0.191556
6	-2.545525	-0.000135	0.434709
1	1.733703	-0.896882	-1.616063
1	1.733639	0.897869	-1.615521
1	-0.080291	2.142151	-0.483360
1	-0.080085	-2.141925	-0.483981
1	1.624281	-0.000018	0.333452
1	3.183113	-0.000480	1.993657
1	-2.393350	2.143211	0.384162
1	-2.393150	-2.143449	0.383530
1	-3.559697	-0.000251	0.815125

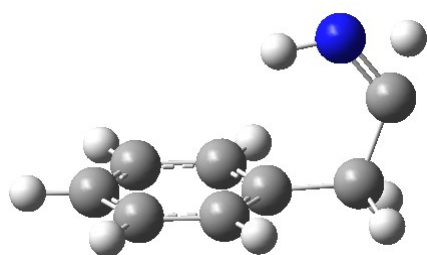
Vibrational frequencies (cm⁻¹)

-1865.50	35.00	93.39
141.39	252.77	345.43
393.51	408.84	456.40
511.06	549.36	632.17
660.23	702.25	715.55
786.24	817.00	866.25
939.78	997.05	1013.49
1017.60	1021.00	1061.29
1111.33	1128.14	1160.65
1181.01	1197.50	1208.00
1218.54	1331.03	1355.41
1443.39	1495.75	1518.43
1538.10	1655.36	1674.64
1902.54	3134.92	3196.47
3197.87	3209.77	3210.89

3219.18

3229.53

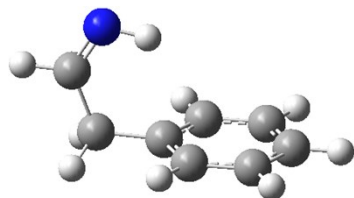
3492.12

III-2-ts2

Atomic Number	X	Y	Z
7	2.215591	0.164789	1.344746
6	1.609878	-0.122246	-1.039191
6	2.610986	0.069215	0.091394
6	0.173514	-0.068092	-0.599058
6	-0.459412	1.162073	-0.409841
6	-0.519246	-1.232632	-0.263084
6	-1.761026	1.226483	0.074649
6	-1.821772	-1.173017	0.220665
6	-2.446877	0.057862	0.388237
1	1.852663	-1.078908	-1.511679
1	1.830550	0.644672	-1.787404
1	0.074682	2.075546	-0.650863
1	-0.033857	-2.194923	-0.391540
1	1.216064	0.005117	1.579438
1	3.285171	-0.330770	1.130043
1	-2.239991	2.189251	0.207476
1	-2.348619	-2.087628	0.465630
1	-3.462068	0.106235	0.763055
Vibrational frequencies (cm ⁻¹)			
-1931.80	30.50		100.90
147.87	270.06		335.88
381.48	413.29		485.80
503.86	632.79		669.84
722.24	751.19		775.77
848.26	875.73		905.92
949.34	990.46		1002.66
1019.76	1024.38		1063.46
1110.70	1174.94		1187.15
1206.22	1230.94		1275.04
1331.11	1331.72		1356.93
1448.15	1494.97		1539.16
1553.81	1658.58		1681.02

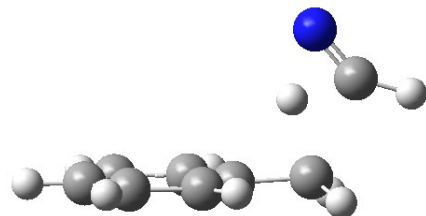
2537.97	3073.52	3111.89
3190.03	3192.03	3207.33
3210.62	3216.37	3228.19

III-2-i2



Atomic Number	X	Y	Z
7	-2.347034	0.000231	1.390799
6	-1.595527	-0.000190	-0.999854
6	-2.587124	0.000008	0.152084
6	-0.157971	-0.000088	-0.556632
6	0.510524	-1.200405	-0.315485
6	0.510468	1.200315	-0.315737
6	1.823159	-1.202481	0.142651
6	1.823104	1.202549	0.142398
6	2.483113	0.000073	0.371086
1	-1.808004	0.874463	-1.623470
1	-1.807960	-0.875104	-1.623123
1	-0.003976	-2.139828	-0.489713
1	-0.004087	2.139676	-0.490138
1	-1.335592	0.000268	1.556357
1	-3.637394	-0.000054	-0.155033
1	2.330726	-2.143053	0.320272
1	2.330614	2.143186	0.319843
1	3.506441	0.000136	0.726354

III-2-ts3



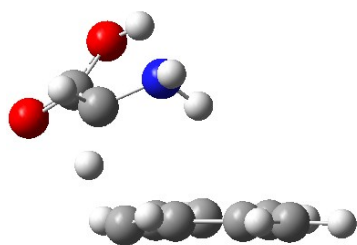
Atomic Number	X	Y	Z
7	2.573815	0.000007	1.433641
6	1.453491	-0.000005	-1.109504
6	2.934270	-0.000000	0.280439
6	0.051075	-0.000002	-0.623984

6	-0.604037	1.203241	-0.327800
6	-0.604039	-1.203244	-0.327793
6	-1.886023	1.202250	0.203869
6	-1.886024	-1.202249	0.203876
6	-2.534072	0.000002	0.468657
1	1.732555	-0.906550	-1.641680
1	1.732556	0.906535	-1.641688
1	-0.101734	2.143454	-0.529993
1	-0.101737	-2.143458	-0.529981
1	1.677274	0.000002	0.385226
1	3.791894	-0.000006	-0.396674
1	-2.380518	2.143043	0.414378
1	-2.380520	-2.143040	0.414390
1	-3.534322	0.000004	0.883964

Vibrational frequencies (cm⁻¹)

-2146.53	33.97	76.56
123.79	227.99	359.55
409.59	424.54	471.36
483.48	536.81	625.85
632.62	714.19	729.76
782.56	827.00	861.86
931.32	943.30	995.42
1013.61	1019.09	1060.74
1062.87	1066.56	1127.64
1163.85	1179.65	1203.95
1252.07	1329.40	1355.10
1460.24	1495.27	1532.73
1650.84	1671.62	1822.50
2144.22	3093.64	3114.44
3194.31	3194.92	3199.89
3208.83	3218.01	3229.00

IV-ts

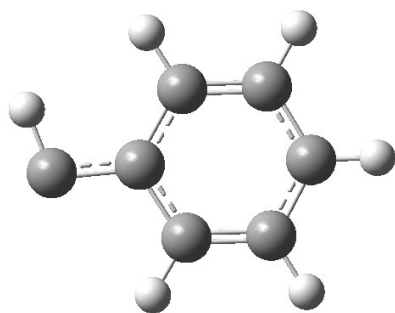


Atomic Number	X	Y	Z
7	-1.385914	1.461410	-1.124377
6	-0.048194	1.276692	1.637601

6	-1.927983	0.905037	0.080474
6	0.916316	0.549884	0.819355
6	1.870367	1.199992	0.010870
6	0.944544	-0.858556	0.884438
6	2.832943	0.476180	-0.681648
6	1.869797	-1.581332	0.150112
6	2.821525	-0.914282	-0.622269
1	-1.336398	0.956585	1.124755
1	-0.035188	2.335892	1.319075
1	1.859640	2.284400	-0.045346
1	0.216022	-1.354958	1.515687
1	-0.385917	1.282613	-1.202230
1	-1.545687	2.457222	-1.199877
1	3.578541	0.988616	-1.277682
1	1.869077	-2.663585	0.191637
1	3.559233	-1.482431	-1.176799
6	-2.163791	-0.600059	-0.046859
8	-2.134666	-1.051850	-1.302823
8	-2.354610	-1.306375	0.897112
1	-1.989903	-0.280754	-1.877633
1	-2.866956	1.390986	0.352301

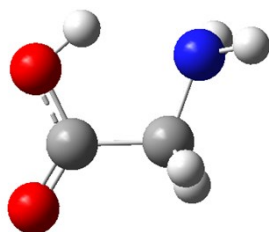
Vibrational frequencies (cm⁻¹)

-404.05	31.11	41.11
76.00	94.35	135.53
215.78	328.49	355.96
356.78	395.74	420.64
497.25	530.21	545.04
592.52	627.74	681.42
713.28	769.25	784.61
824.93	843.24	854.85
878.80	932.05	956.92
967.50	1013.16	1014.81
1033.98	1057.24	1076.02
1109.22	1134.49	1181.78
1195.99	1199.14	1235.81
1258.70	1314.71	1337.62
1348.79	1372.87	1421.51
1464.81	1492.45	1521.19
1634.04	1658.14	1662.60
1711.33	1912.07	2989.71
3125.73	3187.49	3204.06
3214.61	3221.14	3229.78
3498.71	3634.69	3691.61



Atomic Number	X	Y	Z
6	-2.476047	-0.173323	-0.000009
6	-1.038700	-0.039669	-0.000001
6	-0.348214	1.194402	0.000001
6	-0.277860	-1.228216	-0.000005
6	1.034932	1.236821	-0.000007
6	1.107295	-1.191423	0.000005
6	1.756520	0.041639	0.000001
1	-2.882674	0.857882	0.000066
1	-0.925034	2.113303	0.000009
1	-0.823747	-2.164305	-0.000003
1	1.558893	2.184763	-0.000007
1	1.684600	-2.107655	0.000015
1	2.840400	0.074628	0.000010

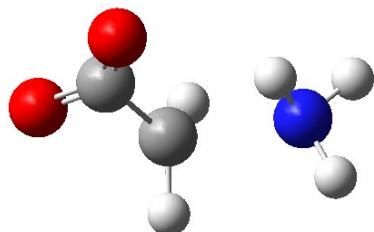
Glycine



Atomic Number	X	Y	Z
7	1.771776	0.127260	-0.083715
6	0.645643	-0.784223	0.118241
1	0.609377	-1.632870	-0.568128
1	2.084719	0.120351	-1.047056
1	2.563311	-0.112152	0.498181
6	-0.688863	-0.040710	0.005283
8	-0.573723	1.286147	0.058238
8	-1.734221	-0.610595	-0.094212
1	0.383472	1.468301	0.117846

1 0.679556 -1.189269 1.131804

IV-1-ts1

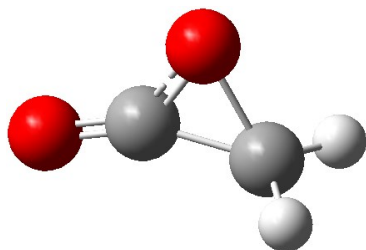


Atomic Number	X	Y	Z
7	2.040531	0.010497	0.000003
6	0.158352	-0.924993	-0.000006
1	0.321067	-1.455779	-0.926622
1	2.624617	-0.088800	-0.823475
1	2.624481	-0.088637	0.823596
6	-0.745179	0.223272	0.000002
8	-0.610204	1.420881	-0.000004
8	-1.675348	-0.635850	0.000006
1	1.630423	0.945611	-0.000111
1	0.321074	-1.455797	0.926598

Vibrational frequencies (cm⁻¹)

-549.13	137.88	181.76
212.31	363.88	465.71
539.09	607.91	680.73
941.16	1010.98	1040.43
1118.71	1174.50	1370.43
1444.11	1650.03	1682.10
1950.31	3204.09	3321.63
3457.61	3593.21	3644.24

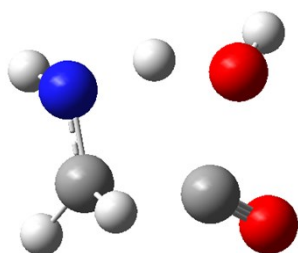
IV-1-i1



Atomic Number	X	Y	Z
6	1.031218	-0.571918	0.000001

1	1.501733	-0.885702	0.923819
6	-0.329066	-0.072248	0.000001
8	-1.505116	-0.157542	0.000004
8	0.603070	0.862094	-0.000006
1	1.501729	-0.885712	-0.923817

IV-2-ts1

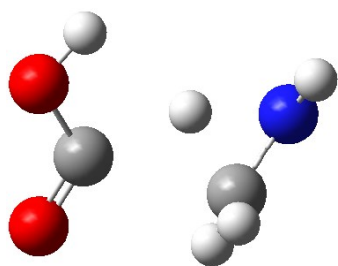


Atomic Number	X	Y	Z
7	-1.726986	0.180258	-0.233661
6	-1.120978	-0.890835	0.255880
1	-0.827427	1.051644	0.006484
1	-1.925542	0.079281	-1.224216
6	0.822173	-0.423144	0.031039
8	0.320976	1.359437	0.242804
8	1.936657	-0.560757	-0.183973
1	0.734743	1.902981	-0.433498
1	-1.156433	-1.860138	-0.240290
1	-1.004674	-0.941137	1.334985

Vibrational frequencies (cm⁻¹)

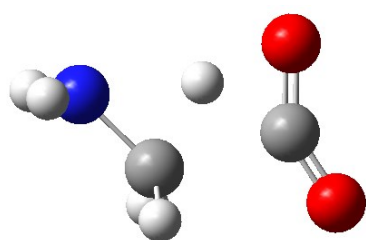
-1285.43	88.73	151.98
241.60	397.08	499.31
561.80	576.07	600.56
745.70	794.61	999.69
1107.17	1214.72	1320.30
1411.20	1493.02	1589.20
1800.95	2121.08	3118.47
3200.28	3558.85	3903.23

IV-3-ts1



Atomic Number	X	Y	Z
7	2.105264	0.359059	-0.334710
6	1.310649	-0.522947	0.323693
1	1.087202	-1.470335	-0.160179
1	0.760253	0.375169	-0.473929
1	2.353991	1.119586	0.294863
6	-0.772490	-0.076766	-0.077707
8	-1.464342	1.085830	0.091884
8	-1.345055	-1.117422	-0.130264
1	-0.853711	1.829040	0.107169
1	1.161638	-0.515856	1.406168
Vibrational frequencies (cm ⁻¹)			
-2280.95	66.80		112.34
240.94	311.50		333.13
514.45	653.70		695.50
932.75	1060.12		1114.10
1118.16	1223.57		1268.02
1321.54	1383.21		1548.14
1869.26	2084.92		3083.20
3201.41	3522.21		3877.08

IV-4-ts1



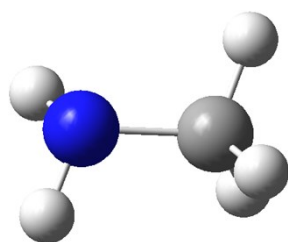
Atomic Number	X	Y	Z
8	0.781290	1.312480	-0.005767
8	1.752455	-0.781423	0.007097
7	-2.014953	0.171533	0.003303
6	-0.825397	-0.688584	-0.007219

6	0.961708	0.086821	0.000143
1	-0.731140	-1.317518	0.874104
1	-2.546976	0.118029	0.859115
1	-2.611571	0.054793	-0.802248
1	-0.353691	0.588580	-0.009374
1	-0.739778	-1.282485	-0.912900

Vibrational frequencies (cm⁻¹)

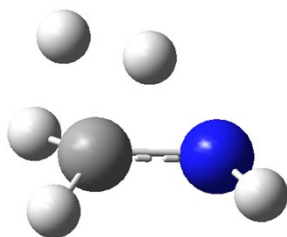
-1761.26	55.90	176.98
209.79	316.71	434.90
611.16	652.81	720.27
814.11	955.29	1032.64
1181.43	1206.49	1329.45
1385.97	1446.64	1555.67
1641.91	2154.41	3125.02
3204.68	3588.26	3696.32

methanamine



Atomic Number	X	Y	Z
7	-0.749951	0.000001	0.124076
6	0.705375	0.000004	-0.018122
1	1.075359	0.000469	-1.052209
1	-1.142901	-0.811018	-0.339832
1	-1.142948	0.811026	-0.339794
1	1.113895	-0.877687	0.485612
1	1.114003	0.877182	0.486422

IV-4-ts2



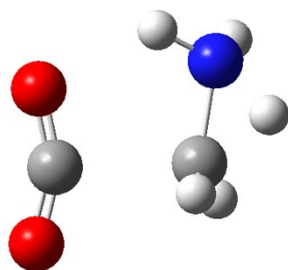
Atomic Number	X	Y	Z
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7	0.806854	-0.005741	-0.143518
6	-0.549639	-0.190074	0.010313
1	-1.007584	-0.591020	0.919004
1	1.226445	0.005380	0.784280
1	-0.223342	1.043730	-0.007526
1	-1.099665	-0.431341	-0.896823
1	-1.246000	1.153878	0.143814

Vibrational frequencies (cm⁻¹)

-2368.42	714.59	775.12
1026.04	1138.98	1190.19
1259.75	1384.49	1413.63
1485.57	1672.31	2213.34
3063.82	3167.83	3510.04

IV-5-ts1

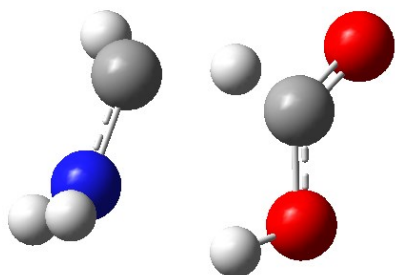


Atomic Number	X	Y	Z
7	1.866013	0.261496	-0.008722
6	0.877983	-0.911180	0.044231
1	0.747046	-1.486916	-0.855204
1	2.151471	0.416995	-0.965986
1	2.167312	-0.844024	0.357023
6	-1.001333	0.156755	-0.004210
8	-0.600188	1.271567	0.035286
8	-1.834131	-0.670374	-0.050362
1	1.398748	1.090741	0.369159
1	0.687978	-1.290267	1.036551

Vibrational frequencies (cm⁻¹)

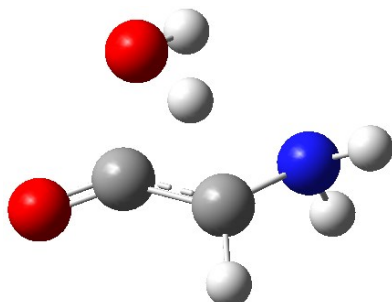
-1700.39	103.41	178.82
235.64	271.87	379.76
492.39	599.53	669.65
734.20	894.67	936.12
1026.50	1267.90	1340.13
1357.75	1442.32	1615.34
2237.72	2306.09	3201.35
3354.28	3401.79	3646.46

IV-6-ts1



Atomic Number	X	Y	Z
7	-1.908649	0.167067	0.055484
6	-1.164019	-0.968169	-0.138301
1	-0.851411	-1.419575	0.808472
1	-2.220067	0.438370	0.979567
1	-2.543460	0.428747	-0.685137
6	0.912533	-0.063713	-0.100711
8	0.659715	1.229304	0.011399
8	1.946497	-0.606971	0.084319
1	-0.304734	1.334725	-0.099180
1	-0.060562	-0.739106	-0.723779
Vibrational frequencies (cm ⁻¹)			
-1048.01	125.13	217.49	
275.81	453.81	559.78	
614.79	650.69	750.86	
776.68	986.59	1070.61	
1119.19	1270.69	1347.08	
1388.13	1442.49	1671.79	
1930.54	1981.86	3107.97	
3552.73	3605.05	3657.27	

IV-7-ts1



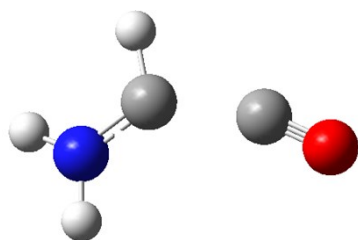
Atomic Number	X	Y	Z
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7	1.741028	-0.068001	-0.312485
6	0.636787	-0.609567	0.468272
1	2.047098	-0.718403	-1.028178
1	2.537631	0.124045	0.281588
6	-0.653135	-0.273667	-0.040040
8	-0.483209	1.371365	0.111657
8	-1.736335	-0.667810	-0.214417
1	0.161038	1.627207	-0.564754
1	0.211979	0.738606	0.896382
1	0.709491	-1.624494	0.855044

Vibrational frequencies (cm⁻¹)

-1763.85	179.97	290.35
387.15	435.10	556.73
581.10	638.76	737.47
879.40	888.34	1001.52
1064.13	1176.23	1218.62
1363.67	1484.91	1680.69
1869.01	2049.47	3142.26
3533.82	3615.16	3811.53

IV-7-ts2

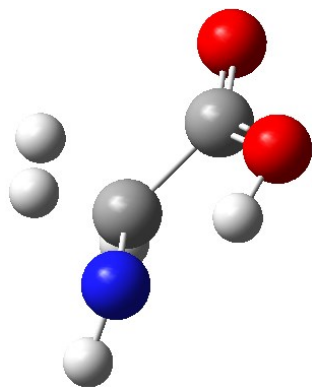


Atomic Number	X	Y	Z
7	-1.718736	-0.318620	-0.036373
6	-0.749957	0.506093	0.335922
1	-1.735759	-1.262240	0.322478
1	-2.432238	-0.107561	-0.724253
6	1.005273	0.149680	-0.381390
8	1.947604	-0.227923	0.132001
1	-0.913586	1.488891	-0.126819

Vibrational frequencies (cm⁻¹)

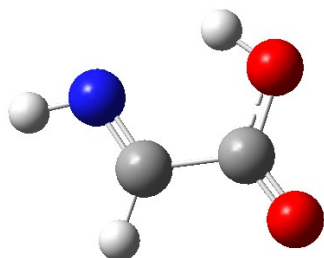
-364.61	87.71	306.11
393.29	604.21	671.21
1011.51	1150.76	1379.86
1388.28	1685.67	2139.74
3057.37	3529.90	3652.98

IV-9-ts1



Atomic Number	X	Y	Z
7	1.745081	0.207520	0.073424
6	0.704241	-0.692495	-0.158027
1	0.734526	-1.457643	-0.938744
1	2.581523	-0.071412	-0.427399
1	1.236773	-0.999094	0.935650
6	-0.684349	-0.001169	-0.028509
8	-0.524828	1.296244	0.013628
8	-1.706774	-0.617730	0.006106
1	0.474826	1.407581	0.021404
1	0.490245	-1.598204	0.856464
Vibrational frequencies (cm ⁻¹)			
-2140.27	128.79		292.18
441.21	514.64		604.38
696.37	843.17		878.42
941.55	967.50		1036.23
1125.16	1209.19		1259.91
1362.76	1451.35		1526.29
1927.36	1998.23		2356.64
3087.16	3105.61		3576.41

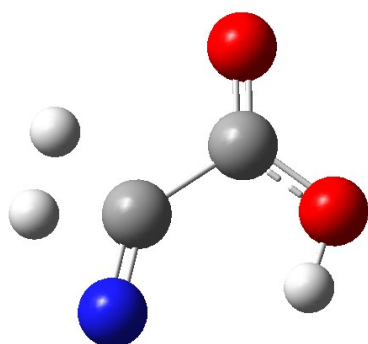
IV-9-i1



Atomic Number	X	Y	Z
7	-1.779711	0.127004	0.000014

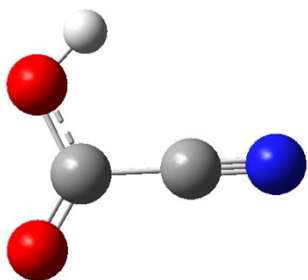
6	-0.797784	-0.664667	-0.000018
1	-0.835362	-1.755450	-0.000035
1	-2.677127	-0.356636	0.000021
6	0.595343	-0.068289	-0.000006
8	0.614228	1.261565	-0.000008
8	1.572593	-0.754465	0.000014
1	-0.309458	1.563994	0.000016

IV-9-ts2



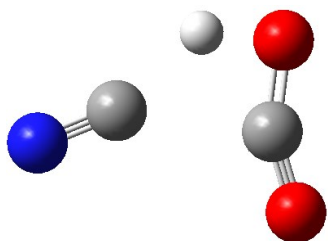
Atomic Number	X	Y	Z
7	1.942944	0.197864	0.000011
6	0.878557	-0.405958	-0.000058
1	0.826143	-1.779771	-0.000100
1	1.725523	-1.281086	0.000236
6	-0.605326	-0.068954	-0.000010
8	-0.772814	1.245872	0.000003
8	-1.464182	-0.888558	0.000017
1	0.104311	1.666766	0.000035
Vibrational frequencies (cm ⁻¹)			
-2234.32	125.78		247.20
253.79	512.63		566.08
645.66	703.71		822.30
871.83	1080.03		1234.28
1402.24	1812.72		1902.90
1957.43	2491.55		3719.53

IV-9-i2



Atomic Number	X	Y	Z
7	-0.438746	-0.697717	-0.008222
6	-1.578784	-0.567957	-0.007486
6	-3.051673	-0.389466	-0.003992
8	-3.435334	0.887642	0.005486
8	-3.799676	-1.306350	-0.009016
1	-2.677041	1.483353	0.008104

IV-9-ts3

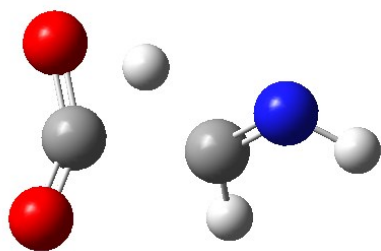


Atomic Number	X	Y	Z
7	-2.287733	-0.237834	0.000000
6	-1.216288	0.196911	-0.000000
6	0.891038	-0.084941	-0.000000
8	1.043327	1.143454	0.000000
8	1.210599	-1.175001	-0.000000
1	-0.065782	1.245395	-0.000002

Vibrational frequencies (cm⁻¹)

-1549.41	121.15	167.61
357.82	462.83	606.79
845.05	954.51	1302.68
2027.44	2303.35	2395.62

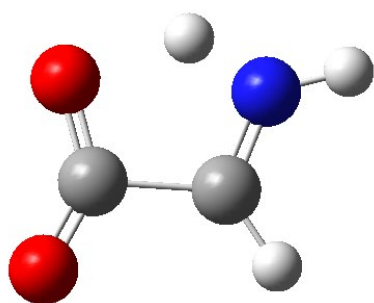
IV-10-ts2



Atomic Number	X	Y	Z
7	1.866996	0.102311	0.420126
6	1.014439	-0.186456	-0.472907
1	1.170004	-0.892489	-1.296657
1	2.756514	-0.385268	0.270270
6	-0.818818	-0.031344	0.010910
8	-0.999274	1.201819	-0.000528
8	-1.291790	-1.084664	0.166083
1	0.159297	0.931130	-0.466952

Vibrational frequencies (cm ⁻¹)			
-2061.19	124.77	209.90	
281.83	599.76	649.65	
685.53	754.92	1005.15	
1149.88	1183.97	1317.00	
1408.47	1649.54	1863.25	
2177.13	3061.92	3434.12	

IV-11-ts2

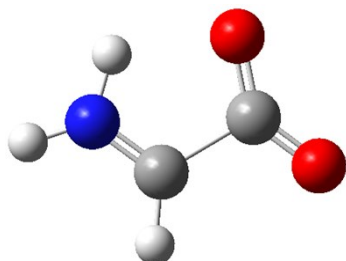


Atomic Number	X	Y	Z
7	1.670628	0.008581	-0.000006
6	0.683584	-0.787864	0.000007
1	0.772775	-1.870096	0.000019
1	2.650022	-0.249259	-0.000007
6	-0.664209	0.054809	0.000002
8	-0.359033	1.268131	-0.000013
8	-1.691799	-0.585677	0.000013
1	1.173215	0.997977	-0.000016

Vibrational frequencies (cm ⁻¹)			

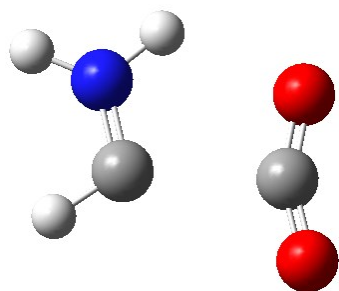
-510.55	183.95	446.55
599.98	712.43	812.44
830.39	902.37	1012.13
1103.09	1209.45	1346.91
1368.81	1728.34	1916.40
2530.98	3215.83	3619.35

IV-11-i2



Atomic Number	X	Y	Z
7	-1.717469	0.008538	0.000006
6	-0.688857	-0.742805	-0.000006
1	-0.784851	-1.825596	-0.000019
1	-2.681828	-0.300572	0.000006
6	0.688408	0.072093	-0.000002
8	0.447330	1.283774	0.000013
8	1.667878	-0.648630	-0.000013
1	-1.430014	1.009524	0.000017

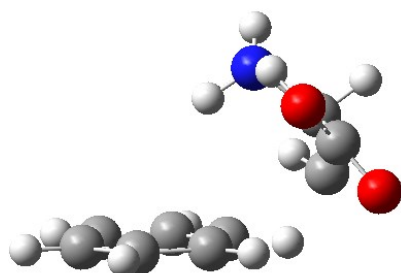
IV-11-ts3



Atomic Number	X	Y	Z
7	-1.854818	0.146364	0.000005
6	-1.001742	-0.820604	-0.000008
1	-1.500824	-1.798908	-0.000019
1	-2.867007	0.054810	0.000006
6	0.979009	0.113278	-0.000001
8	0.604914	1.236012	0.000014
8	1.764653	-0.752094	-0.000012

1	-1.468577	1.092166	0.000016
Vibrational frequencies (cm ⁻¹)			
-206.10	106.13	248.30	
386.34	392.08	623.99	
715.35	883.66	1045.98	
1156.34	1337.16	1379.58	
1521.92	1685.19	2274.66	
3061.85	3445.37	3564.27	

V-1-ts1

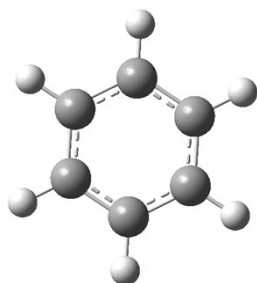


Atomic Number	X	Y	Z
7	-1.096235	0.878131	-1.612547
6	-1.032077	1.696591	0.853882
6	-1.684172	0.947743	-0.260170
6	0.879870	0.435103	0.867029
6	1.955881	1.187348	0.410339
6	0.829649	-0.942324	0.674287
6	3.000673	0.551425	-0.253666
6	1.879738	-1.570667	0.011404
6	2.957716	-0.824970	-0.456862
1	0.056358	0.905596	1.525274
1	-0.424983	2.488787	0.385833
1	1.983592	2.257979	0.577146
1	-0.007527	-1.516901	1.052452
1	-0.089781	0.751078	-1.538437
1	-1.260087	1.733452	-2.128959
1	3.844742	1.127995	-0.612389
1	1.854912	-2.643267	-0.137379
1	3.769390	-1.318469	-0.977841
6	-2.162293	-0.467316	0.150103
8	-2.203721	-1.320091	-0.872811
8	-2.459398	-0.769887	1.265607
1	-1.875801	-0.819695	-1.647581
1	-2.622128	1.528747	-0.330739

Vibrational frequencies (cm⁻¹)

-253.70	33.61	53.85
71.63	97.34	136.75
210.99	292.36	325.73
406.63	414.09	424.85
503.27	549.43	579.65
613.30	618.99	715.23
736.13	762.93	796.16
856.86	884.75	892.77
903.82	946.97	991.38
998.03	1015.18	1021.16
1033.36	1045.69	1067.45
1085.54	1119.46	1144.04
1181.08	1201.59	1206.39
1218.92	1269.63	1292.92
1330.11	1340.63	1373.38
1446.41	1506.45	1513.39
1650.84	1655.02	1664.47
1917.05	2282.67	2991.78
3032.92	3202.85	3210.46
3217.52	3224.34	3231.09
3525.44	3559.31	3627.33

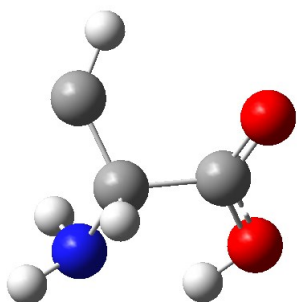
Benzene



Atomic Number	X	Z	Y
6	0.085092	1.388476	0.000002
6	1.245041	0.620550	-0.000003
6	-1.159952	0.767912	-0.000003
6	1.159951	-0.767912	-0.000002
6	-1.245041	-0.620549	-0.000001
6	-0.085092	-1.388476	0.000002
1	0.151344	2.470014	0.000020
1	2.214832	1.103917	-0.000002
1	-2.063415	1.366144	-0.000003
1	2.063414	-1.366144	-0.000000

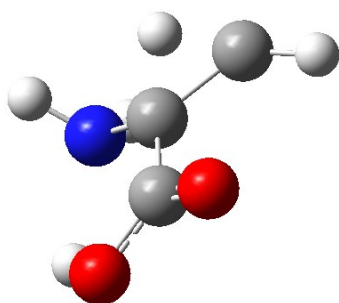
1	-2.214831	-1.103918	-0.000000
1	-0.151345	-2.470021	0.000011

V-1-i1



Atomic Number	X	Y	Z
7	-1.480644	-0.920961	-0.070879
6	-1.124001	1.536340	-0.204636
6	-0.694953	0.248575	0.363145
1	-0.592137	2.320448	-0.721563
1	-1.806148	-0.780146	-1.022774
1	-2.300208	-1.044567	0.510740
6	0.804408	-0.002405	0.055024
8	1.095015	-1.284151	-0.143355
8	1.611461	0.876884	0.031351
1	0.241656	-1.760090	-0.116638
1	-0.743183	0.274151	1.461220

V-1-ts2



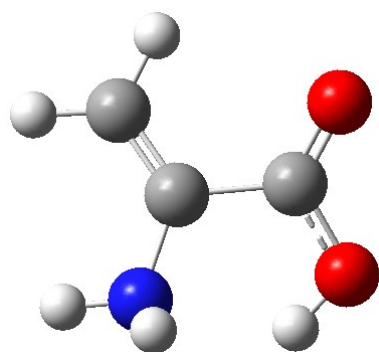
Atomic Number	X	Y	Z
7	1.440793	-1.048458	-0.014384
6	1.269828	1.453968	0.176328
6	0.677393	0.152255	-0.126781
1	0.891313	2.327594	0.686423
1	2.232550	-0.939482	0.608874
1	1.757812	-1.418558	-0.901945

6	-0.804673	0.043709	-0.026524
8	-1.241520	-1.212369	0.147720
8	-1.542142	0.987575	-0.107160
1	-0.456882	-1.770362	0.271351
1	0.903666	1.038778	-1.026639

Vibrational frequencies (cm⁻¹)

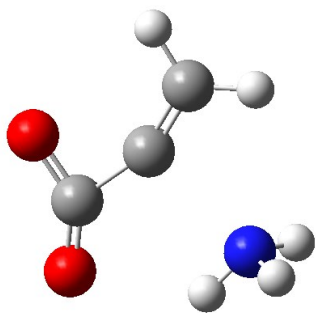
-1844.00	108.51	249.04
288.67	323.47	366.29
407.40	561.23	584.16
719.01	751.25	809.33
819.17	890.34	1013.82
1172.14	1185.47	1290.98
1335.77	1425.52	1654.42
1867.68	2231.08	3251.85
3546.98	3631.69	3732.71

V-1-i2



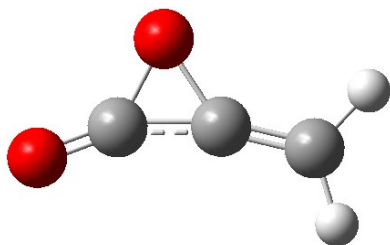
Atomic Number	X	Y	Z
7	-1.286549	-1.166697	0.116724
6	-1.352153	1.265507	-0.173679
6	-0.706142	0.122398	0.028796
1	-2.434162	1.313145	-0.202036
1	-2.279970	-1.157759	-0.075712
1	-1.125964	-1.602423	1.019747
6	0.805079	0.120397	0.026648
8	1.344862	-1.081393	-0.231815
8	1.470516	1.091183	0.225069
1	0.624881	-1.685668	-0.466917
1	-0.782667	2.171457	-0.328775

V-1-ts3



Atomic Number	X	Y	Z
7	1.906930	-0.807885	-0.000007
6	0.687228	1.809435	0.000011
6	0.155447	0.619376	0.000016
1	1.761744	1.913711	0.000028
1	2.497540	-0.859919	0.822632
1	2.497302	-0.859930	-0.822818
6	-0.909332	-0.381444	0.000004
8	-0.921735	-1.580989	0.000014
8	-1.707517	0.594691	-0.000020
1	1.282958	-1.613077	0.000084
1	0.045899	2.680600	-0.000010
Vibrational frequencies (cm ⁻¹)			
-549.94	96.55		144.57
200.02	258.04		284.99
331.37	402.44		530.10
595.06	658.39		731.46
874.30	917.09		935.30
1128.55	1330.96		1373.15
1650.38	1686.57		1780.43
1985.13	3199.28		3304.47
3481.35	3607.09		3646.81

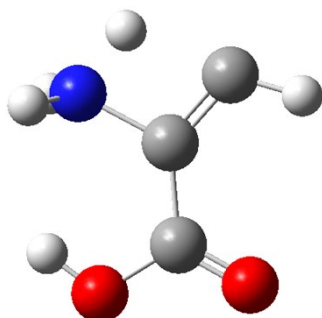
V-1-i3



Atomic Number	X	Y	Z
6	1.931150	-0.393612	0.000008
6	0.655714	-0.096279	0.000002
1	2.237240	-1.429427	0.000028

6	-0.759217	-0.107093	0.000002
8	-1.857621	-0.519347	0.000010
8	-0.127187	1.096814	-0.000021
1	2.675345	0.391598	-0.000007

V-2-ts3

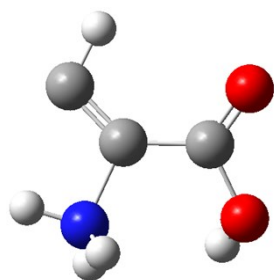


Atomic Number	X	Y	Z
7	-1.556718	-0.912961	-0.000025
6	-1.415152	1.340108	0.000021
6	-0.613418	0.273536	0.000015
1	-2.321810	-0.038786	-0.000026
1	-1.575495	-1.489695	-0.841711
1	-1.575544	-1.489722	0.841642
6	0.859239	0.095298	0.000003
8	1.341184	-1.180366	0.000013
8	1.619088	1.013386	-0.000027
1	0.631236	-1.824728	0.000106
1	-0.927561	2.315853	0.000041

Vibrational frequencies (cm⁻¹)

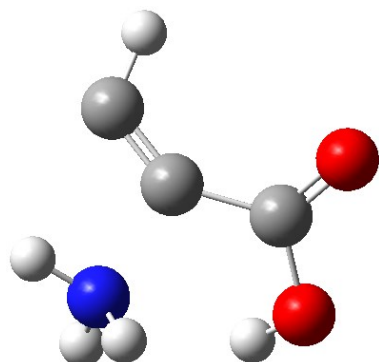
-1149.20	54.78	220.01
245.18	379.96	458.35
483.28	510.24	715.17
753.41	856.50	928.68
950.45	1044.61	1085.77
1147.34	1176.62	1317.76
1472.26	1578.86	1612.75
1901.80	2112.91	3156.54
3449.87	3550.99	3928.94

V-2-i3



Atomic Number	X	Y	Z
7	-1.462682	-0.946213	0.191584
6	-1.418125	1.417065	-0.194756
6	-0.641090	0.352311	-0.062875
1	-2.392351	-0.524286	0.313724
1	-1.505681	-1.601842	-0.590147
1	-1.177532	-1.455948	1.030090
6	0.817726	0.121247	0.007655
8	1.226119	-1.196991	-0.147452
8	1.627138	0.964854	0.225052
1	0.747150	-1.597204	-0.878453
1	-0.809933	2.316128	-0.337243

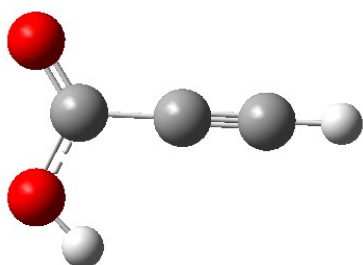
V-2-ts4



Atomic Number	X	Y	Z
7	-1.527674	-0.970046	0.293565
6	-1.345157	1.491862	-0.284135
6	-0.569890	0.496330	-0.088944
1	-2.381301	-0.473123	0.544310
1	-1.740513	-1.578355	-0.495593
1	-1.196151	-1.534521	1.075668
6	0.848454	0.088010	0.016171
8	1.147437	-1.200132	-0.332977
8	1.711235	0.822432	0.381344

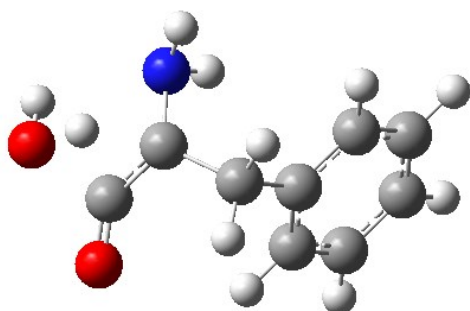
1	0.474979	-1.532215	-0.932935
1	-0.933115	2.472920	-0.491893
Vibrational frequencies (cm ⁻¹)			
-462.05	60.25		118.41
225.31	277.22		365.96
454.28	517.07		576.40
677.04	749.14		784.42
805.77	880.30		946.15
1157.24	1268.84		1289.83
1620.22	1661.40		1746.60
1906.57	3233.67		3428.72
3571.72	3579.85		3909.17

V-2-i4



Atomic Number	X	Y	Z
6	2.139303	0.005930	0.000046
6	0.941992	0.057118	-0.000185
6	-0.522024	0.129371	0.000032
8	-1.129452	-1.069374	-0.000040
8	-1.131534	1.149868	0.000042
1	-0.471523	-1.772539	0.000389
1	3.203781	-0.025925	0.000236

VI-1-ts1



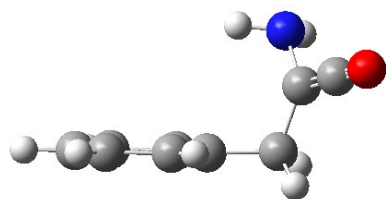
Atomic Number	X	Y	Z
7	-1.339097	1.515379	-0.824723

6	-0.401480	0.498616	1.322683
6	-1.522343	0.612757	0.302686
6	0.921986	0.166865	0.670034
6	1.858618	1.163097	0.396995
6	1.195671	-1.141502	0.261732
6	3.048151	0.863134	-0.261703
6	2.382787	-1.443848	-0.393043
6	3.313139	-0.442016	-0.656982
1	-0.661130	-0.266536	2.058467
1	-0.320257	1.449387	1.858176
1	1.658363	2.181960	0.714050
1	0.466170	-1.920588	0.458430
1	-0.432964	1.359856	-1.262487
1	-1.356311	2.479588	-0.512302
1	3.767708	1.648519	-0.461245
1	2.584483	-2.464225	-0.697007
1	4.239471	-0.679701	-1.165912
6	-2.171434	-0.607864	-0.049578
8	-3.555910	0.046708	-0.633534
8	-2.194986	-1.753183	0.194440
1	-3.300556	0.488276	-1.458021
1	-3.014704	0.752186	0.196720

Vibrational frequencies (cm⁻¹)

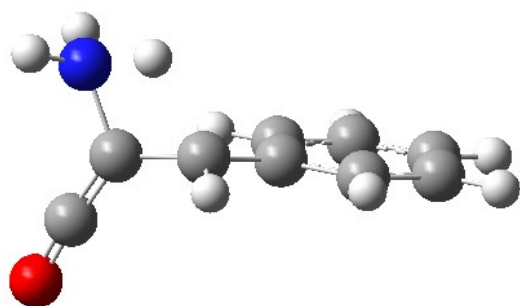
-1736.86	32.57	68.56
76.66	142.98	210.88
235.92	311.53	364.74
385.18	413.87	431.17
452.98	486.94	558.69
576.71	618.49	633.29
660.60	712.47	726.09
780.24	840.25	865.11
875.78	906.12	939.41
949.35	1001.86	1018.95
1022.84	1033.59	1063.42
1107.79	1160.47	1178.74
1206.24	1218.39	1228.48
1233.83	1306.21	1336.65
1357.40	1370.86	1469.12
1478.25	1496.14	1539.57
1659.02	1679.40	1679.83
1871.51	2012.24	3065.99
3116.98	3186.31	3196.35
3206.23	3215.55	3226.74
3496.22	3592.61	3796.88

VI-1-i1



Atomic Number	X	Y	Z
7	1.631878	-1.361798	-1.115473
6	0.806742	-0.358069	1.116466
6	1.794960	-0.451425	-0.027326
6	-0.584879	-0.073917	0.594442
6	-1.525672	-1.094171	0.475257
6	-0.927070	1.209688	0.165761
6	-2.789497	-0.838570	-0.051074
6	-2.187236	1.470112	-0.354928
6	-3.123204	0.444414	-0.465018
1	1.112374	0.422789	1.818116
1	0.801978	-1.304413	1.669349
1	-1.268337	-2.095872	0.804398
1	-0.193965	2.006834	0.240148
1	0.744043	-1.202762	-1.581982
1	1.653242	-2.323178	-0.792104
1	-3.511842	-1.641935	-0.134545
1	-2.441853	2.473092	-0.676286
1	-4.106551	0.646879	-0.871855
6	2.836024	0.357349	-0.083370
8	3.748345	1.069837	-0.111023

VI-1-ts2



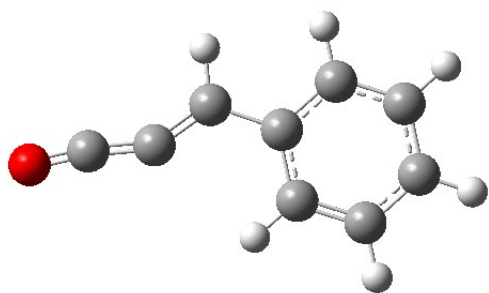
Atomic Number	X	Y	Z
7	-2.346744	0.958167	-1.370466

6	-0.718845	1.066895	0.355371
6	-1.935843	0.360538	-0.075669
6	0.597361	0.442015	0.184065
6	0.807590	-0.686438	-0.625644
6	1.728044	1.009070	0.796553
6	2.078130	-1.211511	-0.818336
6	2.997498	0.487577	0.597868
6	3.186736	-0.628428	-0.212905
1	-0.812169	1.692515	1.240896
1	-1.415808	1.648857	-1.099878
1	-0.043198	-1.170368	-1.096114
1	1.595892	1.875780	1.436283
1	-2.228711	0.366743	-2.196347
1	-3.257650	1.421083	-1.388832
1	2.203176	-2.088186	-1.444507
1	3.847153	0.951468	1.086698
1	4.177248	-1.039749	-0.363454
6	-2.577154	-0.615409	0.521550
8	-3.077478	-1.463897	1.135174

Vibrational frequencies (cm⁻¹)

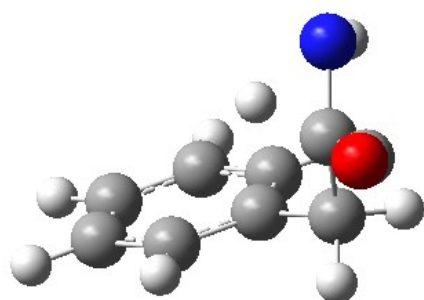
-1357.99	49.13	58.32
91.84	165.50	227.83
283.15	367.63	396.26
415.25	500.82	541.80
581.62	601.92	631.14
649.35	706.34	715.06
779.44	823.04	856.66
894.39	915.96	985.19
1006.56	1009.88	1060.12
1062.39	1069.55	1108.14
1130.38	1173.08	1198.61
1233.07	1306.53	1344.95
1357.14	1425.82	1479.75
1494.56	1532.70	1580.73
1645.12	1674.10	1950.92
2240.79	3123.55	3157.74
3159.70	3177.55	3191.11
3214.37	3393.97	3502.52

VI-1-i2



Atomic Number	X	Y	Z
6	-0.952114	0.828568	-0.000072
6	-2.032154	0.050744	-0.000049
6	0.429161	0.349692	-0.000040
6	0.725845	-1.019419	-0.000049
6	1.475401	1.277407	0.000008
6	2.043151	-1.445102	-0.000009
6	2.796023	0.849234	0.000053
6	3.080019	-0.512121	0.000045
1	-1.060258	1.915567	-0.000113
1	-0.094550	-1.728166	-0.000090
1	1.246386	2.338006	0.000015
1	2.269104	-2.504567	-0.000018
1	3.601920	1.572771	0.000093
1	4.109693	-0.849734	0.000075
6	-3.314650	-0.064942	0.000008
8	-4.447048	-0.328530	0.000083

VI-2-ts2



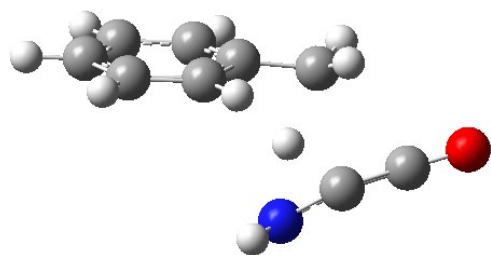
Atomic Number	X	Y	Z
7	1.636250	-1.294703	-1.158374
6	0.789887	-0.199332	1.024015
6	1.753169	-0.295885	-0.152691
6	-0.630464	-0.019529	0.545345
6	-1.511354	-1.096092	0.485621
6	-1.066559	1.234269	0.115297

6	-2.806157	-0.926178	0.005473
6	-2.358500	1.407947	-0.363746
6	-3.231830	0.325940	-0.420412
1	1.079014	0.628393	1.678785
1	0.871833	-1.123292	1.606291
1	-1.183884	-2.073956	0.823479
1	-0.386957	2.079985	0.160493
1	1.411653	0.146269	-1.175702
1	0.954489	-1.981278	-0.823881
1	-3.481191	-1.772644	-0.034868
1	-2.686060	2.387559	-0.690749
1	-4.239663	0.459994	-0.794131
6	3.089877	0.179966	0.137750
8	4.004825	0.830656	-0.112627

Vibrational frequencies (cm⁻¹)

-1681.64	43.27	50.64
90.86	124.11	236.10
284.45	313.44	375.29
414.03	418.23	498.75
544.82	605.52	633.49
642.66	720.94	741.43
805.81	847.53	879.14
908.77	951.43	987.13
1006.07	1021.35	1028.06
1064.83	1070.98	1119.64
1179.92	1188.42	1204.91
1221.49	1239.41	1324.05
1346.88	1357.66	1394.41
1479.98	1502.42	1544.63
1669.31	1689.25	2107.66
2648.50	3046.70	3095.35
3171.61	3182.13	3196.37
3204.60	3216.95	3445.97

VI-3-ts2



Atomic
Number

X

Y

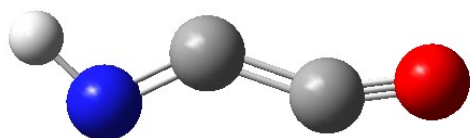
Z

7	1.264305	-1.102767	-1.475794
6	0.827626	0.658220	0.839046
6	2.031746	-0.754110	-0.430532
6	-0.584401	0.422415	0.521260
6	-1.238225	-0.722066	1.009038
6	-1.266898	1.242327	-0.391312
6	-2.547536	-0.997609	0.647454
6	-2.577331	0.963562	-0.750496
6	-3.223668	-0.153002	-0.229501
1	1.195070	1.659296	0.636919
1	1.172011	0.226646	1.771591
1	-0.708510	-1.381495	1.688987
1	-0.761206	2.107834	-0.805529
1	0.868342	-0.188080	-0.440360
1	0.776844	-1.965224	-1.229225
1	-3.043286	-1.874047	1.047213
1	-3.094984	1.615734	-1.443416
1	-4.246683	-0.370098	-0.511756
6	3.075372	-0.000342	-0.119651
8	4.001519	0.491554	0.380539

Vibrational frequencies (cm⁻¹)

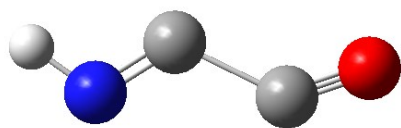
-2161.60	10.88	37.86
47.67	78.45	185.48
226.23	327.03	349.14
380.52	404.06	435.01
470.71	517.61	561.19
618.37	629.50	706.92
763.97	782.10	828.75
860.02	904.36	933.43
988.65	997.70	1008.63
1020.13	1026.87	1050.91
1060.86	1123.19	1178.47
1197.95	1221.89	1251.16
1338.48	1351.89	1462.96
1492.26	1493.89	1529.83
1649.39	1671.20	1906.07
2210.40	3132.27	3168.84
3176.30	3190.36	3196.13
3211.20	3231.12	3462.33

VI-3-i2



Atomic Number	X	Y	Z
7	-1.752668	-0.230756	0.000005
6	-0.629185	0.318480	-0.000009
1	-2.488942	0.482044	0.000025
6	0.669961	-0.143006	-0.000015
8	1.814120	0.010050	0.000011

VI-3-ts3

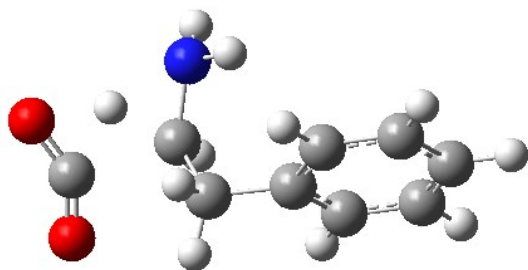


Atomic Number	X	Y	Z
7	-1.749659	-0.237122	-0.000041
6	-0.713534	0.413700	0.000058
1	-2.582964	0.350881	-0.000090
6	0.748720	-0.296225	0.000082
8	1.827433	0.075516	-0.000058

Vibrational frequencies (cm⁻¹)

-456.06	184.48	331.80
565.46	844.31	944.07
1821.46	2126.07	3550.72

VII-ts



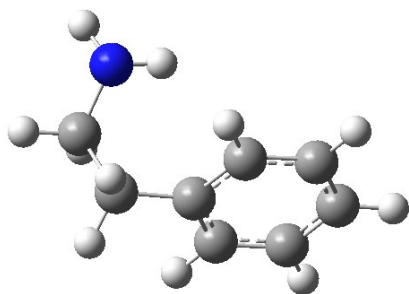
Atomic Number	X	Y	Z
8	-3.741363	0.782265	0.016620
8	-3.226329	-1.431450	0.393828
7	-1.072645	1.405419	-1.044017

6	-0.478306	-0.206765	0.744738
6	-1.314565	0.055508	-0.498357
6	0.999998	-0.166865	0.437064
6	1.780969	0.928884	0.803196
6	1.601089	-1.213565	-0.265878
6	-3.145188	-0.293588	0.098364
6	3.132898	0.983310	0.472450
6	2.949020	-1.164372	-0.594092
6	3.718762	-0.062827	-0.227891
1	-0.765737	-1.181354	1.143118
1	-0.718521	0.546315	1.502820
1	-1.229185	-0.739313	-1.239541
1	1.330133	1.739466	1.368287
1	1.005611	-2.076757	-0.547411
1	-1.174756	1.448343	-2.048429
1	-0.176562	1.789885	-0.762417
1	3.726356	1.840511	0.767873
1	3.404251	-1.987898	-1.131531
1	4.770956	-0.025984	-0.483027
1	-2.390553	0.844000	-0.362771

Vibrational frequencies (cm⁻¹)

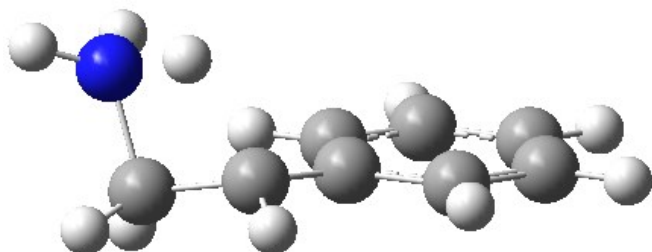
-1615.96	34.11	53.56
69.77	92.30	142.98
225.27	257.91	287.66
293.30	363.15	412.62
423.40	500.40	577.09
633.62	639.22	688.02
722.44	760.80	779.69
795.04	826.28	873.77
881.03	925.81	953.22
986.18	1006.71	1019.54
1025.97	1036.19	1065.88
1105.26	1146.09	1182.57
1194.75	1209.50	1234.97
1255.50	1290.65	1336.88
1354.52	1358.61	1378.96
1441.75	1485.57	1500.15
1543.70	1642.91	1663.44
1684.15	2139.17	3052.23
3112.31	3123.32	3167.23
3187.04	3197.69	3207.82
3219.12	3529.69	3657.68

Phenethylamine



Atomic Number	X	Y	Z
7	2.417367	-0.972157	-0.742693
6	1.472677	0.589813	0.896572
6	2.437559	0.414644	-0.281540
6	0.048596	0.293799	0.497699
6	-0.473969	-0.995447	0.619110
6	-0.756893	1.289884	-0.056845
6	-1.768145	-1.281248	0.197217
6	-2.051291	1.008711	-0.477902
6	-2.560875	-0.279563	-0.352102
1	1.547003	1.614198	1.271783
1	1.783778	-0.087191	1.695707
1	2.178687	1.146223	-1.062301
1	0.148927	-1.776480	1.042186
1	-0.363686	2.297300	-0.153848
1	3.122225	-1.113268	-1.457363
1	1.520165	-1.173094	-1.174008
1	-2.159489	-2.286546	0.301620
1	-2.664867	1.795780	-0.900471
1	-3.570822	-0.500135	-0.676455
1	3.450556	0.644755	0.058743

VII-1-ts1



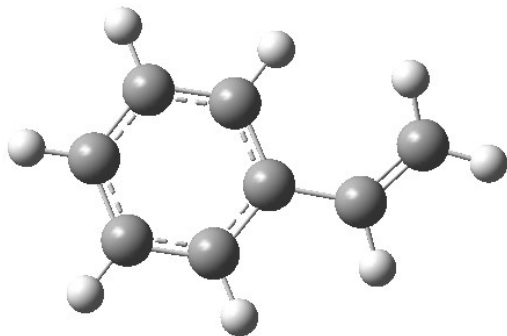
Atomic Number	X	Y	Z
7	-2.868561	0.567959	0.680458
6	-1.333996	-0.991360	-0.115820

6	-2.433186	-0.125832	-0.634308
6	0.017675	-0.452356	-0.094647
6	0.308045	0.922319	-0.217542
6	1.124681	-1.304273	0.110217
6	1.608428	1.408156	-0.138251
6	2.416807	-0.817363	0.194988
6	2.678009	0.548089	0.073331
1	-1.409844	-2.045610	-0.362076
1	-2.217419	-0.281980	1.147267
1	-2.190832	0.652833	-1.363755
1	-0.490426	1.638568	-0.397314
1	0.944574	-2.370462	0.202694
1	-3.869329	0.637869	0.866934
1	-2.423252	1.475586	0.809409
1	1.784238	2.473388	-0.244755
1	3.236269	-1.510629	0.351702
1	3.689884	0.927387	0.139947
1	-3.292707	-0.696938	-0.981063

Vibrational frequencies (cm⁻¹)

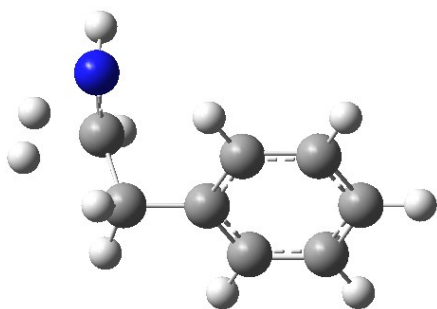
-1250.90	68.45	112.55
191.40	263.36	291.42
392.43	419.84	516.85
547.52	620.21	635.68
712.45	753.03	773.04
782.92	822.73	842.40
886.39	895.24	977.43
998.60	1002.94	1035.37
1064.29	1072.17	1098.02
1134.34	1172.91	1208.15
1233.92	1261.19	1314.43
1326.20	1353.37	1397.58
1487.80	1501.94	1512.15
1536.19	1586.59	1630.53
1672.82	2022.92	3067.11
3151.64	3157.22	3179.54
3184.07	3194.91	3201.88
3225.32	3459.56	3578.94

Styrene



Atomic Number	X	Y	Z
6	1.954207	-0.520468	-0.107516
6	2.942238	0.334340	0.143978
6	0.510886	-0.222244	-0.064205
6	0.011990	1.085003	-0.090103
6	-0.400521	-1.279476	0.002437
6	-1.353027	1.323248	-0.028833
6	-1.768454	-1.042986	0.065096
6	-2.249494	0.260558	0.052495
1	2.204264	-1.549852	-0.352310
1	2.757635	1.364993	0.425117
1	0.697024	1.920092	-0.177720
1	-0.027281	-2.298106	0.012242
1	-1.722180	2.341721	-0.053649
1	-2.458014	-1.876820	0.121210
1	-3.315238	0.449505	0.097158
1	3.976841	0.020615	0.087855

VII-2-ts1

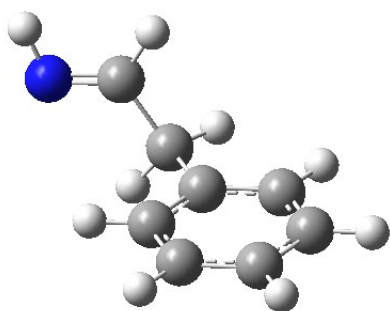


Atomic Number	X	Y	Z
7	-2.707901	1.029197	-0.312317
6	-1.397022	-0.809189	0.660757
6	-2.298063	-0.282816	-0.437010
6	0.017210	-0.370107	0.353387
6	0.372232	0.978584	0.438367

6	0.975872	-1.300650	-0.044767
6	1.667751	1.380368	0.137739
6	2.273471	-0.897935	-0.343213
6	2.621526	0.444364	-0.251599
1	-1.455074	-1.897844	0.713080
1	-1.740197	-0.384203	1.605992
1	-2.108775	-0.731968	-1.417640
1	-0.384163	1.700246	0.722646
1	0.707274	-2.349899	-0.112819
1	-3.550674	-0.148821	-0.110198
1	-2.990142	1.369912	-1.228954
1	1.934490	2.428260	0.207788
1	3.010815	-1.632606	-0.644195
1	3.631877	0.760644	-0.482010
1	-3.497983	-1.173809	-0.149427

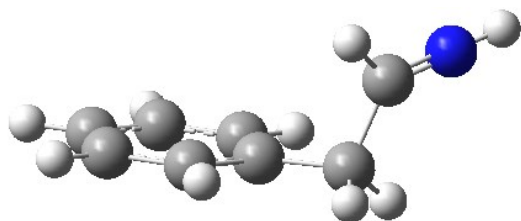
Vibrational frequencies (cm⁻¹)

-2339.66	58.74	123.44
145.46	279.58	319.19
416.46	450.01	490.89
518.61	632.10	643.17
722.14	765.34	772.48
781.65	878.39	903.58
920.89	948.95	1006.28
1019.45	1024.85	1035.28
1064.96	1109.44	1159.08
1174.55	1179.71	1209.47
1213.37	1231.81	1267.40
1315.55	1331.01	1355.34
1373.67	1448.80	1477.98
1497.24	1541.21	1658.72
1680.28	1710.24	2130.35
3072.16	3088.10	3145.70
3189.57	3202.24	3211.27
3220.76	3227.47	3522.42



Atomic Number	X	Y	Z
7	-3.242491	0.659047	-0.175544
6	-1.454773	-0.777422	0.577925
6	-2.378766	-0.216885	-0.469353
6	-0.027047	-0.356131	0.299311
6	0.307471	0.999248	0.334979
6	0.962656	-1.285993	-0.008835
6	1.607404	1.413109	0.077185
6	2.266339	-0.873764	-0.269862
6	2.591607	0.476110	-0.226314
1	-1.522257	-1.868976	0.580882
1	-1.787599	-0.405117	1.548935
1	-2.218776	-0.593767	-1.487844
1	-0.465360	1.725900	0.565080
1	0.713281	-2.341489	-0.039065
1	-3.758991	0.943373	-1.008991
1	1.854754	2.467495	0.112639
1	3.026880	-1.608742	-0.505571
1	3.606163	0.798370	-0.427467

VII-2-ts2



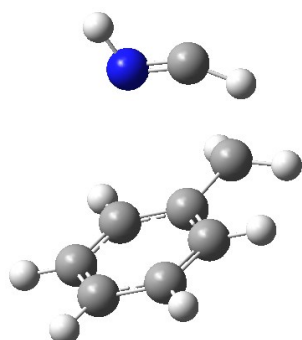
Atomic Number	X	Y	Z
7	-3.279193	0.519991	-0.512629
6	-1.465669	-0.537503	0.764909
6	-2.356022	-0.292855	-0.454518
6	-0.026790	-0.245469	0.417228
6	0.427090	1.074888	0.386274
6	0.854491	-1.264233	0.058411

6	1.733868	1.367924	0.019351
6	2.163615	-0.974184	-0.313641
6	2.607243	0.342434	-0.331875
1	-1.567801	-1.585638	1.064045
1	-1.817655	0.097565	1.578946
1	-2.065326	-0.925029	-1.319778
1	-0.256581	1.874642	0.652201
1	0.514114	-2.294361	0.078651
1	-4.017050	1.178159	-0.547097
1	2.072863	2.397110	0.006666
1	2.837467	-1.778225	-0.585150
1	3.627359	0.569839	-0.616905

Vibrational frequencies (cm⁻¹)

-1158.59	24.65	51.90
140.37	293.36	329.16
413.59	453.86	520.73
577.91	633.71	676.45
719.46	771.83	785.26
863.30	871.35	934.34
997.13	998.98	1019.74
1020.17	1038.69	1062.62
1112.56	1174.23	1186.66
1202.84	1230.21	1293.62
1331.28	1354.85	1419.05
1476.21	1496.27	1539.31
1661.12	1679.70	1846.54
2899.08	3065.51	3137.11
3191.88	3193.21	3206.43
3215.66	3226.93	3954.59

VII-3-ts2

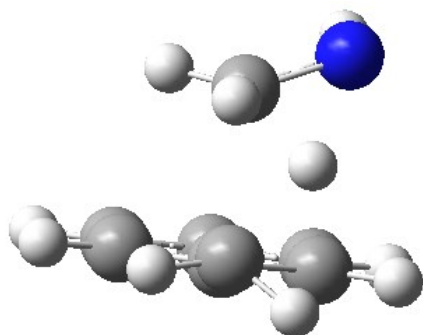


Atomic Number	X	Y	Z
7	-2.347951	1.073687	-0.618264
6	-1.425999	-0.969290	0.864093

6	-2.604576	-0.116645	-0.723080
6	-0.100448	-0.491411	0.512169
6	0.271070	0.838951	0.760346
6	0.805750	-1.315045	-0.178073
6	1.503673	1.322045	0.336360
6	2.033769	-0.830275	-0.596923
6	2.389238	0.493846	-0.342607
1	-1.524284	-2.050922	0.967455
1	-1.959306	-0.420639	1.634495
1	-2.468311	-1.165719	-0.424914
1	-0.413127	1.485028	1.295339
1	0.535660	-2.347375	-0.377620
1	-2.817639	1.653428	-1.316559
1	1.775284	2.350796	0.542965
1	2.720722	-1.484620	-1.120949
1	3.351792	0.871155	-0.666072

Vibrational frequencies (cm⁻¹)

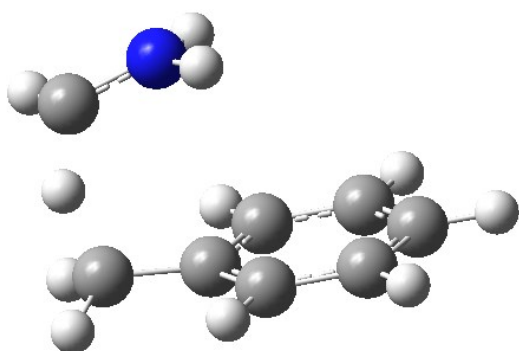
-1301.08	44.73	101.09
115.47	236.23	322.45
372.66	421.50	494.40
526.34	553.01	632.24
711.60	720.81	778.19
819.86	851.39	860.97
889.60	928.20	990.55
998.74	1014.08	1024.98
1036.06	1043.64	1061.62
1123.77	1176.17	1203.30
1273.90	1331.92	1354.78
1474.61	1492.62	1537.77
1644.29	1671.81	1783.87
3083.87	3109.14	3185.54
3199.88	3203.89	3209.53
3222.18	3230.83	3476.12



Atomic Number	X	Y	Z
7	-2.607066	1.049536	-0.806577
6	-1.350822	-0.660623	1.063341
6	-2.583414	-0.305876	-0.605213
6	0.017230	-0.354148	0.624602
6	0.512201	0.954375	0.726495
6	0.800309	-1.305701	-0.045576
6	1.750976	1.292600	0.193179
6	2.037296	-0.966925	-0.574058
6	2.519458	0.334990	-0.457979
1	-1.598967	-1.717622	1.123869
1	-1.671769	-0.136974	1.968673
1	-1.996225	-0.992529	-1.220365
1	-0.076506	1.706323	1.242483
1	0.433867	-2.323459	-0.135752
1	-1.788012	1.302569	-1.358127
1	-2.026074	0.433023	0.297846
1	2.117142	2.307960	0.290033
1	2.631685	-1.721310	-1.076293
1	3.486585	0.597327	-0.868826
1	-3.481660	-0.734211	-0.166251
Vibrational frequencies (cm ⁻¹)			
-2120.14	54.52	70.76	
97.63	224.87	330.10	
394.55	415.95	448.05	
499.09	535.61	627.66	
632.87	718.96	731.99	
779.23	828.91	865.94	
913.24	949.04	995.70	
1000.18	1015.10	1017.28	
1045.82	1062.48	1095.58	
1121.92	1174.72	1178.84	
1204.82	1228.94	1258.39	
1282.45	1326.88	1356.44	

1389.65	1458.36	1494.00
1518.93	1538.56	1647.09
1676.27	2114.40	3065.16
3083.78	3177.60	3179.59
3187.58	3188.23	3206.54
3213.77	3228.29	3512.09

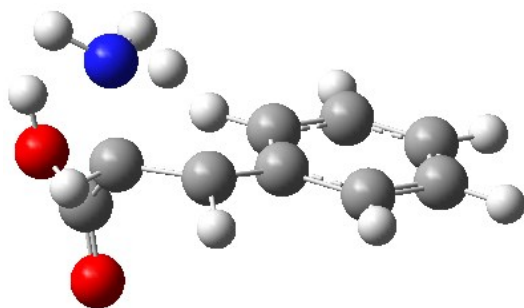
VII-5-ts1



Atomic Number	X	Y	Z
7	-1.719389	1.229320	0.956547
6	-1.431069	-1.240247	-0.805056
6	-2.634073	0.377584	0.499723
6	-0.112521	-0.709396	-0.515796
6	0.668985	-1.237164	0.528915
6	0.360078	0.454137	-1.148112
6	1.868607	-0.647823	0.900446
6	1.567562	1.037948	-0.782127
6	2.329889	0.493354	0.245856
1	-1.849871	-0.983662	-1.773455
1	-1.581872	-2.287764	-0.547718
1	-3.169358	0.766059	-0.368208
1	0.323987	-2.128977	1.042610
1	-0.226150	0.885919	-1.954198
1	-1.120046	0.953262	1.719833
1	-1.367724	2.008854	0.410405
1	2.453712	-1.083985	1.702251
1	1.915057	1.922950	-1.303382
1	3.270418	0.947411	0.532279
1	-2.317175	-0.775671	0.300664
Vibrational frequencies (cm ⁻¹)			
-1287.79	56.30	68.83	
103.20	230.29	289.73	

346.28	366.85	416.18
524.20	553.47	578.86
632.58	647.95	702.28
716.65	773.48	835.48
866.20	904.93	945.88
963.69	993.97	1010.42
1014.81	1018.04	1059.76
1069.65	1120.86	1174.96
1200.93	1273.42	1325.48
1333.04	1351.96	1368.95
1459.42	1485.37	1490.23
1537.10	1637.75	1670.27
1683.64	2169.23	3122.95
3140.19	3178.09	3186.39
3201.87	3207.33	3207.91
3225.72	3525.05	3672.93

VIII-1-ts1



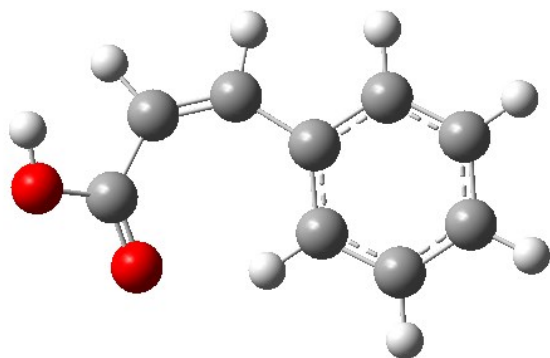
Atomic Number	X	Y	Z
7	-1.781875	0.929429	-1.550034
6	-0.357846	1.489539	0.215424
6	-1.708897	0.896593	0.010534
6	0.811329	0.632227	0.108803
6	0.793140	-0.665828	-0.441848
6	2.075392	1.119703	0.505139
6	1.955977	-1.413400	-0.599053
6	3.229278	0.375336	0.344886
6	3.187428	-0.901815	-0.216671
1	-0.310358	2.269893	0.965050
1	-0.981529	1.716806	-1.440597
1	-0.142854	-1.146440	-0.719463
1	2.131536	2.110398	0.944071
1	-1.320305	0.122964	-1.975294
1	-2.666064	1.147591	-2.014874
1	1.889075	-2.412477	-1.015872

1	4.177802	0.791132	0.667321
1	4.092251	-1.483139	-0.339821
6	-2.078751	-0.458935	0.633321
8	-2.665378	-1.407382	-0.149192
8	-1.893656	-0.667181	1.785379
1	-2.891343	-1.066171	-1.016506
1	-2.475116	1.599436	0.343516

Vibrational frequencies (cm⁻¹)

-1055.59	52.32	63.31
95.87	124.90	195.30
247.33	269.67	332.31
389.74	423.60	447.69
471.96	504.72	535.04
572.75	612.03	634.80
713.82	723.40	764.53
770.52	793.57	832.59
850.17	893.84	906.96
983.70	998.84	1004.29
1031.59	1056.02	1073.49
1099.06	1124.27	1158.36
1176.16	1214.05	1229.39
1264.40	1295.67	1327.78
1341.23	1359.13	1395.27
1494.87	1516.48	1537.76
1607.48	1635.74	1681.03
1939.43	2216.71	3113.49
3137.83	3167.07	3179.54
3184.17	3187.03	3202.63
3406.13	3532.65	3941.10

VIII-1-i1



Atomic
Number

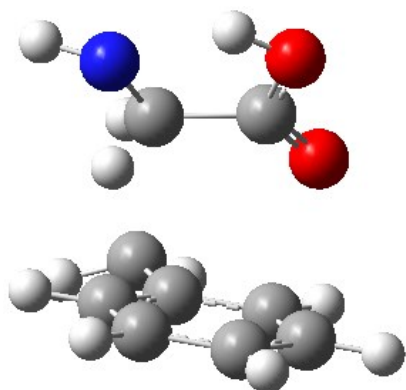
X

Y

Z

6	-0.532261	1.305152	-0.404626
6	-1.837236	1.004636	-0.325156
6	0.704437	0.537511	-0.195838
6	0.822784	-0.854080	-0.307269
6	1.850419	1.285573	0.113749
6	2.049872	-1.466953	-0.087664
6	3.070020	0.668045	0.344045
6	3.171978	-0.715533	0.244390
1	-0.333866	2.353556	-0.619280
1	-0.040227	-1.445010	-0.574456
1	1.775023	2.365851	0.182406
1	2.128254	-2.543485	-0.181711
1	3.939875	1.263913	0.592928
1	4.123928	-1.204259	0.414990
6	-2.489286	-0.288284	0.018032
8	-3.669269	-0.144370	0.666158
8	-2.094598	-1.386715	-0.242990
1	-3.815540	0.777637	0.895591
1	-2.530874	1.824077	-0.493795

IX-ts

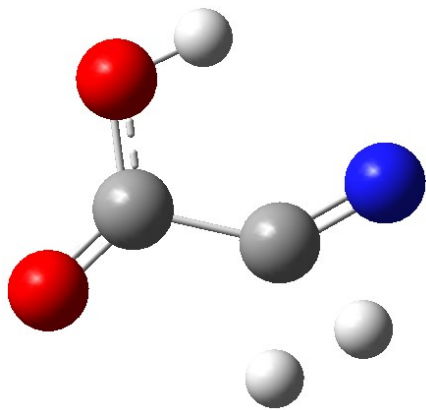


Atomic Number	X	Y	Z
7	-1.816191	1.567001	-0.995434
6	-0.454974	0.834570	1.368016
6	-2.059099	0.824206	0.157621
6	0.802319	0.361925	0.738341
6	1.708799	1.279972	0.197092
6	1.057656	-1.008375	0.597477
6	2.854471	0.841166	-0.454869
6	2.203107	-1.441881	-0.054108
6	3.104462	-0.520245	-0.580548
1	-0.927708	0.113215	2.027439
1	-0.389355	1.821840	1.828694

1	1.517843	2.343416	0.299069
1	0.351787	-1.725918	1.001150
1	-0.904470	1.346393	0.110008
1	-2.152829	2.518638	-0.893671
1	3.551366	1.562587	-0.863904
1	2.394035	-2.503681	-0.151363
1	3.998450	-0.863561	-1.086773
6	-2.074933	-0.688230	-0.129879
8	-1.895457	-0.935208	-1.407643
8	-2.230280	-1.511384	0.727378
1	-1.809928	-0.040562	-1.828054
1	-2.760812	1.132707	0.932721

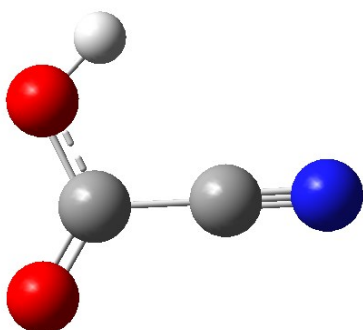
Vibrational frequencies (cm⁻¹)

-1975.10	31.32	51.21
84.65	100.46	180.73
246.45	325.10	379.65
414.89	424.42	443.59
473.82	529.44	544.37
581.99	631.93	694.95
716.19	755.40	786.77
806.98	835.68	860.40
872.93	909.64	941.92
990.57	1004.83	1017.95
1027.49	1063.46	1083.72
1119.17	1135.85	1155.61
1173.34	1180.40	1210.17
1217.60	1259.67	1272.86
1331.05	1361.72	1430.97
1469.89	1496.55	1497.95
1538.50	1654--.16	1676.77
1904.22	2143.87	3106.45
3127.79	3192.61	3202.17
3204.73	3211.85	3221.41
3230.72	3329.62	3573.50



Atomic Number	X	Y	Z
7	1.942944	0.197864	0.000011
6	0.878557	-0.405958	-0.000058
1	0.826143	-1.779771	-0.000100
1	1.725523	-1.281086	0.000236
6	-0.605326	-0.068954	-0.000010
8	-0.772814	1.245872	0.000003
8	-1.464182	-0.888558	0.000017
1	0.104311	1.666766	0.000035
Vibrational frequencies (cm ⁻¹)			
-2234.32	125.78		247.20
253.79	512.63		566.08
645.66	703.71		822.30
871.83	1080.03		1234.28
1402.24	1812.72		1902.90
1957.43	2491.55		3719.53

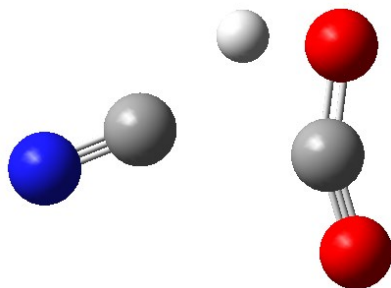
IX-1-i1



Atomic Number	X	Y	Z
7	2.129518	0.002864	0.000521
6	0.983758	-0.058410	-0.000869
6	-0.498331	-0.126864	-0.000194
8	-1.088665	1.068877	0.000213

8	-1.083761	-1.155203	0.000175
1	-0.439775	1.782198	-0.000375

IX-1-ts2

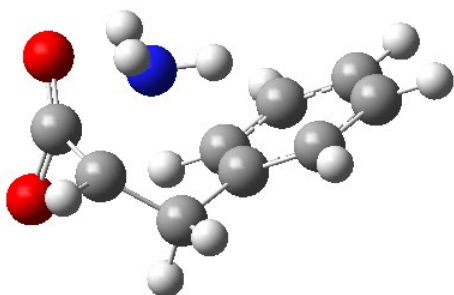


Atomic Number	X	Y	Z
7	-2.287733	-0.237834	0.000000
6	-1.216288	0.196911	-0.000000
6	0.891038	-0.084941	-0.000000
8	1.043327	1.143454	0.000000
8	1.210599	-1.175001	-0.000000
1	-0.065782	1.245395	-0.000002

Vibrational frequencies (cm⁻¹)

-1549.41	121.15	167.61
357.82	462.83	606.79
845.05	954.51	1302.68
2027.44	2303.35	2395.62

X-1-ts1

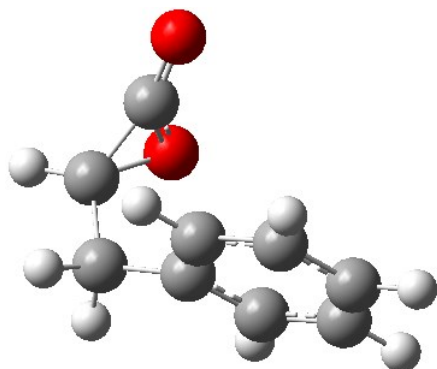


Atomic Number	X	Y	Z
7	-1.211184	1.864718	-1.135226
6	-0.603707	0.714078	1.363695
6	-1.828504	0.556310	0.500455
6	0.677621	0.239635	0.720122
6	1.701614	1.143398	0.439098
6	0.854608	-1.105610	0.391160
6	2.878407	0.719344	-0.170669

6	2.027527	-1.529296	-0.220830
6	3.041099	-0.619475	-0.505238
1	-0.803277	0.148982	2.278317
1	-0.518858	1.764798	1.646456
1	1.582378	2.187892	0.712849
1	0.070069	-1.820261	0.615985
1	-0.231128	2.129976	-1.146525
1	-1.772554	2.662814	-1.411740
1	3.666565	1.433070	-0.379169
1	2.149628	-2.574976	-0.475691
1	3.954831	-0.953967	-0.981308
6	-2.088520	-0.647830	-0.291468
8	-1.979898	-0.962285	-1.449415
8	-2.463109	-1.178731	0.799552
1	-1.340700	1.116632	-1.817510
1	-2.695486	1.156804	0.745869

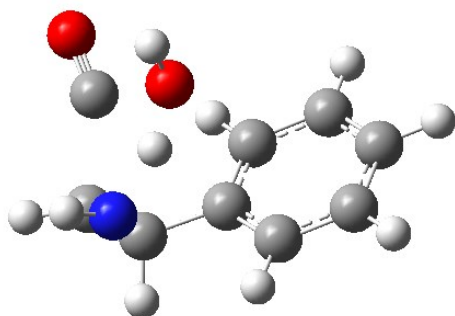
Vibrational frequencies (cm⁻¹)

-538.36	43.64	68.45
101.63	114.30	154.56
200.17	216.61	246.96
333.73	337.77	406.45
419.86	472.12	507.73
585.38	592.30	626.39
640.94	723.99	754.76
773.84	840.18	880.87
898.98	956.23	958.99
992.70	1009.52	1019.76
1033.18	1065.30	1113.68
1126.44	1163.66	1179.24
1208.08	1214.19	1236.22
1319.58	1329.27	1353.76
1368.79	1410.49	1469.28
1499.46	1543.40	1641.43
1661.06	1682.56	1684.74
1937.58	3083.97	3131.26
3178.18	3202.12	3208.86
3218.90	3229.49	3231.35
3461.53	3589.73	3641.41



Atomic Number	X	Y	Z
6	0.885968	1.149179	1.103229
6	2.097255	0.531615	0.447359
6	-0.415252	0.593964	0.579826
6	-0.960206	-0.565547	1.130166
6	-1.058523	1.199621	-0.497474
6	-2.136032	-1.103283	0.621270
6	-2.235453	0.664555	-1.007810
6	-2.777317	-0.486783	-0.447577
1	0.929857	2.231801	0.952417
1	0.974334	0.970545	2.179002
1	-0.456574	-1.052564	1.958990
1	-0.629217	2.090860	-0.942032
1	-2.550051	-2.003966	1.057994
1	-2.727295	1.144849	-1.845048
1	-3.694143	-0.904987	-0.845035
6	2.040293	-0.677971	-0.353171
8	2.001284	-1.842145	-0.543309
8	2.054085	0.444408	-1.053157
1	3.065744	0.873257	0.800531

XI-1-ts1



Atomic Number	X	Y	Z
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7	-1.668396	1.585922	-0.716380
6	-0.652133	0.938712	1.427637
6	-1.835691	0.998558	0.470721
6	0.624199	0.453888	0.792422
6	1.356793	1.282201	-0.058151
6	1.058706	-0.852978	1.003631
6	2.497719	0.805476	-0.690120
6	2.199796	-1.332304	0.370639
6	2.920859	-0.503029	-0.479028
1	-0.916038	0.309313	2.281195
1	-0.527479	1.962411	1.796841
1	1.010455	2.293037	-0.237998
1	0.495089	-1.503385	1.665863
1	-1.160346	0.553921	-1.385375
1	-2.567626	1.829663	-1.121682
1	3.058211	1.455454	-1.351797
1	2.524521	-2.351701	0.541853
1	3.810616	-0.873376	-0.974191
6	-1.949394	-0.894467	-0.003217
8	-1.001564	-0.591090	-1.561506
8	-2.382328	-1.950612	0.075986
1	-1.509115	-0.908653	-2.314802
1	-2.793513	1.089134	0.991710

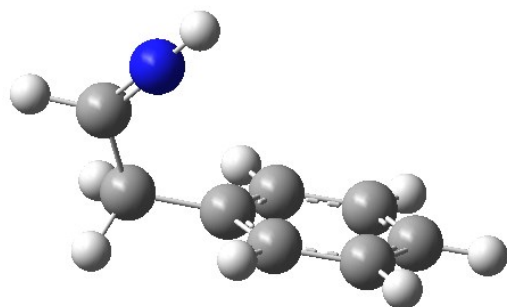
Vibrational frequencies (cm⁻¹)

-1206.27	42.68	62.60
76.53	116.48	158.39
169.04	272.24	312.43
375.66	416.40	424.08
477.12	498.42	514.67
553.36	599.15	618.96
632.12	703.42	720.86
773.47	779.20	842.74
861.49	867.28	937.16
946.30	952.14	995.00
1017.11	1021.64	1065.10
1112.15	1141.93	1173.73
1204.55	1212.45	1224.65
1241.59	1326.81	1343.10
1354.40	1385.39	1475.74
1498.23	1504.40	1535.54
1545.03	1668.22	1690.81
1798.36	2113.66	3054.75
3093.25	3115.39	3167.50
3180.52	3189.71	3198.22

3206.57

3537.25

3896.07

XI-1-ts2

Atomic Number	X	Y	Z
7	-2.363673	-0.761973	1.033347
6	-1.552210	0.682940	-0.790710
6	-2.595003	0.050793	0.140763
6	-0.133926	0.346269	-0.435902
6	0.353288	-0.945733	-0.640310
6	0.708496	1.293756	0.140618
6	1.654732	-1.278348	-0.288229
6	2.013323	0.965593	0.495952
6	2.490195	-0.321579	0.281327
1	-1.713188	1.765902	-0.784110
1	-1.792769	0.348816	-1.807454
1	-0.298417	-1.693585	-1.079553
1	0.339987	2.299955	0.311165
1	-2.185201	-1.410141	1.759252
1	2.019647	-2.284616	-0.457920
1	2.656842	1.716852	0.938492
1	3.506547	-0.579012	0.554435
1	-3.621105	0.407495	-0.088783
Vibrational frequencies (cm ⁻¹)			
-1149.40	31.37	104.99	
123.15	254.24	335.27	
413.57	474.84	497.23	
633.53	677.19	687.54	
719.84	735.24	771.57	
841.13	869.46	921.05	
942.79	995.03	1010.98	
1018.03	1021.15	1063.01	
1112.01	1176.69	1201.27	
1205.14	1233.79	1317.12	
1333.08	1357.96	1425.05	
1468.96	1496.79	1543.82	

1662.58	1683.10	1855.92
2894.06	3048.47	3091.92
3190.52	3193.36	3204.69
3213.77	3224.77	3952.99