Supporting Information

MATRIX-IR SPECTROSCOPIC INVESTIGATIONS OF THE THERMOLYSIS AND PHOTOLYSIS OF DIAZOAMIDES

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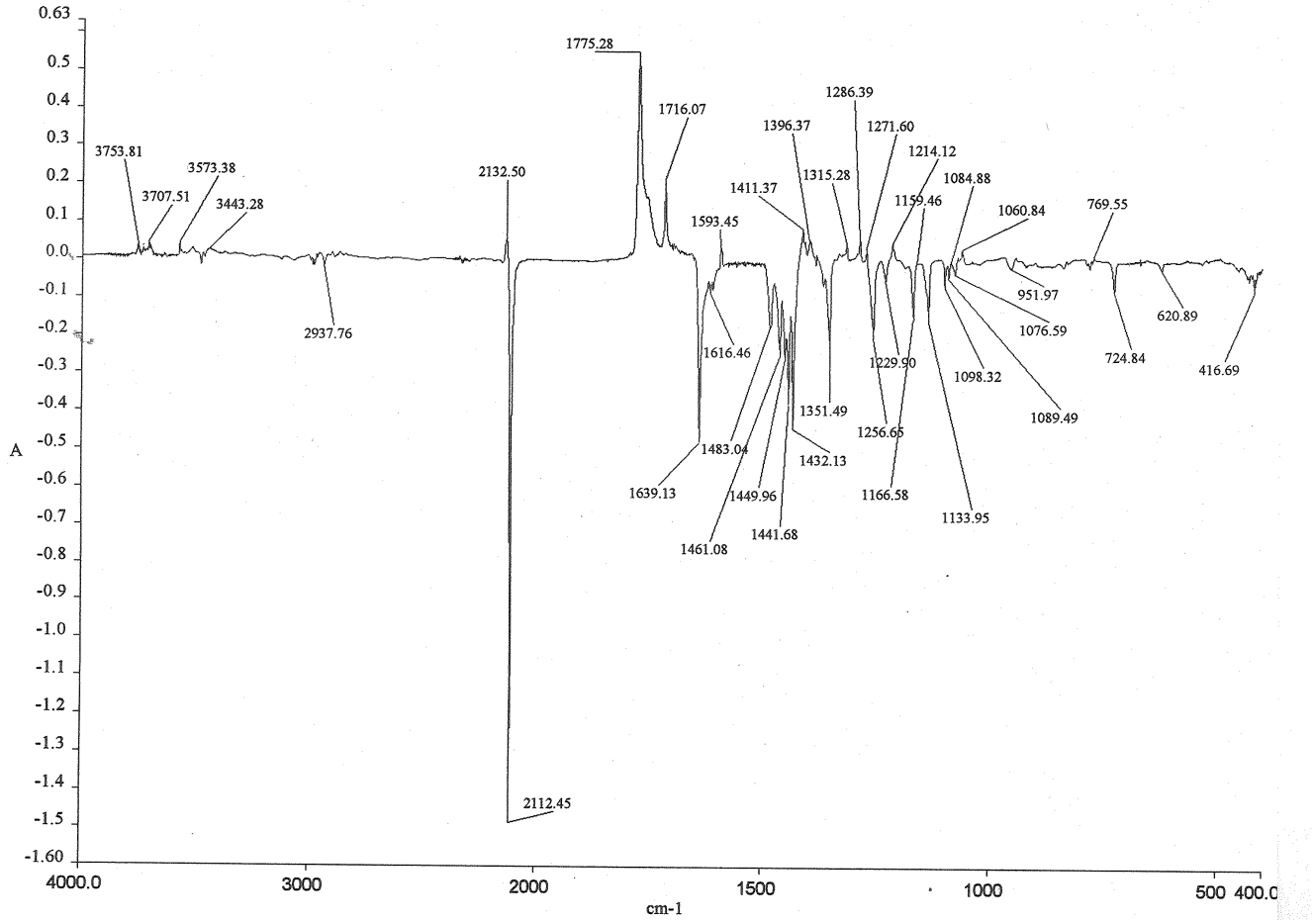


Figure S1. IR-Difference spectrum (Ar matrix, 10 K). Negative peaks: *N,N*-diethyldiazoacetamide **1b**. Positive peaks: products after 15 min photolysis at $\lambda \geq 305$ nm.

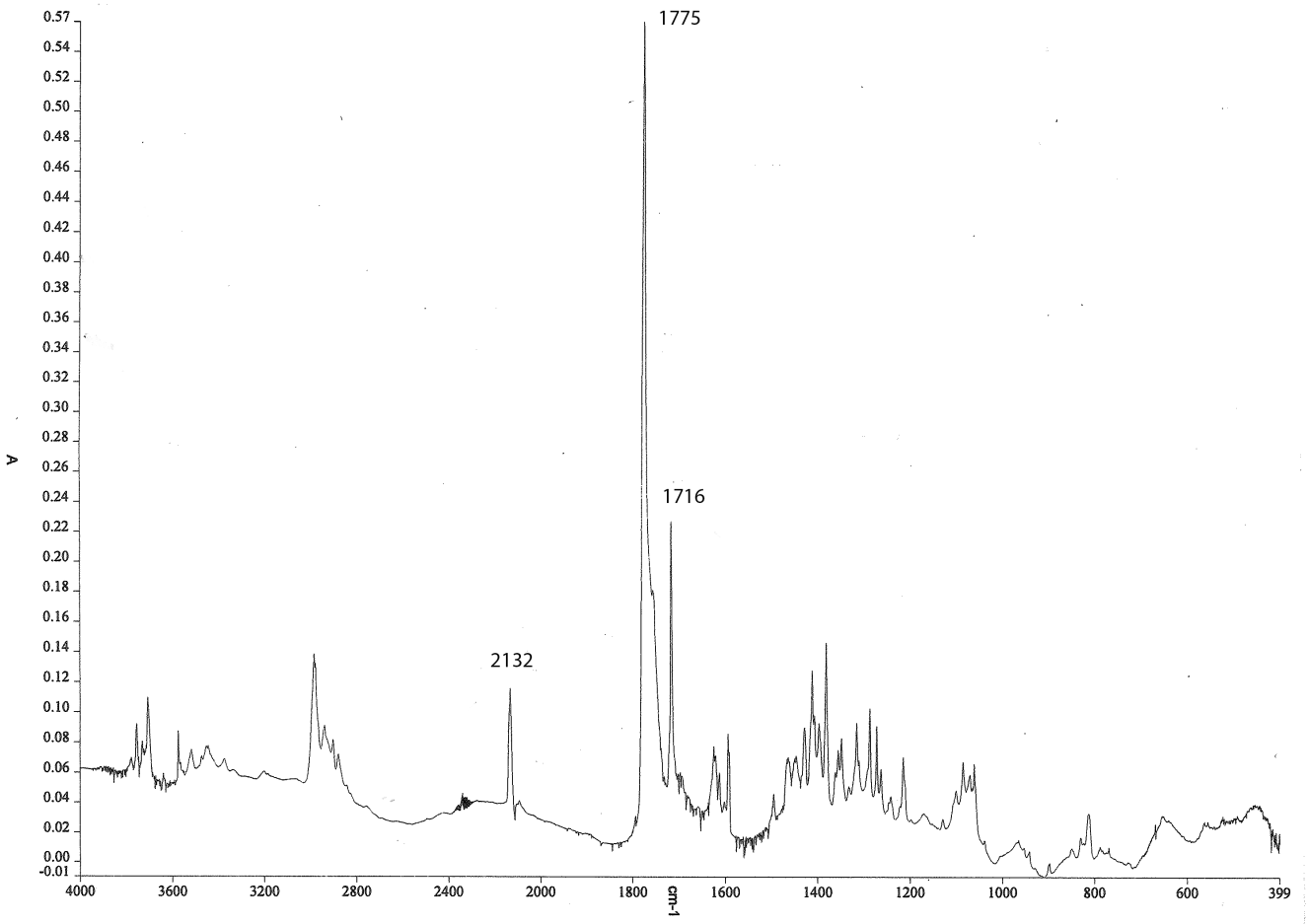


Figure S2. IR spectrum (Ar matrix, 10 K) resulting from15 min photolysis of **1b** at $\lambda \geq 305$ nm; peaks due to **1b** have been subtracted (cf Figure S1).

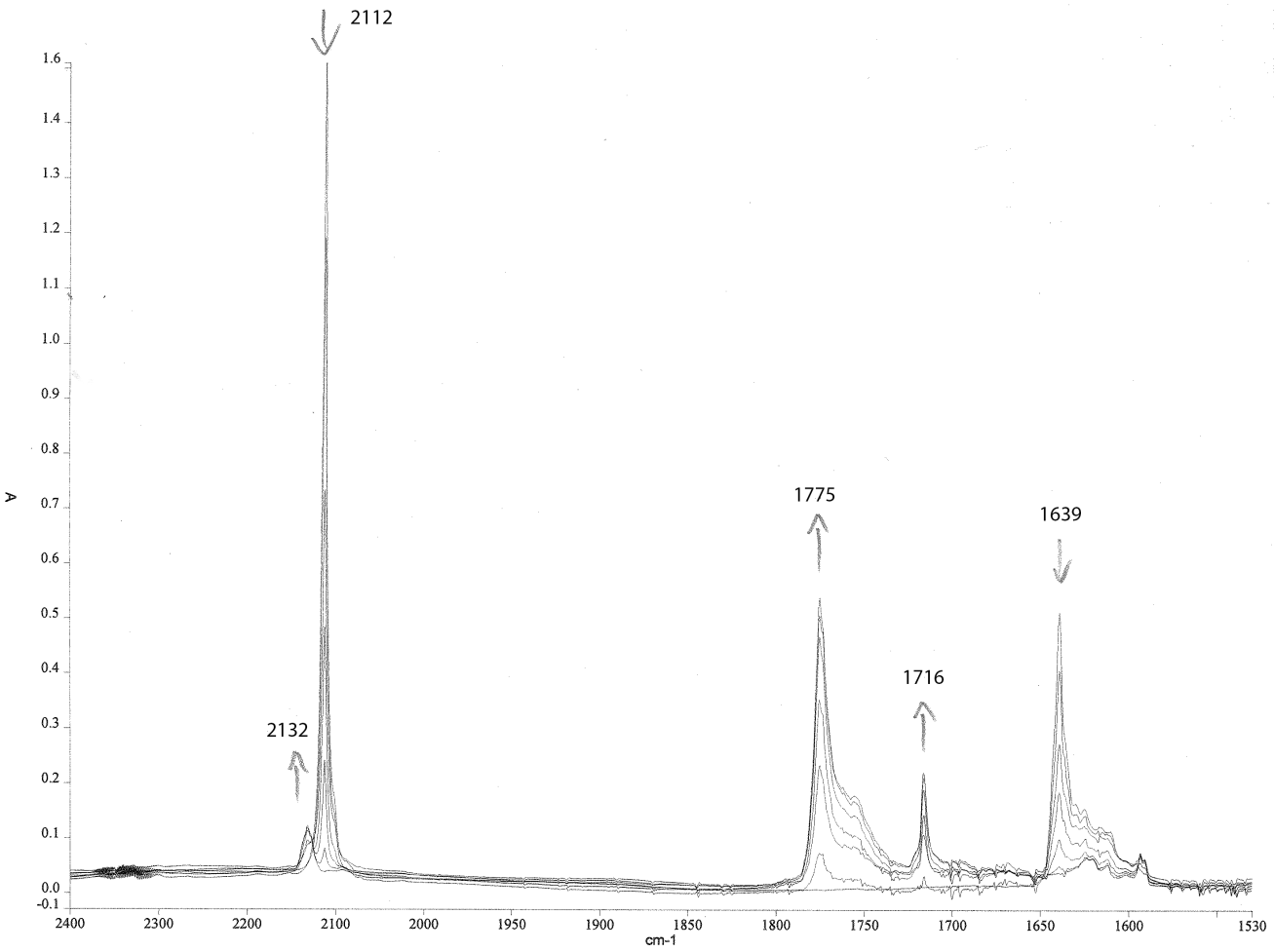


Figure S3. IR spectra (Ar matrix, 10 K) resulting photolysis of **1b** at λ ≥ 305 nm for 0, 2, 4, 6, 8, 10, and 12 min. Decreasing bands arw due to diazo compound **1b** (2112, 1639 cm^{-1}). Increasing bands are due to the photoproducts, ketene **2b** (2132 cm^{-1}) and lactones **3b** and **6b** (1775 and 1716 cm^{-1}).

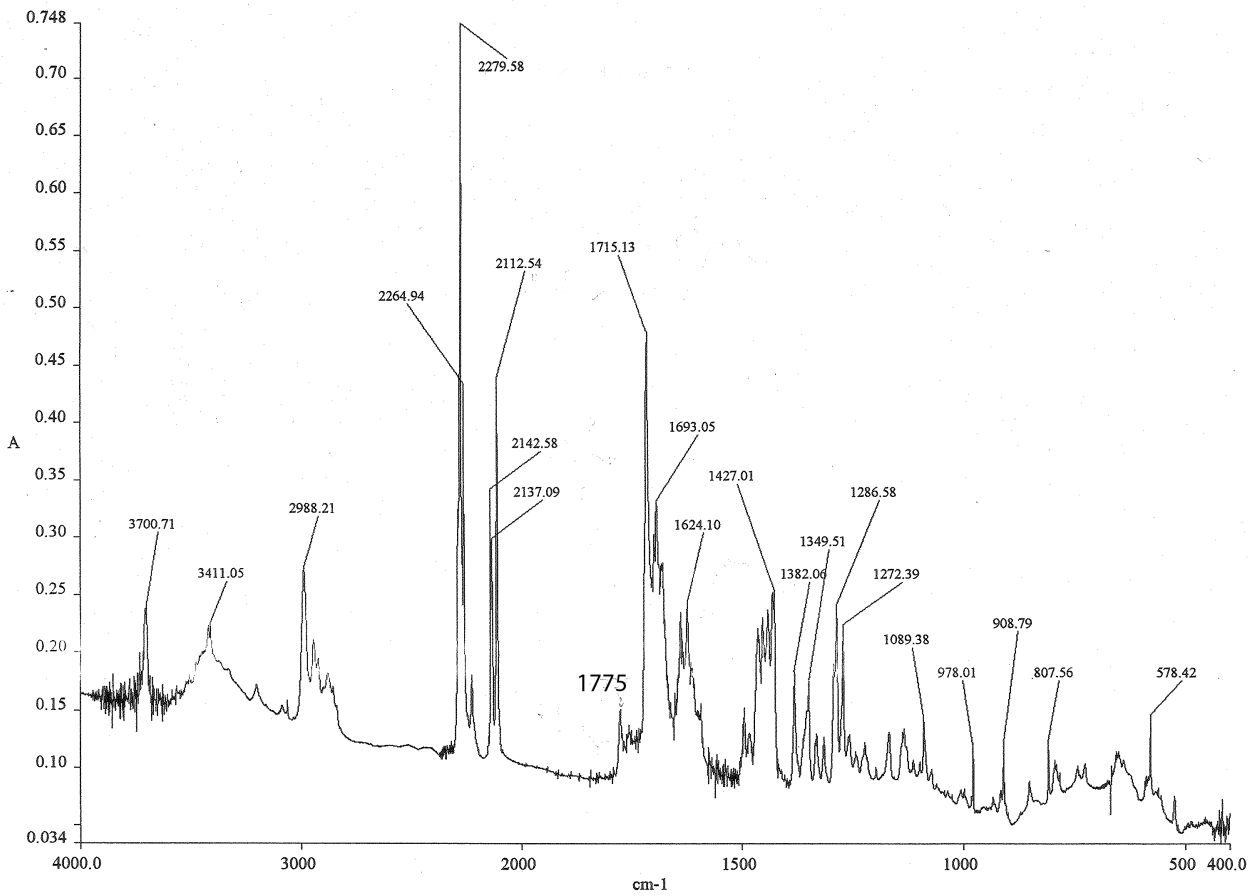
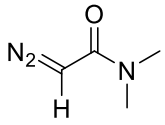


Figure S4. IR spectrum (Ar matrix, 10 K) of the product of FVT of diazoamide **1b** at 400-420 ^{o}C. Bands at 1775 and 1715 cm^{-1} are due to lactams **3b** and **6b**, respectively. 2279 = ethyl isocyanate. 2112 = residual **1b**. 2137 = CO. 2142 = ketene CH_2CO. 1464, 1453, 1441 = propene.

COMPUTATIONAL DATA

(*s-Z*)-*N,N*-dimethyldiazoacetamide 1a

GAUSSIAN 98; B3LYP/6-31g(d)



C	-0.03320100	-0.33229300	-0.02101400
O	0.27584100	-1.52383000	-0.02962600
N	-1.34084300	0.10290100	-0.06463000
C	1.00413300	0.71592500	0.03308500
N	2.24347200	0.30174600	0.01622200
N	3.31402200	-0.08083400	-0.00401300
C	-2.40013300	-0.88939300	0.05387100
C	-1.73859200	1.49989000	-0.01937000
H	0.87235100	1.78084400	0.14617700
H	-3.12438500	-0.77281400	-0.76074700
H	-2.93294100	-0.78815900	1.00895600
H	-1.94724100	-1.87766200	-0.00067800
H	-2.73764100	1.59389900	-0.45334700
H	-1.07000400	2.12107500	-0.61950500
H	-1.77665900	1.90198500	1.00366200

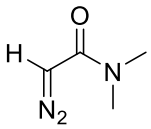
State= 1-A
HF= =-396.0745917 (B3LYP/6-31G**)
Zero-point correction= 0.116839 (Hartree/Particle)
Sum of electronic and zero-point Energies= -395.957752

Vibrational Frequencies (scaled by 0.9613):

Mode Nr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	?A	64.4	0.4	0
2	?A	92.9	3.8	1
3	?A	101.0	0.8	0
4	?A	133.2	1.5	0
5	?A	149.0	0.4	0
6	?A	199.9	5.2	1
7	?A	290.7	3.0	1
8	?A	377.7	7.8	1
9	?A	410.3	4.5	1
10	?A	439.5	33.7	6
11	?A	478.7	5.5	1
12	?A	540.3	1.1	0
13	?A	610.9	5.3	1
14	?A	695.6	29.4	6
15	?A	842.8	4.0	1
16	?A	957.4	4.4	1
17	?A	1045.2	9.5	2

18	?A	1085.4	4.9	1
19	?A	1102.4	208.1	39
20	?A	1127.5	8.4	2
21	?A	1168.7	35.4	7
22	?A	1247.4	31.1	6
23	?A	1326.5	2.9	1
24	?A	1381.7	194.0	36
25	?A	1388.9	218.6	41
26	?A	1425.9	75.7	14
27	?A	1452.7	12.9	2
28	?A	1455.3	12.1	2
29	?A	1460.8	11.7	2
30	?A	1482.8	80.1	15
31	?A	1662.6	226.0	42
32	?A	2160.0	532.1	100
33	?A	2892.0	52.8	10
34	?A	2904.5	79.7	15
35	?A	2956.6	42.4	8
36	?A	2976.4	24.6	5
37	?A	3011.9	17.8	3
38	?A	3061.1	1.1	0
39	?A	3141.0	2.3	0

(*s*-*E*)-*N*,*N*-dimethyldiazoacetamide 1a



C	0.36795000	0.83181400	0.11241200
O	1.03833500	1.85532100	0.00956600
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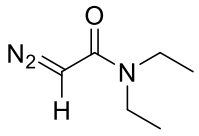
C	-1.09198500	0.96192800	0.34582900
N	-1.96753400	0.11248100	-0.11062700
N	-2.71973900	-0.65065700	-0.50943100
C	2.29774300	-0.54084100	-0.42784400
C	0.29735700	-1.64605100	0.51442800
H	-1.47703600	1.92108900	0.66345900
H	2.40079900	-1.34842600	-1.16103300
H	2.95614100	-0.75852400	0.42387000
H	2.60555600	0.40371200	-0.87265300
H	1.05281300	-2.21702800	1.06563700
H	-0.10344700	-2.29093200	-0.27874100
H	-0.50434700	-1.40699700	1.21383000

State= 1-A
HF= -396.0704469 (B3LYP/6-31G**)
Zero-point correction= 0.117076 (Hartree/Particle)
Sum of electronic and zero-point Energies= -395.953371

Vibrational Frequencies (scaled by 0.9613):

Mode Nr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	?A	70.4	0.8	0
2	?A	100.9	0.2	0
3	?A	114.6	4.4	1
4	?A	145.6	3.5	1
5	?A	190.4	2.1	0
6	?A	213.4	7.8	2
7	?A	302.3	5.1	1
8	?A	381.0	5.6	1
9	?A	420.1	9.5	2
10	?A	457.1	14.9	3
11	?A	516.7	24.9	6
12	?A	535.7	2.1	0
13	?A	669.8	11.9	3
14	?A	683.9	33.5	8
15	?A	731.5	22.9	5
16	?A	968.4	31.6	7
17	?A	1044.4	7.5	2
18	?A	1089.8	1.5	0
19	?A	1121.6	7.0	2
20	?A	1134.7	75.5	17
21	?A	1170.7	56.8	13
22	?A	1236.1	41.4	9
23	?A	1328.8	42.5	10
24	?A	1361.9	211.3	48
25	?A	1389.9	11.2	3
26	?A	1423.4	34.0	8
27	?A	1445.3	9.0	2
28	?A	1452.1	17.5	4
29	?A	1462.2	5.9	1
30	?A	1485.2	36.5	8
31	?A	1674.4	390.3	89
32	?A	2123.5	439.7	100
33	?A	2903.9	38.8	9
34	?A	2910.6	61.3	14
35	?A	2960.4	53.8	12
36	?A	2965.0	9.3	2
37	?A	3030.8	10.5	2
38	?A	3060.2	1.4	0
39	?A	3125.2	8.0	2

(s-*Z*)-*N*,*N*-Diethyldiazoacetamide 1b



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C	-1.89343000	-0.83781800	-0.50508200
C	-2.38463900	-1.80697900	0.57326600
C	0.46582100	-0.38218900	-0.15995400
O	0.74425100	-1.49639000	-0.60628800
C	1.53030300	0.55397800	0.25567000
N	2.75554800	0.10829000	0.17456400
N	3.81306700	-0.30357400	0.09848700
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H	-0.36354000	2.68596400	-0.89867300
H	-1.66046400	3.40022700	0.08021000
H	-2.04805700	2.25597400	-1.21567100
H	-2.71751400	-0.21338100	-0.86830100
H	-1.49722600	-1.39938100	-1.35284600
H	-1.56611200	-2.45838900	0.88902800
H	-3.19367600	-2.43363900	0.18301900
H	-2.76546100	-1.27463600	1.45172500

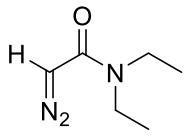
State= 1-A
HF= -474.7126025 (B3LYP/6-31G**)
Zero-point correction= 0.174297 (Hartree/Particle)
Sum of electronic and zero-point Energies= -474.538306

Vibrational Frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	53.6	0.6	0
2	A	69.0	0.2	0
3	A	76.4	3.7	1
4	A	89.9	3.5	1
5	A	123.8	0.7	0
6	A	146.8	0.8	0
7	A	220.5	0.0	0
8	A	230.8	1.3	0
9	A	286.4	1.0	0
10	A	317.9	3.1	1
11	A	371.4	7.0	1
12	A	407.4	4.2	1
13	A	432.1	6.0	1
14	A	439.7	33.4	6
15	A	513.8	1.7	0
16	A	539.1	1.0	0
17	A	601.6	4.9	1
18	A	695.6	28.6	5
19	A	754.0	6.6	1
20	A	760.6	2.9	1
21	A	813.4	8.4	1
22	A	893.8	2.8	0
23	A	925.4	9.8	2
24	A	991.9	0.9	0
25	A	1051.6	11.7	2
26	A	1064.1	6.0	1
27	A	1076.7	21.1	4
28	A	1112.8	107.1	19
29	A	1168.8	31.6	6
30	A	1207.8	22.1	4
31	A	1237.3	91.8	16
32	A	1292.9	19.5	3

33	A	1332.6	20.7	4
34	A	1346.3	87.2	15
35	A	1353.5	11.5	2
36	A	1367.8	15.9	3
37	A	1370.8	20.3	4
38	A	1410.2	351.9	62
39	A	1431.4	65.3	12
40	A	1446.5	1.2	0
41	A	1448.8	3.4	1
42	A	1454.1	16.3	3
43	A	1460.4	5.8	1
44	A	1469.1	29.8	5
45	A	1654.5	225.3	40
46	A	2157.5	567.2	100
47	A	2927.9	20.8	4
48	A	2929.1	11.6	2
49	A	2933.8	44.1	8
50	A	2941.8	27.2	5
51	A	2973.1	8.9	2
52	A	2988.8	22.8	4
53	A	3000.5	34.7	6
54	A	3007.5	37.6	7
55	A	3012.2	14.9	3
56	A	3023.8	20.0	4
57	A	3137.7	2.0	0

(s-*E*)- *N,N*-Diethyldiazoacetamide 1b



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C	1.80331300	-0.76505100	0.13001200
C	2.37192400	-0.36844300	1.49446200
C	-0.54222500	-1.03206200	-0.45725200
O	-0.36439300	-2.21474200	-0.73785300
C	-1.94156600	-0.53001000	-0.43672900
N	-2.36734700	0.36001300	0.41332800
N	-2.71708300	1.15563700	1.15662100
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H	-0.59389800	1.54019300	-0.61921300
H	0.47679600	1.75056100	0.76055200
H	2.45547300	1.79777000	-0.80573700
H	1.23602000	2.98409300	-1.27071100
H	1.37503400	1.46323300	-2.17175500
H	1.66519200	-1.84417500	0.06906000
H	2.50394800	-0.48999200	-0.66755500
H	2.54740000	0.70921500	1.57694900
H	3.33134100	-0.87034300	1.65547800
H	1.69310800	-0.66426500	2.30013700

State= 1-A
HF= -474.7044313 (B3LYP/6-31G**)

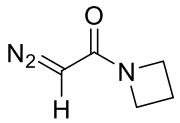
Zero-point correction= 0.174636 (Hartree/Particle)
Sum of electronic and zero-point Energies= -474.529795

Vibrational Frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	36.2	0.3	0
2	A	55.1	0.4	0
3	A	77.2	0.1	0
4	A	111.7	5.9	1
5	A	145.8	0.6	0
6	A	169.2	5.0	1
7	A	228.8	2.3	1
8	A	252.7	3.2	1
9	A	283.2	0.1	0
10	A	324.9	1.5	0
11	A	372.1	7.0	2
12	A	429.4	15.1	4
13	A	431.2	4.1	1
14	A	468.8	13.5	3
15	A	528.4	17.2	4
16	A	533.1	4.9	1
17	A	653.2	13.0	3
18	A	674.5	16.3	4
19	A	713.4	44.2	10
20	A	764.2	5.0	1
21	A	779.7	8.8	2
22	A	910.3	5.3	1
23	A	928.3	1.3	0
24	A	1007.6	24.1	6
25	A	1035.4	5.1	1
26	A	1058.8	8.2	2
27	A	1101.9	12.1	3
28	A	1126.3	67.9	16
29	A	1163.3	10.1	2
30	A	1200.8	22.3	5
31	A	1253.0	197.7	47
32	A	1283.0	16.4	4
33	A	1326.2	50.2	12
34	A	1334.6	11.1	3
35	A	1358.8	27.1	6
36	A	1370.2	21.4	5
37	A	1371.5	10.4	2
38	A	1391.4	172.3	41
39	A	1440.2	5.0	1
40	A	1446.4	4.8	1
41	A	1453.6	3.5	1
42	A	1457.7	5.0	1
43	A	1461.8	2.6	1
44	A	1476.9	9.4	2
45	A	1665.5	380.1	90
46	A	2122.1	423.8	100
47	A	2911.1	25.0	6
48	A	2930.2	23.0	5
49	A	2931.3	15.8	4
50	A	2937.9	37.6	9
51	A	2992.7	25.4	6
52	A	3004.4	12.6	3
53	A	3005.4	34.1	8

54	A	3009.5	13.4	3
55	A	3031.8	26.0	6
56	A	3033.6	6.6	2
57	A	3123.1	7.2	2

(s-*Z*)-*N*-Diazocarbonylazetidine 1c



C	-0.37603500	0.41946400	-0.10810900
O	-0.71641700	1.59234700	0.02548600
N	0.93288700	0.05110100	-0.27821400
C	1.64204800	-1.20455700	0.02632300
C	2.09027500	0.90950000	0.00673300
H	1.29562100	-1.69376400	0.94565100
C	2.94714300	-0.37559700	0.18790000
H	1.63576800	-1.93639700	-0.78975800
H	1.95650300	1.51684300	0.90866200
H	2.36902100	1.56842500	-0.82127600
H	3.44236500	-0.47516300	1.15479100
H	3.67586300	-0.54156600	-0.60732300
C	-1.32719000	-0.70620900	-0.13017800
H	-1.08055500	-1.74445000	-0.30183500
N	-2.59236400	-0.42791900	0.02482000
N	-3.68633700	-0.15008200	0.16927800

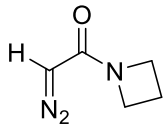
State= 1-A
HF= -434.1547687 (B3LYP/6-31G**)
Zero-point correction= 0.123969 (Hartree/Particle)
Sum of electronic and zero-point Energies= -434.030799

Vibrational Frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	56.3	0.8	0
2	A	105.7	0.9	0
3	A	113.7	3.9	1
4	A	116.8	0.1	0
5	A	169.3	9.7	1
6	A	196.8	6.7	1
7	A	346.2	4.7	1
8	A	446.7	32.6	5
9	A	449.0	1.8	0
10	A	525.5	6.8	1
11	A	540.1	0.8	0
12	A	697.9	31.5	4
13	A	739.4	2.1	0
14	A	796.4	11.2	2
15	A	822.6	0.0	0
16	A	868.9	4.6	1
17	A	906.0	3.1	0
18	A	931.5	2.5	0
19	A	1003.0	34.6	5
20	A	1096.3	1.9	0
21	A	1099.9	4.0	1

22	A	1139.7	32.4	5
23	A	1158.8	0.8	0
24	A	1160.2	18.8	3
25	A	1190.4	1.8	0
26	A	1227.6	8.2	1
27	A	1249.8	3.3	0
28	A	1287.5	2.8	0
29	A	1314.5	116.6	17
30	A	1392.3	700.0	100
31	A	1447.5	4.3	1
32	A	1465.7	1.1	0
33	A	1488.6	6.8	1
34	A	1674.3	232.2	33
35	A	2156.4	562.0	80
36	A	2911.6	59.1	8
37	A	2939.3	35.4	5
38	A	2955.5	31.6	5
39	A	2980.6	23.2	3
40	A	2983.6	33.5	5
41	A	3035.2	24.0	3
42	A	3123.5	2.3	0

(s-*E*)-*N*-Diazocarbonylazetidine 1c



C	-1.66811700	0.70263700	0.27644400
C	-0.27011100	1.09762200	0.01166500
O	0.05275000	2.28134500	0.02165700
N	0.62996600	0.09616800	-0.26965700
C	0.75357000	-1.26457200	0.30552200
C	2.08561400	0.32664100	-0.28489900
H	-2.37818900	1.44376800	0.61502100
H	0.40309400	-1.32984700	1.34274400
C	2.29298000	-1.14990400	0.14935100
H	0.26657600	-2.04963200	-0.28192700
H	2.39623800	1.07954500	0.44680700
H	2.47803100	0.60764600	-1.26683000
H	2.86605000	-1.29234200	1.06671500
H	2.70356800	-1.79109800	-0.63260200
N	-2.14151800	-0.47184700	-0.02803100
N	-2.53430300	-1.50908500	-0.30398200

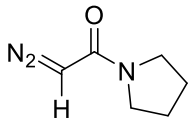
State= 1-A
HF= -434.1526737 (B3LYP/6-31G**)
Zero-point correction= 0.124198 (Hartree/Particle)
Sum of electronic and zero-point Energies= -434.028476

Vibrational Frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	67.5	1.2	0
2	A	94.4	0.1	0
3	A	115.5	1.5	0

4	A	144.0	6.2	1
5	A	187.1	7.4	2
6	A	220.1	11.4	3
7	A	366.3	6.8	2
8	A	459.7	3.3	1
9	A	485.3	35.1	8
10	A	538.6	1.1	0
11	A	594.2	3.2	1
12	A	661.4	22.9	5
13	A	713.1	41.1	10
14	A	743.4	0.5	0
15	A	820.9	0.1	0
16	A	847.8	3.5	1
17	A	913.7	2.3	1
18	A	938.2	2.9	1
19	A	1058.8	8.4	2
20	A	1094.8	5.6	1
21	A	1098.8	4.6	1
22	A	1124.1	13.3	3
23	A	1153.3	4.1	1
24	A	1163.1	3.4	1
25	A	1190.8	2.3	1
26	A	1228.0	4.9	1
27	A	1249.6	0.9	0
28	A	1293.6	8.7	2
29	A	1320.7	131.1	31
30	A	1346.8	399.2	93
31	A	1447.7	2.3	1
32	A	1463.8	0.7	0
33	A	1486.8	7.5	2
34	A	1676.4	385.5	90
35	A	2124.3	427.0	100
36	A	2922.8	42.5	10
37	A	2944.6	31.6	7
38	A	2971.7	20.7	5
39	A	2980.8	28.5	7
40	A	2988.2	19.2	5
41	A	3034.3	24.5	6
42	A	3131.6	8.7	2

(s-*Z*)-*N*-Diazocarbonylpyrrolidine 1d



C	-1.64303300	-0.72368600	0.04955900
C	-0.71163500	0.41796900	-0.04344400
O	-1.10862100	1.58232200	-0.10177400
N	0.61772300	0.09549300	-0.05669200
C	1.20582600	-1.24618000	0.01698800
C	1.62944200	1.16066100	-0.07403200
H	-1.38685600	-1.76929000	0.13583400
H	1.03642000	-1.70013200	1.00466400
C	2.70323400	-0.99034800	-0.22460700
H	0.77702000	-1.91478800	-0.73815600
H	1.34075800	1.96340500	0.60843200
C	2.91595300	0.42865400	0.32970700

H	1.70801300	1.59864300	-1.07813600
H	2.91286200	-1.00881400	-1.29989300
H	3.33453500	-1.74487700	0.25195800
H	3.81394300	0.91211000	-0.06343100
H	3.00302800	0.39683900	1.42175100
N	-2.91848600	-0.44596600	0.04823000
N	-4.02344800	-0.17439800	0.04362600

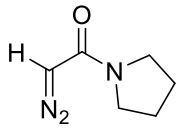
State= 1-A
HF= -473.5022663 (B3LYP/6-31G**)
Zero-point correction= 0.153884 (Hartree/Particle)
Sum of electronic and zero-point Energies= -473.348383

Vibrational Frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	31.6	0.2	0
2	A	94.5	2.5	0
3	A	105.8	1.5	0
4	A	116.9	0.4	0
5	A	178.3	4.5	1
6	A	210.7	3.7	1
7	A	242.6	0.4	0
8	A	332.6	6.1	1
9	A	434.0	0.7	0
10	A	435.6	30.9	4
11	A	495.2	8.3	1
12	A	539.6	0.9	0
13	A	557.2	1.2	0
14	A	696.1	29.2	4
15	A	706.3	9.9	1
16	A	814.5	5.7	1
17	A	846.9	3.0	0
18	A	851.2	4.8	1
19	A	885.1	3.4	0
20	A	896.9	1.1	0
21	A	937.1	7.8	1
22	A	974.8	6.0	1
23	A	1009.9	12.7	2
24	A	1104.2	7.8	1
25	A	1139.6	6.1	1
26	A	1149.8	17.5	2
27	A	1165.0	23.0	3
28	A	1175.1	18.4	3
29	A	1205.2	26.4	4
30	A	1231.3	12.2	2
31	A	1274.4	1.2	0
32	A	1299.9	31.3	4
33	A	1305.3	6.7	1
34	A	1322.4	1.9	0
35	A	1335.4	49.7	7
36	A	1397.6	707.9	100
37	A	1445.4	3.3	0
38	A	1453.3	1.8	0
39	A	1474.4	0.8	0
40	A	1486.3	5.3	1
41	A	1662.4	239.7	34
42	A	2156.0	568.7	80
43	A	2886.1	52.0	7

44	A	2913.7	35.4	5
45	A	2937.4	17.4	2
46	A	2942.3	9.4	1
47	A	2951.1	53.5	8
48	A	2993.6	18.2	3
49	A	2996.7	23.6	3
50	A	3004.5	41.6	6
51	A	3131.8	2.0	0

(s-*E*)-*N*-diazocarbonylpyrrolidine 1d



C	-1.97328100	0.56110700	0.36564000
C	-0.63903700	1.12053600	0.04161200
O	-0.51550800	2.34408000	0.02176500
N	0.40366700	0.26527000	-0.22266400
C	0.48147500	-1.15303500	0.17822200
C	1.74400100	0.83901700	-0.44792200
H	-2.71959100	1.23874700	0.75735500
H	0.11947900	-1.27805100	1.20703600
C	1.97932000	-1.49304100	0.06174700
H	-0.11985300	-1.79901300	-0.46853600
H	1.77042000	1.85569300	-0.05481800
C	2.68103700	-0.14175200	0.26365200
H	1.95857700	0.88610300	-1.52405700
H	2.19424200	-1.88000700	-0.94046000
H	2.28159400	-2.25662700	0.78322900
H	3.69691900	-0.12216200	-0.13969000
H	2.73653900	0.10288200	1.33057700
N	-2.40355200	-0.61017100	-0.00357900
N	-2.77659500	-1.64041200	-0.33125200

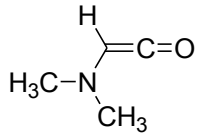
State= 1-A
HF= -473.4973119 (B3LYP/6-31G**)
Zero-point correction= 0.154263 (Hartree/Particle)
Sum of electronic and zero-point Energies= -473.343049

Vibrational Frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	42.2	0.4	0
2	A	66.1	0.6	0
3	A	123.6	4.1	1
4	A	139.5	3.7	1
5	A	193.7	5.2	1
6	A	222.1	3.7	1
7	A	267.7	6.7	2
8	A	369.9	7.2	2
9	A	447.5	2.7	1
10	A	484.3	31.4	7
11	A	532.1	2.9	1
12	A	553.5	7.6	2
13	A	556.5	0.6	0

14	A	658.0	23.5	5
15	A	707.9	44.6	10
16	A	742.3	2.2	0
17	A	834.7	4.1	1
18	A	852.5	1.7	0
19	A	888.9	3.0	1
20	A	900.3	1.4	0
21	A	948.8	5.0	1
22	A	987.0	2.7	1
23	A	1028.2	1.8	0
24	A	1100.2	2.0	0
25	A	1144.1	9.5	2
26	A	1148.4	24.5	6
27	A	1155.9	6.0	1
28	A	1169.2	21.6	5
29	A	1211.7	18.6	4
30	A	1232.3	31.1	7
31	A	1277.3	1.0	0
32	A	1305.9	5.9	1
33	A	1316.5	39.1	9
34	A	1321.5	10.9	2
35	A	1338.0	64.5	15
36	A	1357.6	370.8	85
37	A	1446.2	3.2	1
38	A	1453.9	5.0	1
39	A	1473.6	1.0	0
40	A	1485.1	9.4	2
41	A	1662.0	377.2	87
42	A	2121.4	434.8	100
43	A	2911.8	65.5	15
44	A	2915.1	5.3	1
45	A	2940.1	20.1	5
46	A	2944.6	22.1	5
47	A	2969.3	27.8	6
48	A	2995.4	24.3	6
49	A	3003.0	40.0	9
50	A	3022.9	6.7	2
51	A	3122.9	8.0	2

N,N-DIMETHYLAMINOKETENE (2a)



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_4H_7NO, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	Z
1	C	0.567830802	0.33136164	–1.841523335
2	N	0.568214405	0.330059961	–0.380201986
3	C	1.918876795	0.331363692	0.177625321

4	C	–0.25158576	–0.704142112	0.168341026
5	C	–1.311847853	–0.349054352	0.87777952
6	O	–2.249218534	–0.031407667	1.504989376
7	H	–0.043413092	–1.76902294	0.029050443
8	H	–0.459967248	0.406916456	–2.206087082
9	H	1.023545338	–0.579618537	–2.274312815
10	H	1.130724752	1.19904385	–2.20451006
11	H	1.863780381	0.406920126	1.266771636
12	H	2.492785754	–0.579616363	–0.078521518
13	H	2.469147646	1.199045809	–0.204226904

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –2.0199 y = 0.0000 z = 0.9919 Tot = 2.2503

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –286.6612621 Hartree

Zero-point correction = 0.106661 Hartree

Sum of electronic and zero-point energies = –286.5546011 Hartree

Zero-point vibrational energy = 280.0396 kJ/mol = 66.93107 kcal/mol

Enthalpy = -1.798107652×10^5 kcal/mol = -7.523282416×10^5 kJ/mol

Entropy = 81.376 cal/mol K = 340.477184 J/mol K

Gibbs Free Energy (T = 298.15 K) = -1.798350275×10^5 kcal/mol = -7.524297549×10^5 kJ/mol

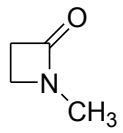
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	83.9076	0.0459	0	80
2	137.635	0.068	0	132
3	242.1432	0.0067	0	232
4	246.5824	0.4394	0	237
5	342.9214	11.1397	1	329
6	370.8903	7.9604	1	356
7	404.094	1.3612	0	388
8	542.1304	8.2992	1	521
9	635.5341	7.2995	1	610
10	652.8238	39.257	6	627

11	873.6918	23.3722	4	839
12	1052.403	9.299	1	1011
13	1059.471	14.7269	2	1018
14	1131.685	5.2418	0	1087
15	1158.651	9.8381	1	1113
16	1188.15	14.2516	2	1142
17	1241.665	12.3578	2	1193
18	1305.312	1.119	0	1254
19	1422.761	27.9911	4	1367
20	1461.903	1.3625	0	1405
21	1495.046	0.1708	0	1437
22	1510.449	10.8798	1	1451
23	1524.478	3.6846	0	1465
24	1525.243	15.9141	2	1466
25	1538.401	2.3515	0	1478
26	2223.209	578.6639	100	2137
27	2950.193	41.9709	7	2836
28	2958.497	135.3728	23	2844
29	3079.755	12.2223	2	2960
30	3082.831	77.1513	13	2963
31	3098.072	22.7558	3	2978
32	3137.846	21.7377	3	3016
33	3140.581	27.9685	4	3019

[*] scaling factor = 0.9613, [#] rounded

N-METHYLAZETIDINONE (3a)



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_4H_7NO, framework group C_S

STANDARD ORIENTATION

center No.	**atom type**			**coordinates [Å]**
		x	**y**	**z**
1	C	0.268044104	–1.951896976	0.165286037
2	N	0.268044104	–0.510685976	0.165286037

3	C	1.185273812	0.484387036	0.730884242
4	C	0.245619615	1.581068313	0.151458258
5	C	–0.607655297	0.402183	–0.374703024
6	O	–1.632135017	0.268028786	–1.006435604
7	H	–0.619763431	–2.279462327	–0.382169352
8	H	1.160691156	–2.353753433	–0.331625566
9	H	0.224860898	–2.353753433	1.186008875
10	H	0.678628944	2.208557702	–0.63156741
11	H	–0.259599723	2.208557702	0.889956528
12	H	1.254204323	0.452988544	1.825241071
13	H	2.194055848	0.452988544	0.301085348

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 3.1899 y = 2.5153 z = 0.0000 Tot = 4.0623

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –286.7056929 Hartree

Zero-point correction = 0.109372 Hartree

Sum of electronic and zero-point energies = –286.5963209 Hartree

Zero-point vibrational energy = 287.1556 kJ/mol = 68.63184 kcal/mol

Enthalpy = -1.798374411×10^5 kcal/mol = -7.524398537×10^5 kJ/mol

Entropy = 77.847 cal/mol K = 325.711848 J/mol K

Gibbs Free Energy (T = 298.15 K) = -1.798606512×10^5 kcal/mol = -7.525369645×10^5 kJ/mol

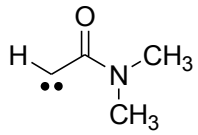
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	114.2901	2.6582	0	109
2	155.283	4.2819	0	149
3	194.1299	0.8257	0	186
4	251.9659	5.511	1	242
5	477.4697	2.325	0	458
6	552.0748	3.9053	0	530
7	717.8107	0.8197	0	690
8	776.104	1.7232	0	746
9	832.968	1.1318	0	800

10	950.7559	0.5513	0	913
11	992.2646	23.0969	4	953
12	1056.963	3.415	0	1016
13	1086.693	61.7996	12	1044
14	1133.061	0.0846	0	1089
15	1183.313	3.3285	0	1137
16	1196.521	0.0001	0	1150
17	1209.118	1.1516	0	1162
18	1270.712	16.951	3	1221
19	1313.478	25.8574	5	1262
20	1434.052	113.4418	22	1378
21	1466.999	10.808	2	1410
22	1494.196	0.4724	0	1436
23	1511.658	8.3162	1	1453
24	1538.455	12.1417	2	1478
25	1560.092	5.953	1	1499
26	1879.407	502.6969	100	1806
27	3031.698	53.7129	10	2914
28	3046.968	65.4533	13	2929
29	3081.972	49.3786	9	2962
30	3087.191	24.3491	4	2967
31	3103.83	13.0264	2	2983
32	3148.126	5.3355	1	3026
33	3159.046	12.9603	2	3036

* scaling factor = 0.9613, # rounded

N,N-DIMETHYLAMINOCARBONYLCARBENE (5a), Singlet



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_4H_7NO, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	z
1	C	–0.46867246	0.017027712	–1.969111175
2	C	–0.468619682	0.016996265	–0.562454603
3	N	0.420993581	0.017032423	0.435028454

4	C	–0.006498743	–0.22340456	1.804993153
5	O	–1.719813731	–0.178004975	–0.497597728
6	C	1.829823061	0.2372809	0.157509584
7	H	–0.734648284	1.013749018	–2.351040386
8	H	1.984465091	0.244319308	–0.924692266
9	H	2.431147908	–0.572044596	0.588586755
10	H	2.175066849	1.191231665	0.576297323
11	H	–1.08406493	–0.39593573	1.806393395
12	H	0.222277983	0.641412875	2.439614169
13	H	0.501117117	–1.105321602	2.214801908

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 4.7206 y = 0.8458 z = 1.4263 Tot = 5.0034

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –286.591526 Hartree

Zero-point correction = 0.105265 Hartree

Sum of electronic and zero-point energies = –286.486261 Hartree

Zero-point vibrational energy = 276.3744 kJ/mol = 66.05507 kcal/mol

Enthalpy = -1.797676571×10^5 kcal/mol = -7.521478774×10^5 kJ/mol

Entropy = 82.291 cal/mol K = 344.305544 J/mol K

Gibbs Free Energy (T = 298.15 K) = -1.797921922×10^5 kcal/mol = -7.52250532×10^5 kJ/mol

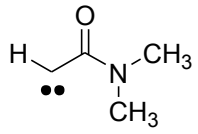
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	119.5928	0.7542	0	114
2	151.4396	2.1864	0	145
3	168.4012	1.3976	0	161
4	200.7734	5.6284	1	193
5	226.0417	0.8423	0	217
6	318.5244	35.582	7	306
7	388.0249	17.1404	3	373
8	492.3973	37.0723	8	473
9	591.2005	8.1446	1	568
10	743.6193	1.3797	0	714

11	872.9787	12.9886	2	839
12	954.4648	133.4604	29	917
13	1036.961	57.9874	12	996
14	1097.038	5.2562	1	1054
15	1139.012	0.322	0	1094
16	1187.839	2.5272	0	1141
17	1266.304	10.9955	2	1217
18	1336.135	11.9249	2	1284
19	1460.616	24.5591	5	1404
20	1481.548	28.4925	6	1424
21	1484.661	35.8278	7	1427
22	1506.34	1.5414	0	1448
23	1519.856	17.6697	3	1461
24	1530.6	19.3754	4	1471
25	1546.369	11.5718	2	1486
26	1723.8	454.0374	100	1657
27	3039.104	30.3612	6	2921
28	3045.245	63.1669	13	2927
29	3067.41	25.4378	5	2948
30	3095.485	55.7077	12	2975
31	3098.423	1.5621	0	2978
32	3145.181	10.5088	2	3023
33	3170.803	1.2627	0	3048

[*] scaling factor = 0.9613, [#] rounded

N,N-DIMETHYLAMINOCARBONYLCARBENE (5a), Triplet



GAUSSIAN 98; UB3LYP/6-31g(d)

stoichiometry C_4H_7NO, framework group C_S

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	1.262160967	–1.514998381	0
2	C	–0.004041787	–0.814779436	0
3	N	–0.007232905	0.555435304	0
4	C	–1.270603154	1.270271321	0

5	O	–1.035740594	–1.504294783	0
6	C	1.207347185	1.346654043	0
7	H	1.371866918	–2.595034924	0
8	H	2.076095137	0.684260847	0
9	H	1.253724187	1.988474904	0.890208694
10	H	1.253724187	1.988474904	–0.890208694
11	H	–2.080449284	0.54071671	0
12	H	–1.353792663	1.908266708	–0.890086439
13	H	–1.353792663	1.908266708	0.890086439

DIPOLE MOMENT [DEBYE] [UB3LYP/6-311+g(3df,2p)]

x = 1.6430 y = 2.9053 z = 0.0000 Tot = 3.3377

THERMOCHEMICAL DATA [UB3LYP/6-311+g(3df,2p)]

HF = –286.5932251 Hartree

Zero-point correction = 0.105117 Hartree

Sum of electronic and zero-point energies = –286.4881081 Hartree

Zero-point vibrational energy = 275.9834 kJ/mol = 65.96162 kcal/mol

Enthalpy = -1.797688877×10^5 kcal/mol = -7.521530263×10^5 kJ/mol

Entropy = 84.240 cal/mol K = 352.46016 J/mol K

Gibbs Free Energy (T = 298.15 K) = -1.797940039×10^5 kcal/mol = -7.522581121×10^5 kJ/mol

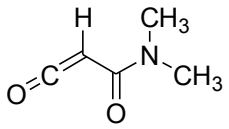
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	95.2493	0.0549	0	91
2	135.7054	1.3683	0	130
3	157.9701	0.0648	0	151
4	223.8716	6.3937	2	215
5	299.1214	1.3752	0	287
6	378.9724	6.2083	2	364
7	448.6148	39.6949	17	431
8	488.645	7.875	3	469
9	603.5935	11.1564	4	580
10	707.1289	21.0585	9	679
11	742.2301	13.9985	6	713

12	951.1592	63.7205	27	914
13	1033.186	24.3191	10	993
14	1090.252	2.06	0	1048
15	1138.451	0.0263	0	1094
16	1186.49	1.9198	0	1140
17	1224.786	47.6276	20	1177
18	1307.541	47.6921	20	1256
19	1440.034	112.2306	48	1384
20	1455.731	14.1377	6	1399
21	1481.708	3.918	1	1424
22	1505.256	2.8661	1	1447
23	1526.269	14.8577	6	1467
24	1527.527	17.6464	7	1468
25	1557.811	9.8641	4	1497
26	1663.667	232.0436	100	1599
27	3024.845	32.1503	13	2907
28	3032.816	78.99	34	2915
29	3073.679	66.7302	28	2954
30	3077.363	7.7113	3	2958
31	3143.072	8.7881	3	3021
32	3181.985	0.5499	0	3058
33	3236.084	3.9223	1	3110

* scaling factor = 0.9613, # rounded

N,N-DIMETHYLAMINOCARBONYLKETENE (13a), *s-cis* conformer



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_5H_7NO_2$, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	z
1	H	–1.81344246	1.257441815	–1.777291719
2	C	–1.825555899	1.280718542	–0.67716996
3	N	–0.491429577	1.282324129	–0.100448714
4	C	0.262936525	0.15270572	0.124526948
5	C	–0.357149955	–1.151551318	–0.204106054

6	C	0.356182631	–2.237621859	0.075685546
7	O	0.956982885	–3.204220469	0.31273302
8	C	0.145401923	2.581589951	0.068998573
9	H	–0.452919816	3.214367655	0.736180703
10	O	1.405908262	0.198112043	0.583897636
11	H	–1.313605576	–1.304403839	–0.687226427
12	H	–2.414388769	0.436858333	–0.310264983
13	H	–2.342646157	2.1934806	–0.365690981
14	H	1.131506836	2.423487788	0.502913496
15	H	0.251482451	3.096319937	–0.896134655

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –2.8484 y = 3.8560 z = 0.1547 Tot = 4.7965

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –400.0708495 Hartree

Zero-point correction = 0.117177 Hartree

Sum of electronic and zero-point energies = –399.9536725 Hartree

Zero-point vibrational energy = 307.6493 kJ/mol = 73.52995 kcal/mol

Enthalpy = -2.50968422×10^5 kcal/mol = -1.050051877×10^6 kJ/mol

Entropy = 94.059 cal/mol K = 393.542856 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.509964657×10^5 kcal/mol = -1.050169212×10^6 kJ/mol

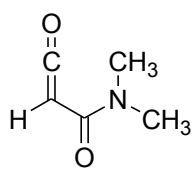
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	61.212	0.0321	0	58
2	88.1392	0.3828	0	84
3	95.0956	3.4781	0	91
4	134.0308	1.3369	0	128
5	146.5003	1.0699	0	140
6	212.439	5.7477	0	204
7	310.6439	2.7108	0	298
8	395.548	8.6544	1	380
9	442.8253	10.9452	1	425
10	499.716	4.8449	0	480

11	524.6418	14.9789	1	504
12	559.0609	19.552	2	537
13	643.9684	6.2036	0	619
14	740.6198	39.9646	4	711
15	876.7186	1.3459	0	842
16	996.2937	0.892	0	957
17	1091.851	11.0044	1	1049
18	1136.177	12.7141	1	1092
19	1145.376	163.1663	19	1101
20	1151.54	50.9212	6	1106
21	1180.727	6.0129	0	1135
22	1298.954	46.6054	5	1248
23	1380.886	14.3801	1	1327
24	1448.633	162.0854	19	1392
25	1456.477	174.8462	20	1400
26	1497.199	63.2914	7	1439
27	1527.605	11.3827	1	1468
28	1529.135	13.442	1	1469
29	1534.381	15.2964	1	1475
30	1556.16	62.205	7	1495
31	1717.544	242.0116	28	1651
32	2240.622	845.5024	100	2153
33	3018.765	50.9054	6	2901
34	3030.908	75.559	8	2913
35	3081.256	42.8715	5	2962
36	3102.622	25.0178	2	2982
37	3142.396	18.2574	2	3020
38	3194.72	0.9724	0	3071
39	3243.557	6.3381	0	3118

* scaling factor = 0.9613, # rounded

N,N-DIMETHYLAMINOCARBONYLKETENE (13a), *s-trans* conformer



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_5H_7NO_2$, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	z
1	H	–0.796304649	0.842513957	–2.410367213
2	C	–0.896730228	0.582641822	–1.350478221
3	N	0.416647221	0.62801099	–0.728639845
4	C	1.338041139	1.631939799	–1.245042972
5	H	1.592112227	1.42890507	–2.294334677
6	C	0.883097905	–0.259917722	0.215080548
7	C	–0.086341521	–1.188664693	0.873533508
8	C	–1.367191146	–0.959834349	1.106018618
9	O	–2.501088013	–0.759630688	1.309351991
10	O	2.062666835	–0.312160381	0.546425523
11	H	–1.314329854	–0.425019564	–1.300250585
12	H	–1.60707318	1.287903316	–0.896011914
13	H	0.881565494	2.627819686	–1.185027172
14	H	2.248524937	1.607643281	–0.648506962
15	H	0.361087014	–2.028503275	1.394088432

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –0.2292 y = –2.8365 z = 0.6156 Tot = 2.9116

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –400.0678313 Hartree

Zero-point correction = 0.117339 Hartree

Sum of electronic and zero-point energies = –399.9504923 Hartree

Zero-point vibrational energy = 308.0732 kJ/mol = 73.63126 kcal/mol

Enthalpy = -2.509665519×10^5 kcal/mol = -1.050044053×10^6 kJ/mol

Entropy = 92.726 cal/mol K = 387.965584 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.50994198×10^5 kcal/mol = -1.050159725×10^6 kJ/mol

IR SPECTRUM

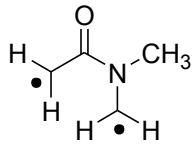
mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	49.8209	1.268	0	47
2	110.1525	0.0857	0	105
3	114.0013	3.9829	0	109

4	155.9088	3.9059	0	149
5	191.4335	2.8258	0	184
6	213.0215	6.1422	0	204
7	319.4232	5.5227	0	307
8	405.814	3.8059	0	390
9	462.3277	11.7076	1	444
10	493.5649	8.5526	1	474
11	530.8638	1.2272	0	510
12	559.3026	26.265	3	537
13	699.9678	5.0318	0	672
14	726.5575	33.2753	4	698
15	771.9388	19.885	2	742
16	1002.764	14.2172	2	963
17	1090.084	7.8021	1	1047
18	1124.783	86.8097	12	1081
19	1140.428	1.535	0	1096
20	1176.598	3.9791	0	1131
21	1203.891	110.0666	15	1157
22	1293.142	46.4105	6	1243
23	1386.187	24.8969	3	1332
24	1421.388	205.6483	29	1366
25	1454.588	11.983	1	1398
26	1492.293	34.4455	4	1434
27	1523.135	8.6368	1	1464
28	1526.121	20.6007	2	1467
29	1536.695	6.6665	0	1477
30	1558.547	31.2839	4	1498
31	1748.65	403.6135	58	1680
32	2216.524	691.038	100	2130
33	3027.085	38.4992	5	2909
34	3035.424	62.2024	9	2917
35	3082.162	49.5449	7	2962
36	3091.376	13.7961	1	2971
37	3149.342	13.1202	1	3027
38	3194.848	1.0749	0	3071
39	3225.657	16.1585	2	3100

[*] scaling factor = 0.9613, [#] rounded

TRIPLET DIRADICAL

GAUSSIAN 98; UB3LYP/6-31g(d)



stoichiometry C_4H_7NO, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	0.680462421	0.104330729	–1.823950181
2	C	0.676330516	–0.036909259	–0.378519559
3	O	1.747100658	–0.169683487	0.234971905
4	N	–0.5429553	0.012665716	0.300332357
5	C	–1.77661059	0.050859136	–0.327210737
6	C	–0.516736923	0.044360904	1.762205197
7	H	1.628583866	–0.060664311	–2.319494001
8	H	–1.85033252	–0.278677182	–1.353680936
9	H	–2.646330843	0.000967038	0.313652541
10	H	0.518960057	0.118505799	2.0876459
11	H	–0.963133378	–0.869530639	2.170883521
12	H	–1.08526399	0.908695631	2.122570053
13	H	–0.159273895	0.47366249	–2.398827135

DIPOLE MOMENT [DEBYE] [UB3LYP/6-311+g(3df,2p)]

x = –1.3540 y = 2.1155 z = –0.0190 Tot = 2.5118

THERMOCHEMICAL DATA [UB3LYP/6-311+g(3df,2p)]

HF = –286.6157109 Hartree

Zero-point correction = 0.103182 Hartree

Sum of electronic and zero-point energies = –286.5125289 Hartree

Zero-point vibrational energy = 270.9041 kJ/mol = 64.74762 kcal/mol

Enthalpy = $–1.797840627 \times 10^5$ kcal/mol = $–7.522165182 \times 10^5$ kJ/mol

Entropy = 84.663 cal/mol K = 354.229992 J/mol K

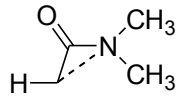
Gibbs Free Energy (T = 298.15 K) = $–1.79809305 \times 10^5$ kcal/mol = $–7.52322132 \times 10^5$ kJ/mol

IR SPECTRUM

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	88.74	0.3287	0	85
2	121.28	5.3398	3	116
3	238.9181	1.5014	0	229
4	278.2657	4.4167	2	267
5	290.2523	6.2701	3	279
6	363.1931	2.1187	1	349
7	425.8921	8.8416	5	409
8	472.9688	10.4261	6	454
9	505.4685	61.6811	38	485
10	584.266	5.7353	3	561
11	605.8058	4.7261	2	582
12	723.7207	39.0612	24	695
13	764.6232	5.9785	3	735
14	998.0344	10.1397	6	959
15	1019.568	31.4798	19	980
16	1101.072	5.857	3	1058
17	1159.472	0.7021	0	1114
18	1230.574	51.5614	31	1182
19	1344.305	86.2425	53	1292
20	1420.371	98.5801	61	1365
21	1450.573	11.9421	7	1394
22	1492.333	71.6051	44	1434
23	1518.652	4.7811	2	1459
24	1527.827	10.8073	6	1468
25	1539.399	13.7189	8	1479
26	1625.512	161.2336	100	1562
27	3053.478	47.6768	29	2935
28	3107.862	29.0149	17	2987
29	3199.664	0.5658	0	3075
30	3203.144	0.5722	0	3079
31	3207.599	8.922	5	3083
32	3309.506	3.3814	2	3181
33	3319.275	5.629	3	3190

[*] scaling factor = 0.9613, [#] rounded

TRANSITION STATE ^{1}5a→^{1}2a



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_4H_7NO, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–0.388241567	–0.730652287	–1.73076847
2	C	0.409695548	0.012744434	–0.805145291
3	O	1.312028907	0.791888086	–1.089472711
4	N	–0.238724219	–0.01664489	0.44852787
5	H	–0.308691342	–1.826830685	–1.626279906
6	C	–0.350792594	1.228745535	1.19451414
7	C	–0.575425582	–1.237705889	1.167416253
8	H	–1.652337738	–1.308303795	1.366981223
9	H	–0.268850748	–2.111368529	0.588436097
10	H	–0.048122511	–1.258128853	2.131494465
11	H	–1.379708918	1.372381944	1.546828177
12	H	0.319038536	1.219232098	2.066140792
13	H	–0.057903837	2.055636605	0.54638597

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –4.2920 y = 1.9216 z = –0.5709 Tot = 4.7371

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –286.5696877 Hartree

Zero-point correction = 0.103845 Hartree

Sum of electronic and zero-point energies = –286.4658427 Hartree

Zero-point vibrational energy = 272.6449 kJ/mol = 65.16369 kcal/mol

Enthalpy = -1.79755268×10^5 kcal/mol = -7.520960414×10^5 kJ/mol

Entropy = 79.463 cal/mol K = 332.473192 J/mol K

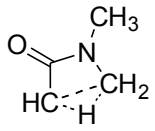
Gibbs Free Energy (T = 298.15 K) = -1.797789599×10^5 kcal/mol = -7.521951682×10^5 kJ/mol

IR SPECTRUM

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	–236.8086	2.1114	0	–228
2	103.5695	0.7481	0	99
3	183.9551	2.1599	1	176
4	230.417	2.9154	1	221
5	247.2226	3.5614	1	237
6	304.3238	6.3926	3	292
7	376.8364	3.0572	1	362
8	554.5388	3.678	1	533
9	653.9758	29.2553	13	628
10	660.3979	41.919	19	634
11	772.3526	24.7848	11	742
12	930.9329	138.379	65	894
13	1014.12	60.6355	28	974
14	1091.196	5.9259	2	1048
15	1116.156	17.8054	8	1072
16	1148.252	18.4807	8	1103
17	1189.944	31.6134	14	1143
18	1273.743	22.3515	10	1224
19	1370.064	61.3957	28	1317
20	1462.871	2.0311	0	1406
21	1487.319	11.1357	5	1429
22	1502.024	0.0673	0	1443
23	1509.995	17.3297	8	1451
24	1529.687	15.6601	7	1470
25	1556.752	5.5637	2	1496
26	1728.102	212.2031	100	1661
27	3025.372	21.273	10	2908
28	3030.21	82.9504	39	2912
29	3039.932	36.1621	17	2922
30	3076.788	45.7698	21	2957
31	3083.549	18.2231	8	2964
32	3152.252	12.8707	6	3030
33	3175.806	1.9158	0	3052

[*] scaling factor = 0.9613, [#] rounded

TRANSITION STATE ^{1}5a→^{1}3a



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_4H_7NO, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	Z
1	C	0.622463867	0.029181861	–1.699856008
2	C	0.761607043	–0.116622629	–0.246718985
3	O	1.843268326	–0.293209843	0.304111212
4	N	–0.474463333	0.068378693	0.328543211
5	C	–1.442519546	0.117870683	–0.724287609
6	C	–0.739600148	0.216557416	1.740424866
7	H	0.633849118	–0.942437836	–2.218177429
8	H	–0.792084264	0.456666334	–1.672379262
9	H	–2.169048263	0.933888839	–0.626060283
10	H	–1.937594322	–0.829746873	–0.962973435
11	H	0.225381635	0.167998027	2.251960717
12	H	–1.38450973	–0.585238973	2.121279831
13	H	–1.212604753	1.183974384	1.956284106

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 3.8439 y = 3.1956 z = 1.1021 Tot = 5.1188

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –286.578289 Hartree

Zero-point correction = 0.102733 Hartree

Sum of electronic and zero-point energies = –286.475556 Hartree

Zero-point vibrational energy = 269.7242 kJ/mol = 64.46563 kcal/mol

Enthalpy = $–1.797615747 \times 10^5$ kcal/mol = $–7.521224284 \times 10^5$ kJ/mol

Entropy = 78.321 cal/mol K = 327.695064 J/mol K

Gibbs Free Energy (T = 298.15 K) = $–1.797849261 \times 10^5$ kcal/mol = $–7.522201308 \times 10^5$ kJ/mol

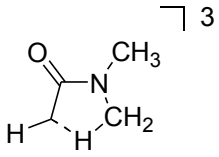
IR SPECTRUM

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	–438.2418	32.2106	10	–422
2	96.9283	3.9734	1	93
3	166.2042	1.9867	0	159
4	216.3861	1.372	0	208
5	272.7397	10.5324	3	262
6	458.1196	6.0677	2	440
7	521.7068	3.8882	1	501
8	601.471	30.3208	10	578
9	643.4549	12.2403	4	618
10	750.8643	7.6246	2	721
11	803.0405	13.5406	4	771
12	997.4168	8.7251	2	958
13	1016.254	59.4274	19	976
14	1080.8	8.2338	2	1038
15	1130.829	7.6999	2	1087
16	1171.768	4.882	1	1126
17	1199.055	6.5393	2	1152
18	1330.02	31.2857	10	1278
19	1367.011	7.0817	2	1314
20	1434.956	136.7635	45	1379
21	1464.345	15.7569	5	1407
22	1490.536	13.9122	4	1432
23	1515.979	8.5775	2	1457
24	1532.477	30.2785	10	1473
25	1560.493	24.8121	8	1500
26	1767.421	298.6082	100	1699
27	1989.15	41.1924	13	1912
28	3031.938	55.7674	18	2914
29	3058.961	28.5006	9	2940
30	3071.094	20.4253	6	2952
31	3084.443	38.9595	13	2965
32	3117.958	18.6907	6	2997
33	3150.538	1.6917	0	3028

[*] scaling factor = 0.9613, [#] rounded

TRANSITION STATE ^{3}5a→triplet DIRADICAL

GAUSSIAN 98; UB3LYP/6-31g(d)



stoichiometry C_4H_7NO, framework group C_S

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	Z
1	C	0.734761639	0	–1.676162771
2	C	0.794356939	0	–0.220817935
3	O	1.802760307	0	0.479140583
4	N	–0.515135771	0	0.254808554
5	C	–1.527033645	0	–0.758085372
6	C	–0.814857419	0	1.669793094
7	H	1.560015224	0	–2.379221918
8	H	–0.613286848	0	–1.773761647
9	H	–2.120363483	0.916663443	–0.831222812
10	H	–2.120363483	–0.916663443	–0.831222812
11	H	0.137465978	0	2.205567524
12	H	–1.391482263	–0.890673341	1.952357517
13	H	–1.391482263	0.890673341	1.952357517

DIPOLE MOMENT [DEBYE] [UB3LYP/6-311+g(3df,2p)]

x = 2.3411 y = 2.7166 z = 0.0000 Tot = 3.5862

THERMOCHEMICAL DATA [UB3LYP/6-311+g(3df,2p)]

HF = –286.5656265 Hartree

Zero-point correction = 0.099190 Hartree

Sum of electronic and zero-point energies = –286.4664365 Hartree

Zero-point vibrational energy = 260.4232 kJ/mol = 62.24265 kcal/mol

Enthalpy = -1.797556494×10^5 kcal/mol = -7.520976372×10^5 kJ/mol

Entropy = 81.388 cal/mol K = 340.527392 J/mol K

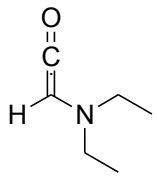
Gibbs Free Energy (T = 298.15 K) = -1.797799152×10^5 kcal/mol = -7.521991652×10^5 kJ/mol

IR SPECTRUM

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	–1807.071	17.1275	11	–1738
2	117.6178	5.9031	3	113
3	150.9651	1.6461	1	145
4	197.3953	0.9387	0	189
5	308.8269	6.4516	4	296
6	402.4427	0.0114	0	386
7	464.6576	11.6472	7	446
8	491.0094	7.4432	4	472
9	615.3956	15.9439	10	591
10	643.7889	10.036	6	618
11	702.4775	21.6501	14	675
12	779.4051	4.3131	2	749
13	1000.751	53.6203	35	962
14	1033.213	24.939	16	993
15	1061.521	13.2171	8	1020
16	1127.487	0.6197	0	1083
17	1163.683	13.641	8	1118
18	1164.024	0.9129	0	1118
19	1188.158	11.5119	7	1142
20	1321.323	35.933	23	1270
21	1355.128	85.6817	56	1302
22	1458.983	8.8414	5	1402
23	1513.393	20.9241	13	1454
24	1518.832	8.7499	5	1460
25	1543.7	2.69	1	1483
26	1708.041	152.0801	100	1641
27	1783.233	63.7549	41	1714
28	3030.36	54.0489	35	2913
29	3067.959	40.8995	26	2949
30	3079.434	37.5188	24	2960
31	3144.316	29.342	19	3022
32	3154.172	0.5018	0	3032
33	3247.668	1.6914	1	3121

[*] scaling factor = 0.9613, [#] rounded

N,*N*-DIETHYLAMINOKETENE (2b), 1st of 2 calculated conformers



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	Z
1	C	–1.836074066	–0.198665801	–1.255803298
2	C	–1.677052724	–0.482696412	0.2460131
3	N	–0.335910379	–0.344715381	0.803493366
4	C	0.596484135	–1.466446057	0.774427781
5	C	1.454066755	–1.622390752	–0.491135345
6	C	0.170165693	0.957723098	1.050806346
7	C	0.708134137	1.67409408	0.070012525
8	O	1.177768147	2.28336788	–0.816130344
9	H	0.132140207	1.404515449	2.046043471
10	H	–2.339692829	0.190953571	0.805423029
11	H	–2.016406681	–1.505270284	0.460615635
12	H	–1.256311244	–0.900105443	–1.865004484
13	H	–2.889412304	–0.286366742	–1.550374373
14	H	–1.506650734	0.817580928	–1.500820325
15	H	0.010637329	–2.382353474	0.931816253
16	H	1.261764359	–1.367313387	1.642418847
17	H	2.147140735	–2.465740278	–0.37980216
18	H	0.83871636	–1.806788976	–1.378045915
19	H	2.052958706	–0.722755669	–0.673607445

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –1.5638 y = 0.0000 z = –0.7213 Tot = 1.7221

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.3114735 Hartree

Zero-point correction = 0.163356 Hartree

Sum of electronic and zero-point energies = –365.1481175 Hartree

Zero-point vibrational energy = 428.8918 kJ/mol = 102.50759 kcal/mol

Enthalpy = $–2.291270646 \times 10^5$ kcal/mol = $–9.586676384 \times 10^5$ kJ/mol

Entropy = 98.955 cal/mol K = 414.02772 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.29156568×10^5 kcal/mol = -9.587910806×10^5 kJ/mol

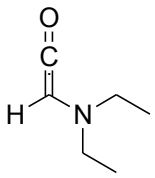
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	40.6766	0.7927	0	39
2	64.3305	0.0844	0	61
3	69.2923	1.5857	0	66
4	88.5468	0.6166	0	85
5	180.2887	4.5765	0	173
6	231.6273	0.719	0	222
7	237.0186	0.0733	0	227
8	300.1134	1.3445	0	288
9	405.6594	3.4414	0	389
10	414.582	6.8382	1	398
11	444.4482	7.6399	1	427
12	562.2007	8.1443	1	540
13	629.0135	42.2937	8	604
14	636.0454	1.3032	0	611
15	769.5021	8.0989	1	739
16	784.0069	5.7468	1	753
17	813.6143	1.0645	0	782
18	919.0175	2.608	0	883
19	985.3336	6.2078	1	947
20	1078.463	14.5594	2	1036
21	1089.946	2.8651	0	1047
22	1108.479	6.2211	1	1065
23	1108.882	29.3198	5	1065
24	1176.85	10.6275	2	1131
25	1249.052	34.4913	6	1200
26	1278.174	12.843	2	1228
27	1365.343	20.3438	4	1312
28	1391.821	7.2025	1	1337
29	1402.022	18.9199	3	1347
30	1410.899	12.7496	2	1356
31	1420.769	15.5077	3	1365

32	1430.981	18.6397	3	1375
33	1437.053	11.4414	2	1381
34	1496.808	0.8358	0	1438
35	1505.762	2.5662	0	1447
36	1518.193	0.6024	0	1459
37	1526.179	3.1866	0	1467
38	1528.158	8.4987	1	1469
39	1535.921	1.0371	0	1476
40	2189.424	499.1341	100	2104
41	3024.714	23.483	4	2907
42	3030.448	79.1752	15	2913
43	3045.751	15.628	3	2927
44	3048.167	21.8966	4	2930
45	3063.796	16.331	3	2945
46	3069.961	28.5627	5	2951
47	3110.02	52.3692	10	2989
48	3112.136	50.7036	10	2991
49	3119.814	26.1638	5	2999
50	3123.706	28.4915	5	3002
51	3132.082	49.146	9	3010

[*] scaling factor = 0.9613, [#] rounded

N,*N*-DIETHYLAMINOKETENE (2b), 2nd of 2 calculated conformers



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	z
1	C	–0.825468644	–0.679288451	–2.428184497
2	C	–0.853806681	–0.559845925	–0.903680147
3	N	0.486107986	–0.532310818	–0.305105857
4	C	1.373823489	0.561248318	–0.735409467
5	C	0.926806177	1.982481692	–0.368069999
6	C	0.524757908	–0.782169069	1.100954332
7	C	–0.400018141	–0.36039845	1.954182691

8	O	–1.282492532	–0.068041603	2.675153599
9	H	1.371953002	–1.327389144	1.510986295
10	H	–1.464753295	0.317879236	–0.620806224
11	H	–1.357839766	–1.43744501	–0.485322435
12	H	–0.202942367	–1.525991127	–2.736434974
13	H	–1.842169413	–0.842549871	–2.802537803
14	H	–0.441503181	0.224742845	–2.912768847
15	H	1.502794391	0.479746226	–1.820594433
16	H	2.35635337	0.361056744	–0.291686114
17	H	1.681389924	2.710979455	–0.686753112
18	H	–0.018378231	2.251778927	–0.85316725
19	H	0.795715276	2.085531579	0.714839626

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 1.6677 y = 0.6320 z = 0.4511 Tot = 1.8396

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.3131732 Hartree

Zero-point correction = 0.163898 Hartree

Sum of electronic and zero-point energies = –365.1492752 Hartree

Zero-point vibrational energy = 430.3145 kJ/mol = 102.84764 kcal/mol

Enthalpy = -2.291279536×10^5 kcal/mol = -9.586713579×10^5 kJ/mol

Entropy = 97.143 cal/mol K = 406.446312 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291569168×10^5 kcal/mol = -9.587925398×10^5 kJ/mol

IR SPECTRUM

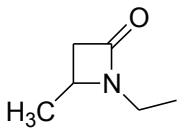
mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	32.571	2.0383	0	31
2	72.8024	0.0222	0	69
3	97.0323	0.436	0	93
4	141.1275	1.1036	0	135
5	207.8645	3.1198	0	199
6	234.2042	0.3905	0	225
7	275.2926	0.5572	0	264
8	304.6109	1.7483	0	292

9	382.9959	6.2558	1	368
10	443.5457	2.3655	0	426
11	467.1395	12.9498	2	449
12	501.6106	8.7535	1	482
13	611.8021	31.1899	6	588
14	672.827	2.6738	0	646
15	777.3529	6.8363	1	747
16	799.8534	2.39	0	768
17	826.5569	1.6358	0	794
18	925.6308	2.2651	0	889
19	1001.323	2.5352	0	962
20	1062.565	9.2094	1	1021
21	1078.296	7.7293	1	1036
22	1104.788	11.8068	2	1062
23	1148.818	4.1344	0	1104
24	1174.641	20.0908	4	1129
25	1213.066	30.5537	6	1166
26	1261.449	18.0175	3	1212
27	1329.592	9.5798	1	1278
28	1381.939	4.0525	0	1328
29	1395.52	14.0022	2	1341
30	1406.593	9.6255	1	1352
31	1423.591	6.2368	1	1368
32	1431.535	18.715	3	1376
33	1442.597	24.8213	5	1386
34	1508.041	4.6983	0	1449
35	1519.258	5.8304	1	1460
36	1526.642	4.5474	0	1467
37	1531.12	1.3187	0	1471
38	1535.144	2.4592	0	1475
39	1548.365	0.8607	0	1488
40	2186.056	490.0068	100	2101
41	2946.724	54.6598	11	2832
42	3051.04	17.8091	3	2932
43	3053.284	13.7922	2	2935
44	3058.587	38.5716	7	2940
45	3086.251	10.3427	2	2966

46	3091.801	16.0023	3	2972
47	3116.954	40.8247	8	2996
48	3121.872	40.0757	8	3001
49	3125.992	33.3864	6	3005
50	3130.791	34.9542	7	3009
51	3173.905	13.4995	2	3051

* scaling factor = 0.9613, # rounded

1-ETHYL-4-METHYL-2-AZETIDINONE (3b)



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

center No.	atom type			coordinates [Å]
		x	y	z
1	O	–0.720304463	–2.055450368	–1.011159585
2	C	–0.762075117	–0.941453168	–0.535080015
3	N	0.220232662	–0.112672671	–0.047256692
4	C	–0.691159442	0.991047945	0.320475258
5	C	–1.853468519	0.10536276	–0.223165028
6	C	–0.432927465	2.315066364	–0.387832177
7	C	1.651469466	–0.299412414	0.071477268
8	C	2.125333438	–0.489765706	1.516662606
9	H	0.523472159	2.754510001	–0.08043234
10	H	–0.411638287	2.177374305	–1.474955542
11	H	–1.222027317	3.036178978	–0.145372571
12	H	–0.7400045	1.143104488	1.407216894
13	H	1.887316973	–1.185045346	–0.52779971
14	H	2.16943245	0.553301365	–0.388496631
15	H	1.885904826	0.383316514	2.134679646
16	H	1.650290137	–1.367556973	1.966556531
17	H	3.211625416	–0.632083564	1.545406726
18	H	–2.363251375	0.501031738	–1.10638877
19	H	–2.593347582	–0.216894547	0.514431818

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –0.2113 y = –4.2022 z = 0.7165 Tot = 4.2681

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.3654919 Hartree

Zero-point correction = 0.166140 Hartree

Sum of electronic and zero-point energies = –365.1993519 Hartree

Zero-point vibrational energy = 436.2005 kJ/mol = 104.25442 kcal/mol

Enthalpy = -2.291599219×10^5 kcal/mol = -9.588051132×10^5 kJ/mol

Entropy = 92.302 cal/mol K = 386.191568 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291874417×10^5 kcal/mol = -9.589202562×10^5 kJ/mol

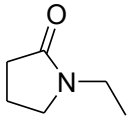
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	48.9544	0.5721	0	47
2	88.0517	0.6443	0	84
3	117.8174	4.687	0	113
4	182.6544	1.271	0	175
5	238.287	0.2103	0	229
6	266.3097	0.0315	0	256
7	291.7395	4.1873	0	280
8	394.1636	1.4603	0	378
9	455.5445	3.2778	0	437
10	520.9048	1.3699	0	500
11	562.5093	6.9859	1	540
12	683.9582	0.2017	0	657
13	730.0549	1.0724	0	701
14	786.5038	4.482	0	756
15	842.6201	4.191	0	810
16	922.3743	2.2826	0	886
17	957.8103	4.0593	0	920
18	977.447	8.1042	1	939
19	1064.138	3.0043	0	1022
20	1081.429	14.2925	2	1039
21	1090.407	23.4783	4	1048
22	1108.474	6.9978	1	1065

23	1121.624	13.2979	2	1078
24	1197.221	2.0276	0	1150
25	1207.083	0.5694	0	1160
26	1251.618	18.8809	3	1203
27	1280.778	12.2544	2	1231
28	1349.479	60.6411	11	1297
29	1396.503	30.0087	5	1342
30	1408.013	24.9121	4	1353
31	1434.109	110.8369	21	1378
32	1438.132	22.8296	4	1382
33	1438.401	7.1744	1	1382
34	1493.611	0.315	0	1435
35	1507.816	6.9617	1	1449
36	1519.656	1.521	0	1460
37	1523.047	6.723	1	1464
38	1527.354	2.1778	0	1468
39	1532.942	1.8954	0	1473
40	1872.419	511.576	100	1799
41	3036.613	51.8284	10	2919
42	3038.947	9.6114	1	2921
43	3047.6	24.9871	4	2929
44	3052.749	26.6261	5	2934
45	3094.857	11.6861	2	2975
46	3102.823	0.7088	0	2982
47	3113.33	26.4273	5	2992
48	3121.522	25.3876	4	3000
49	3122.902	37.4271	7	3002
50	3134.044	29.1692	5	3012
51	3149.671	12.3512	2	3027

[*] scaling factor = 0.9613, [#] rounded

1-ETHYL-2-PYROLLIDINONE (6b)



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	z
1	C	–2.215031789	1.344338934	–0.851092957
2	C	–1.703553117	–0.046351479	–0.463216137
3	N	–0.353974985	–0.034038839	0.076895326
4	C	0.692056613	–0.672874103	–0.546935512
5	C	1.896598965	–0.60741744	0.395465189
6	C	1.499797935	0.438451152	1.449132258
7	C	–0.044151646	0.416823133	1.427251479
8	O	0.644886262	–1.211865365	–1.64208974
9	H	–2.24326589	2.023137676	0.009217906
10	H	–1.573453694	1.790359717	–1.617915275
11	H	–3.232521274	1.274078143	–1.252154195
12	H	–1.670245835	–0.697726595	–1.340933128
13	H	–2.37892253	–0.506564411	0.272987027
14	H	–0.455925518	–0.280853603	2.174814607
15	H	–0.477990238	1.403455123	1.625241288
16	H	2.80588501	–0.36664171	–0.160903939
17	H	2.036729786	–1.604732501	0.832569125
18	H	1.898979935	0.231696563	2.44580425
19	H	1.855163288	1.429165206	1.146097056

Dipole Moment [Debye] [B3LYP/6-311+g(3df,2p)]

x = 0.0267 y = –4.0143 z = –0.4326 Tot = 4.0376

Thermochemical Data [B3LYP/6-311+g(3df,2p)]

HF = –365.3891362 Hartree

Zero-point correction = 0.168381 Hartree

Sum of electronic and zero-point energies = –365.2207552 Hartree

Zero-point vibrational energy = 442.0848 kJ/mol = 105.66081 kcal/mol

Enthalpy = -2.291737468×10^5 kcal/mol = -9.588629564×10^5 kJ/mol

Entropy = 89.169 cal/mol K = 373.083096 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.292003325×10^5 kcal/mol = -9.589741913×10^5 kJ/mol

IR Spectrum

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	56.6244	0.6929	0	54
2	109.0006	2.2745	0	104
3	151.3431	2.1532	0	145
4	189.9581	0.9063	0	182
5	209.5623	1.3763	0	201
6	321.902	5.4633	1	309
7	368.6416	5.8393	1	354
8	500.6587	3.4542	0	481
9	562.1865	4.8155	1	540
10	612.1061	2.1477	0	588
11	654.7364	8.794	2	629
12	747.1913	1.3802	0	718
13	802.4075	8.4266	2	771
14	862.6805	11.2584	3	829
15	915.012	1.0154	0	879
16	937.3679	3.1934	0	901
17	951.9167	2.9082	0	915
18	1025.307	2.5204	0	985
19	1050.847	2.2024	0	1010
20	1096.949	2.5085	0	1054
21	1111.65	6.5423	1	1068
22	1154.726	18.6994	5	1110
23	1195.899	6.4319	1	1149
24	1232.129	10.4801	3	1184
25	1252.323	25.4247	7	1203
26	1274.839	9.8446	2	1225
27	1306.588	83.6998	24	1256
28	1324.634	39.0117	11	1273
29	1356.005	10.7824	3	1303
30	1370.447	40.1523	11	1317
31	1412.551	9.4574	2	1357
32	1439.808	8.7652	2	1384
33	1467.639	89.9991	25	1410
34	1502.458	2.0623	0	1444
35	1513.633	7.0186	2	1455

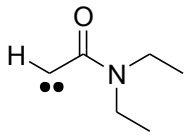
36	1522.871	6.5186	1	1463
37	1527.834	6.3834	1	1468
38	1532.536	3.6882	1	1473
39	1562.218	6.9226	1	1501
40	1807.638	348.3813	100	1737
41	2995.44	60.7728	17	2879
42	3023.615	51.9718	14	2906
43	3051.537	16.9386	4	2933
44	3060.508	17.3217	4	2942
45	3071.2	13.6027	3	2952
46	3083.5	48.5076	13	2964
47	3109.692	15.6962	4	2989
48	3123.97	24.8069	7	3003
49	3126.753	25.8089	7	3005
50	3134.476	17.7923	5	3013
51	3135.287	26.9366	7	3013

[*] scaling factor = 0.9613, [#] rounded

N,*N*-DIETHYLAMINOCARBONYLCARBENE (5b), 1st of 2 calculated conformers

GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1



STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–0.7727803	0.058855371	–2.321215941
2	C	–0.769988544	0.056249103	–0.914835429
3	N	0.105364863	0.05251732	0.093231377
4	C	–0.355004256	–0.242464608	1.455015437
5	C	–0.542024207	1.013513334	2.309233761
6	O	–2.02478981	–0.136312807	–0.866392224
7	C	1.533073852	0.224690311	–0.189417311
8	C	2.27477726	–1.102917748	–0.367091154
9	H	–1.0236616	1.058540786	–2.706365017
10	H	1.621742141	0.829825759	–1.097725743
11	H	1.971629986	0.812301544	0.62508555

12	H	–1.300789626	–0.783180987	1.36293825
13	H	0.369552963	–0.922137526	1.91856125
14	H	3.33617374	–0.91919224	–0.568156979
15	H	2.205564515	–1.725004365	0.531902194
16	H	1.853307247	–1.663022305	–1.207457184
17	H	–0.866023788	0.737120457	3.318886144
18	H	0.388868933	1.584779855	2.400380935
19	H	–1.303922897	1.665295667	1.870332578

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 4.1526 y = 2.5175 z = 1.5570 Tot = 5.0996

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.2480546 Hartree

Zero-point correction = 0.162735 Hartree

Sum of electronic and zero-point energies = –365.0853196 Hartree

Zero-point vibrational energy = 427.2608 kJ/mol = 102.11778 kcal/mol

Enthalpy = -2.2908776×10^5 kcal/mol = -9.585031878×10^5 kJ/mol

Entropy = 96.814 cal/mol K = 405.069776 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291166251×10^5 kcal/mol = -9.586239594×10^5 kJ/mol

IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	48.6158	2.3199	0	46
2	60.8153	0.4634	0	58
3	124.5156	3.3611	0	119
4	136.9623	3.0001	0	131
5	194.4794	0.2207	0	186
6	212.7361	0.6811	0	204
7	266.0698	2.2698	0	255
8	317.6756	28.0363	5	305
9	323.9634	13.9952	2	311
10	410.7564	11.5231	2	394
11	443.6052	6.0252	1	426
12	524.7065	35.778	7	504

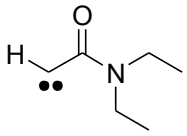
13	588.0655	4.2681	0	565
14	707.1009	1.4095	0	679
15	796.1757	3.2606	0	765
16	799.066	12.0427	2	768
17	877.0808	11.628	2	843
18	934.227	88.2437	18	898
19	958.4777	46.1041	9	921
20	975.3499	12.0846	2	937
21	1070.01	26.1317	5	1028
22	1099.199	11.1449	2	1056
23	1112.923	10.9128	2	1069
24	1133.427	16.0748	3	1089
25	1233.334	17.9231	3	1185
26	1262.054	6.0546	1	1213
27	1341.662	1.1079	0	1289
28	1383.906	25.8405	5	1330
29	1397.403	10.4829	2	1343
30	1421.914	19.0308	4	1366
31	1439.119	6.2204	1	1383
32	1442.975	25.1399	5	1387
33	1477.181	57.03	12	1420
34	1510.271	2.8758	0	1451
35	1516.163	13.9012	2	1457
36	1521.301	0.8235	0	1462
37	1524.758	3.1485	0	1465
38	1532.501	2.4874	0	1473
39	1535.612	8.5254	1	1476
40	1710.479	473.4134	100	1644
41	3054.018	13.5526	2	2935
42	3057.862	7.9411	1	2939
43	3062.978	22.8285	4	2944
44	3063.822	49.3159	10	2945
45	3068.125	17.1452	3	2949
46	3104.382	6.0529	1	2984
47	3114.335	11.4555	2	2993
48	3126.917	34.9447	7	3005
49	3129.573	18.8224	3	3008

50	3140.639	11.3007	2	3019
51	3143.134	34.3506	7	3021

* scaling factor = 0.9613, # rounded

N,*N*-DIETHYLAMINOCARBONYLCARBENE (5b), 2nd of 2 calculated conformers

GAUSSIAN 98; B3LYP/6-31g(d)



stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–0.789789872	–0.030704734	–2.307360143
2	C	–0.790382557	0.024736502	–0.902032835
3	N	0.096859646	0.044235931	0.095886334
4	C	–0.352415273	–0.192597264	1.472775944
5	C	–0.22752766	–1.657293152	1.900120527
6	O	–2.046587631	–0.146599919	–0.83424302
7	C	1.517823524	0.212120648	–0.21274505
8	C	2.024159658	1.640720946	0.002804096
9	H	–1.046666505	0.950406818	–2.732526277
10	H	2.087071584	–0.493657874	0.403440691
11	H	1.659792984	–0.092389809	–1.256046571
12	H	0.22919899	0.459270994	2.134124864
13	H	–1.395846822	0.128980179	1.52933159
14	H	3.092164377	1.702682863	–0.234385131
15	H	1.48764531	2.344658946	–0.641849443
16	H	1.891983127	1.962311545	1.041822472
17	H	–0.560121389	–1.776261116	2.93747609
18	H	–0.849306436	–2.293764198	1.263264821
19	H	0.807561389	–2.010988196	1.836711477

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 4.8458 y = 1.3805 z = –0.8748 Tot = 5.1140

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.2484851 Hartree

Zero-point correction = 0.162774 Hartree

Sum of electronic and zero-point energies = –365.0857111 Hartree

Zero-point vibrational energy = 427.3626 kJ/mol = 102.14211 kcal/mol

Enthalpy = -2.290880207×10^5 kcal/mol = -9.585042787×10^5 kJ/mol

Entropy = 96.215 cal/mol K = 402.56356 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291167072×10^5 kcal/mol = -9.586243029×10^5 kJ/mol

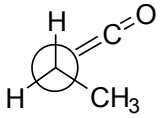
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	59.6716	1.8757	0	57
2	71.6108	0.8486	0	68
3	122.8185	2.098	0	118
4	137.9325	3.5375	0	132
5	187.4974	1.1568	0	180
6	213.7717	0.2992	0	205
7	259.4206	5.1597	1	249
8	315.1337	17.9249	3	302
9	324.2388	15.8571	3	311
10	414.9846	14.0445	2	398
11	432.2754	23.5459	5	415
12	535.9336	20.4225	4	515
13	585.1794	7.2426	1	562
14	706.2363	0.6531	0	678
15	797.7866	4.5064	0	766
16	801.3951	8.4983	1	770
17	873.3437	12.5024	2	839
18	937.5888	60.565	12	901
19	962.4325	72.608	15	925
20	975.158	10.0258	2	937
21	1071.386	29.0571	6	1029
22	1099.133	9.7933	2	1056
23	1112.152	8.2572	1	1069
24	1134.787	14.6811	3	1090
25	1232.859	17.8747	3	1185
26	1262.552	6.6936	1	1213

27	1342.222	2.3574	0	1290
28	1384.951	25.2884	5	1331
29	1398.818	11.1663	2	1344
30	1423.872	18.3785	3	1368
31	1439.114	7.9237	1	1383
32	1443.023	18.8846	4	1387
33	1478.702	56.4053	12	1421
34	1510.275	3.4822	0	1451
35	1516.938	12.2228	2	1458
36	1521.072	1.3579	0	1462
37	1524.527	3.8843	0	1465
38	1532.578	2.0355	0	1473
39	1535.02	9.317	1	1475
40	1709.897	468.23	100	1643
41	3054.562	10.6776	2	2936
42	3056.218	6.0666	1	2937
43	3059.606	38.201	8	2941
44	3070.295	25.3822	5	2951
45	3071.635	23.9581	5	2952
46	3097.536	4.3977	0	2977
47	3117.142	10.0596	2	2996
48	3124.578	31.5037	6	3003
49	3130.669	19.54	4	3009
50	3133.849	27.6778	5	3012
51	3145.06	26.0736	5	3023

* scaling factor = 0.9613, # rounded

ETHYL ISOCYANATE, 1st of 2 calculated conformers



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_3H_5NO, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	z

1	C	0.806523595	–0.319500292	0.868216401
2	O	1.190650551	–0.290158263	1.985533061
3	N	0.558179646	–0.37231929	–0.311118061
4	C	–0.583184015	–0.267585907	–1.19620194
5	C	–1.414704204	0.993505853	–0.956306461
6	H	–2.24167225	1.039173913	–1.673693152
7	H	–1.837184851	0.998114488	0.054412976
8	H	–0.801495773	1.89197453	–1.077654554
9	H	–1.20545987	–1.164587262	–1.083193945
10	H	–0.198461446	–0.275692456	–2.220557389

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –3.1506 y = –0.2096 z = 0.4473 Tot = 3.1891

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –247.4000175 Hartree

Zero-point correction = 0.079927 Hartree

Sum of electronic and zero-point energies = –247.3200905 Hartree

Zero-point vibrational energy = 209.8495 kJ/mol = 50.15524 kcal/mol

Enthalpy = -1.55191534×10^5 kcal/mol = -6.493213783×10^5 kJ/mol

Entropy = 76.551 cal/mol K = 320.289384 J/mol K

Gibbs Free Energy (T = 298.15 K) = -1.552143577×10^5 kcal/mol = -6.494168725×10^5 kJ/mol

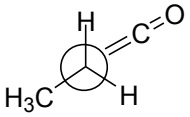
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	36.9052	1.8594	0	35
2	134.1804	7.8761	0	128
3	278.1065	2.6876	0	267
4	416.6995	4.6277	0	400
5	569.1479	24.476	2	547
6	623.7019	26.685	2	599
7	809.0667	10.5947	1	777
8	815.5544	11.6239	1	783
9	998.6664	18.7381	1	960
10	1112.939	12.6184	1	1069

11	1174.151	13.5899	1	1128
12	1322.542	8.6308	0	1271
13	1402.018	42.731	4	1347
14	1438.276	7.2128	0	1382
15	1492.447	8.2881	0	1434
16	1519.382	6.8539	0	1460
17	1530.391	0.697	0	1471
18	1547.27	2.4695	0	1487
19	2384.916	948.8455	100	2292
20	3052.213	38.4438	4	2934
21	3057.059	14.5023	1	2938
22	3100.678	9.5343	1	2980
23	3129.227	36.582	3	3008
24	3138.56	30.213	3	3017

* scaling factor = 0.9613, # rounded

ETHYL ISOCYANATE, 2nd of 2 calculated conformers



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_3H_5NO, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	z
1	C	–1.018219857	0.010909891	–2.060803018
2	C	–1.063449794	–0.022604444	–0.535827303
3	N	0.27716889	0.008689963	0.016846558
4	C	0.822715757	0.003221812	1.092457607
5	O	1.481119685	0.00340274	2.073565607
6	H	–2.035707282	–0.013103931	–2.465486517
7	H	–0.524826986	0.921543665	–2.414607517
8	H	–0.468176567	–0.850704695	–2.451880213
9	H	–1.575077198	–0.931007803	–0.193297469
10	H	–1.631628313	0.836057551	–0.156142751

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –2.9310 y = 1.0598 z = 0.0002 Tot = 3.1167

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –247.3999319 Hartree

Zero-point correction = 0.079724 Hartree

Sum of electronic and zero-point energies = –247.3202079 Hartree

Zero-point vibrational energy = 209.3155 kJ/mol = 50.02761 kcal/mol

Enthalpy = -1.551915493×10^5 kcal/mol = -6.493214424×10^5 kJ/mol

Entropy = 77.361 cal/mol K = 323.678424 J/mol K

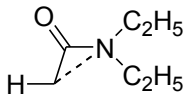
Gibbs Free Energy (T = 298.15 K) = -1.552146145×10^5 kcal/mol = -6.49417947×10^5 kJ/mol

IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	22.8119	1.2976	0	21
2	127.6239	5.2139	0	122
3	265.1302	1.0121	0	254
4	385.7043	17.711	1	370
5	567.6188	23.6018	2	545
6	617.664	25.8368	2	593
7	806.1005	0.8612	0	774
8	807.8149	14.0801	1	776
9	1026.069	18.2112	1	986
10	1124.789	7.49	0	1081
11	1159.953	2.4398	0	1115
12	1323.564	0.0138	0	1272
13	1401.391	87.2877	8	1347
14	1446.562	24.9405	2	1390
15	1488.003	18.2988	1	1430
16	1518.547	5.4593	0	1459
17	1522.792	6.5414	0	1463
18	1538.009	4.2473	0	1478
19	2388.861	997.2002	100	2296
20	3040.25	35.8787	3	2922
21	3063.066	17.2357	1	2944
22	3075.937	20.5954	2	2956
23	3135.111	28.7824	2	3013
24	3141.443	29.2973	2	3019

* scaling factor = 0.9613, # rounded

TRANSITION STATE ^{1}5b→^{1}2b, 1st of 2 calculated conformers



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–1.387173592	0.010025943	–1.803546014
2	C	–1.310040297	0.00199242	–0.373684994
3	N	0.054747137	–0.007990886	–0.019293435
4	C	1.038284001	0.957972397	–0.519055556
5	O	–2.217164538	–0.260936107	0.409590859
6	C	0.466448126	–0.936981349	1.041739299
7	H	–1.149646009	0.991783056	–2.251861409
8	C	1.972424022	0.404551479	–1.599856953
9	H	0.494852999	1.829061007	–0.900273848
10	H	1.626688729	1.305155055	0.339744562
11	H	1.472649334	–1.303197942	0.805263862
12	C	0.427414017	–0.307067567	2.439084498
13	H	–0.216965239	–1.789749118	1.008575585
14	H	2.70974877	1.161657794	–1.890542308
15	H	2.517437148	–0.476753076	–1.244509893
16	H	1.404082796	0.111660751	–2.489706493
17	H	0.766931624	–1.034861008	3.185440813
18	H	1.079313507	0.571289593	2.509481636
19	H	–0.595144976	–0.005580993	2.678632984

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –2.6508 y = –3.9740 z = –1.1849 Tot = 4.9217

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.2267494 Hartree

Zero-point correction = 0.161221 Hartree

Sum of electronic and zero-point energies = –365.0655284 Hartree

Zero-point vibrational energy = 423.2858 kJ/mol = 101.16773 kcal/mol

Enthalpy = -2.290757726×10^5 kcal/mol = -9.584530324×10^5 kJ/mol

Entropy = 92.528 cal/mol K = 387.137152 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291033598×10^5 kcal/mol = -9.585684575×10^5 kJ/mol

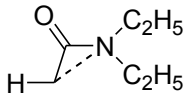
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	–205.4925	1.521	0	–198
2	81.4364	0.1157	0	78
3	92.1547	1.3896	0	88
4	135.0968	1.2806	0	129
5	161.2042	2.8061	1	154
6	219.0185	0.447	0	210
7	229.6633	2.3188	1	220
8	305.3767	3.9397	1	293
9	341.1046	1.103	0	327
10	383.056	3.6033	1	368
11	446.0786	5.3926	2	428
12	585.5591	6.8988	3	562
13	644.2201	13.8326	6	619
14	670.4661	42.5998	19	644
15	735.1277	32.4274	14	706
16	796.4924	11.4536	5	765
17	800.4582	9.3592	4	769
18	928.6939	50.323	22	892
19	949.6572	54.8079	24	912
20	965.1888	27.8152	12	927
21	1045.574	23.0187	10	1005
22	1093.624	16.2855	7	1051
23	1104.227	11.7519	5	1061
24	1117.494	27.9348	12	1074
25	1153.988	48.0402	21	1109
26	1240.815	12.8697	5	1192
27	1271.972	48.1572	21	1222
28	1342.496	8.3861	3	1290

29	1392.25	14.2315	6	1338
30	1413.785	22.8783	10	1359
31	1418.974	26.6944	12	1364
32	1430.609	4.3933	1	1375
33	1439.509	17.7215	8	1383
34	1500.602	4.3388	1	1442
35	1510.144	6.3432	2	1451
36	1518.301	8.654	3	1459
37	1520.739	4.9173	2	1461
38	1531.873	3.3384	1	1472
39	1536.746	7.6786	3	1477
40	1722.756	220.0943	100	1656
41	3026.158	32.6664	14	2909
42	3047.991	17.9235	8	2930
43	3051.318	7.8931	3	2933
44	3055.43	36.9845	16	2937
45	3061.153	33.7106	15	2942
46	3096.305	5.1491	2	2976
47	3111.531	16.2571	7	2991
48	3123.924	34.457	15	3003
49	3128.588	35.6581	16	3007
50	3130.54	15.1446	6	3009
51	3158.377	14.5701	6	3036

* scaling factor = 0.9613, # rounded

TRANSITION STATE ^{1}5b→^{1}2b, 2nd of 2 calculated conformers



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–1.356704114	–0.031732174	–1.964698604

2	C	–1.370194663	0.024674735	–0.538377953
3	N	–0.041492261	0.015985116	–0.059614554
4	C	0.958918916	1.013905987	–0.45961044
5	O	–2.35358593	–0.188590237	0.164696818
6	C	0.286651206	–0.948407401	0.997752422
7	H	–1.138961083	0.923990537	–2.471093014
8	H	1.819242611	0.520777035	–0.929742526
9	H	0.50095788	1.645288709	–1.225654194
10	C	1.43678022	1.895856981	0.699985593
11	C	1.417030735	–1.905134666	0.611697429
12	H	0.540594754	–0.40816821	1.919283707
13	H	–0.635255963	–1.495320151	1.207172791
14	H	2.111900268	2.668149745	0.314648085
15	H	0.591085175	2.389413313	1.189972844
16	H	1.987224473	1.324770515	1.454007703
17	H	1.575118221	–2.634289103	1.414068848
18	H	1.165936953	–2.450702698	–0.304007133
19	H	2.366396182	–1.382064388	0.450579544

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 4.4209 y = –1.7957 z = 0.9819 Tot = 4.8716

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.225131 Hartree

Zero-point correction = 0.161240 Hartree

Sum of electronic and zero-point energies = –365.063891 Hartree

Zero-point vibrational energy = 423.3357 kJ/mol = 101.17966 kcal/mol

Enthalpy = -2.29074671×10^5 kcal/mol = -9.584484236×10^5 kJ/mol

Entropy = 94.450 cal/mol K = 395.1788 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291028313×10^5 kcal/mol = -9.58566246×10^5 kJ/mol

IR SPECTRUM

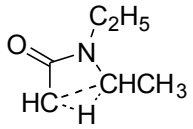
mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	–242.8267	4.2451	2	–234
2	47.9382	0.5487	0	46

3	52.6017	0.8946	0	50
4	146.7097	1.7877	0	141
5	172.0333	4.2455	2	165
6	225.2705	1.6552	0	216
7	242.2656	2.2992	1	232
8	291.7521	0.9654	0	280
9	327.7504	2.0388	1	315
10	389.9305	3.4253	1	374
11	445.1089	6.0873	3	427
12	567.1384	5.8777	2	545
13	652.1595	28.2506	14	626
14	656.9961	37.9931	19	631
15	735.8857	25.534	12	707
16	794.8276	3.4266	1	764
17	815.7667	17.0914	8	784
18	914.4656	108.4931	54	879
19	946.7188	25.5065	12	910
20	970.3102	15.1129	7	932
21	1046.299	45.8081	22	1005
22	1081.388	8.9737	4	1039
23	1100.693	11.2587	5	1058
24	1139.291	1.4533	0	1095
25	1172.778	58.9488	29	1127
26	1242.072	18.3047	9	1194
27	1273.36	51.805	25	1224
28	1331.309	18.6219	9	1279
29	1382.41	2.7042	1	1328
30	1400.082	6.7833	3	1345
31	1424.713	41.8285	20	1369
32	1438.362	20.2887	10	1382
33	1440.522	20.2994	10	1384
34	1513.21	4.2853	2	1454
35	1516.545	7.1497	3	1457
36	1525.989	3.1959	1	1466
37	1530.048	1.9524	0	1470
38	1533.403	13.2955	6	1474
39	1545.67	2.0255	1	1485

40	1713.561	199.5429	100	1647
41	3041.632	18.4153	9	2923
42	3048.261	32.1838	16	2930
43	3050.763	6.101	3	2932
44	3056.5	38.4217	19	2938
45	3060.635	25.9886	13	2942
46	3112.627	5.8494	2	2992
47	3115.922	15.2701	7	2995
48	3128.728	28.4352	14	3007
49	3130.337	22.7119	11	3009
50	3140.464	33.3704	16	3018
51	3142.988	14.3928	7	3021

* scaling factor = 0.9613, # rounded

TRANSITION STATE ^{1}5b→^{1}3b, 1st of 2 calculated conformers



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–1.285840645	–0.118723743	–1.709480248
2	C	–1.24372223	–0.051348083	–0.2481048
3	N	0.05778317	0.067742511	0.180588151
4	C	0.506087181	–0.187154264	1.540530136
5	O	–2.260402752	–0.174158306	0.430670794
6	C	0.903517935	0.255211804	–0.971894269
7	H	–1.594666882	0.839510133	–2.15804344
8	H	0.216016488	–0.125837567	–1.862069463
9	H	1.720881913	–0.478279222	–1.012208682
10	C	1.394266212	1.67286985	–1.229673188
11	H	–0.381611662	–0.051561061	2.1669145
12	H	1.232845907	0.582050672	1.831471731
13	C	1.090803811	–1.588800962	1.747168657
14	H	1.895423452	1.742749258	–2.201388304
15	H	0.565098042	2.385949007	–1.205202953

16	H	2.117783537	1.966402014	–0.459060695
17	H	1.396960664	–1.719609654	2.791276166
18	H	0.34618163	–2.354561923	1.50801114
19	H	1.973153155	–1.760070404	1.119538866

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –0.1856 y = –5.3825 z = –0.4148 Tot = 5.4016

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.2376125 Hartree

Zero-point correction = 0.159995 Hartree

Sum of electronic and zero-point energies = –365.0776175 Hartree

Zero-point vibrational energy = 420.0665 kJ/mol = 100.39829 kcal/mol

Enthalpy = -2.290834684×10^5 kcal/mol = -9.584852318×10^5 kJ/mol

Entropy = 92.315 cal/mol K = 386.24596 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291109921×10^5 kcal/mol = -9.58600391×10^5 kJ/mol

IR SPECTRUM

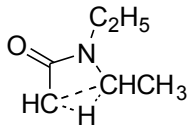
mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	–322.9472	37.7707	12	–311
2	54.6281	1.2696	0	52
3	99.3673	1.3163	0	95
4	129.2868	2.37	0	124
5	190.8559	1.1177	0	183
6	227.67	0.9586	0	218
7	239.7431	5.474	1	230
8	297.5279	9.3094	3	286
9	332.8109	0.2826	0	319
10	463.0607	5.2213	1	445
11	495.0062	7.4373	2	475
12	595.1342	24.662	8	572
13	618.7679	19.0357	6	594
14	705.0727	2.1814	0	677
15	763.739	5.4466	1	734
16	794.1309	4.6385	1	763

17	880.3943	19.837	6	846
18	955.9389	4.4484	1	918
19	964.4949	3.0353	1	927
20	1009.47	65.1364	22	970
21	1045.533	4.8091	1	1005
22	1101.548	17.9543	6	1058
23	1104.668	2.028	0	1061
24	1133.949	8.2821	2	1090
25	1192.351	0.1662	0	1146
26	1221.695	1.925	0	1174
27	1271.722	15.6826	5	1222
28	1352.236	90.5921	30	1299
29	1392.419	32.3797	10	1338
30	1414.186	26.2321	8	1359
31	1434.322	6.6249	2	1378
32	1441.564	10.9618	3	1385
33	1463.429	82.7661	28	1406
34	1510.709	9.8059	3	1452
35	1514.592	16.6302	5	1455
36	1516.742	11.9187	4	1458
37	1524.817	14.2222	4	1465
38	1531.899	5.868	1	1472
39	1547.381	57.1042	19	1487
40	1751.88	295.5573	100	1684
41	2054.335	125.7986	42	1974
42	3047.713	31.1396	10	2929
43	3049.748	1.0716	0	2931
44	3052.954	25.2225	8	2934
45	3056.05	36.5914	12	2937
46	3059.457	14.7099	4	2941
47	3106.256	4.6207	1	2986
48	3115.669	18.3263	6	2995
49	3122.094	27.3232	9	3001
50	3137.615	22.1304	7	3016
51	3142.988	17.6313	5	3021

[*] scaling factor = 0.9613, [#] rounded

TRANSITION STATE ^{1}5b→^{1}3b, 2nd of 2 calculated conformers

GAUSSIAN 98; B3LYP/6-31g(d)



stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–1.435077988	0.034720343	–1.765818267
2	C	–1.343185976	–0.023905389	–0.307935347
3	N	–0.03124861	–0.129349368	0.08760131
4	C	0.39651417	–0.267206785	1.469772606
5	O	–2.355011025	–0.058893731	0.390614792
6	C	0.819927458	0.114509908	–1.05374988
7	H	–1.6514523	1.060994134	–2.10679913
8	H	0.090377777	–0.101974662	–1.952102933
9	C	1.989438504	–0.844194721	–1.227704598
10	H	1.125382407	1.164101272	–1.154533969
11	H	–0.505348902	–0.551118392	2.020641
12	C	0.999912175	1.010842396	2.061570194
13	H	1.106701583	–1.100182379	1.552022994
14	H	2.512976462	–0.643017032	–2.167589371
15	H	2.711864075	–0.720958914	–0.411864686
16	H	1.644193821	–1.882390911	–1.230484445
17	H	1.278325915	0.846885313	3.108666352
18	H	1.902943662	1.322679111	1.523175527
19	H	0.277693902	1.832983372	2.023932903

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 4.9367 y = 1.8658 z = 1.5080 Tot = 5.4888

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.238142 Hartree

Zero-point correction = 0.160206 Hartree

Sum of electronic and zero-point energies = –365.077936 Hartree

Zero-point vibrational energy = 420.6200 kJ/mol = 100.53059 kcal/mol

Enthalpy = -2.290836331×10^5 kcal/mol = -9.58485921×10^5 kJ/mol

Entropy = 92.819 cal/mol K = 388.342144 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291113071×10^5 kcal/mol = -9.586017088×10^5 kJ/mol

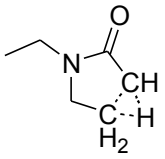
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	–309.516	35.9376	12	–298
2	49.6392	0.213	0	47
3	97.0976	2.9086	1	93
4	118.465	2.3183	0	113
5	191.5566	1.6794	0	184
6	211.2376	0.0949	0	203
7	255.8072	3.4367	1	245
8	299.313	5.5264	1	287
9	327.6071	5.6287	1	314
10	433.443	6.7387	2	416
11	497.2684	8.0481	2	478
12	595.6853	28.5902	10	572
13	615.1357	14.2398	5	591
14	724.2518	1.4547	0	696
15	759.9616	6.428	2	730
16	793.0287	3.0907	1	762
17	846.4272	11.5738	4	813
18	958.48	17.8774	6	921
19	980.3902	3.5908	1	942
20	1010.296	55.1548	19	971
21	1056.391	1.9745	0	1015
22	1099.573	6.8317	2	1057
23	1110.438	1.787	0	1067
24	1138.587	6.0319	2	1094
25	1199.113	0.8961	0	1152
26	1267.382	8.0306	2	1218
27	1348.324	34.9537	12	1296
28	1367.119	50.5061	17	1314
29	1403.022	22.8197	8	1348
30	1405.264	14.3952	5	1350
31	1425.818	2.9589	1	1370

32	1435.113	15.0775	5	1379
33	1440.211	7.1449	2	1384
34	1479.865	235.5893	82	1422
35	1508.266	14.4864	5	1449
36	1518.042	7.8522	2	1459
37	1522.709	0.6321	0	1463
38	1523.149	6.4023	2	1464
39	1533.305	3.8665	1	1473
40	1743.44	284.1907	100	1675
41	2133.291	159.5634	56	2050
42	3047.399	30.3709	10	2929
43	3049.69	6.5616	2	2931
44	3053.219	14.6362	5	2935
45	3055.574	47.2975	16	2937
46	3058.366	20.2456	7	2940
47	3107.417	10.2765	3	2987
48	3122.747	24.3063	8	3001
49	3124.472	15.9533	5	3003
50	3133.829	23.9246	8	3012
51	3145.939	15.5095	5	3024

* scaling factor = 0.9613, # rounded

TRANSITION STATE ^{1}5b→^{1}6b, 1st of 2 calculated conformers



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z

1	C	0.84075601	0.371750205	–2.02076963
2	C	0.958674046	0.205976124	–0.586671153
3	O	2.147432551	0.249349604	–0.225504094
4	N	–0.120610422	0.119579903	0.250794183
5	C	–1.453773628	0.267911834	–0.320887049
6	C	–1.467477717	–0.246215166	–1.755455447
7	C	0.070142808	0.289626399	1.69016997
8	C	–0.35607553	–0.935404979	2.502008863
9	H	1.135071794	–0.555564903	–2.533554489
10	H	–2.172660989	–0.292579709	0.288028474
11	H	–1.766738085	1.324552642	–0.300102859
12	H	1.134643118	0.490287422	1.834647154
13	H	–0.484587974	1.180430216	2.019921793
14	H	–2.390660556	0.01664598	–2.281921158
15	H	–0.669704617	0.340703135	–2.347867354
16	H	–1.290693951	–1.320531453	–1.825638311
17	H	–0.196320516	–0.752778261	3.570637437
18	H	–1.417598013	–1.172158869	2.362518815
19	H	0.230586396	–1.812728864	2.211430637

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –1.1013 y = –5.1225 z = 0.6905 Tot = 5.2849

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.2426025 Hartree

Zero-point correction = 0.161689 Hartree

Sum of electronic and zero-point energies = –365.0809135 Hartree

Zero-point vibrational energy = 424.5153 kJ/mol = 101.46160 kcal/mol

Enthalpy = -2.290857958×10^5 kcal/mol = -9.584949698×10^5 kJ/mol

Entropy = 89.961 cal/mol K = 376.396824 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291126177×10^5 kcal/mol = -9.586071923×10^5 kJ/mol

IR SPECTRUM

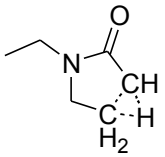
mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	–296.1366	78.6773	32	–285

2	64.4016	1.1379	0	61
3	110.0977	3.1142	1	105
4	176.3369	0.0219	0	169
5	187.6734	2.8845	1	180
6	217.114	2.8172	1	208
7	326.1737	15.3731	6	313
8	335.7185	16.4353	6	322
9	420.838	5.0024	2	404
10	456.0225	0.7768	0	438
11	527.373	0.7865	0	506
12	599.1975	12.1763	4	576
13	621.69	26.6145	10	597
14	711.3818	7.2208	2	683
15	802.0636	6.9739	2	771
16	837.1366	0.6256	0	804
17	884.8007	26.6082	10	850
18	957.9243	12.3941	5	920
19	969.803	22.8964	9	932
20	1033.606	31.302	12	993
21	1068.242	30.21	12	1026
22	1104.686	6.8491	2	1061
23	1115.114	2.6121	1	1071
24	1171.088	17.1346	6	1125
25	1207.611	5.7749	2	1160
26	1268.865	13.6658	5	1219
27	1302.015	12.3935	5	1251
28	1343.959	115.5908	47	1291
29	1366.499	18.5929	7	1313
30	1408.214	22.0594	9	1353
31	1414.781	11.8021	4	1360
32	1442.088	10.433	4	1386
33	1473.188	1.8593	0	1416
34	1500.842	85.7901	35	1442
35	1517.147	22.7853	9	1458
36	1523.345	8.5162	3	1464
37	1532.064	4.5272	1	1472
38	1551.926	19.7228	8	1491

39	1576.833	10.4306	4	1515
40	1662.616	244.9753	100	1598
41	2298.054	117.8821	48	2209
42	3000.638	48.7116	19	2884
43	3023.638	51.0708	20	2906
44	3051.877	16.8136	6	2933
45	3075.833	27.114	11	2956
46	3082.468	14.3607	5	2963
47	3099.984	13.7898	5	2980
48	3110.304	22.2115	9	2989
49	3130.101	23.594	9	3008
50	3138.568	15.562	6	3017
51	3171.465	9.2865	3	3048

* scaling factor = 0.9613, # rounded

TRANSITION STATE ^{1}5b→^{1}6b, 2nd of 2 calculated conformers



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_{11}NO$, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–1.202023268	0.419865227	–1.801750479
2	C	–1.049282772	0.373645074	–0.35863714
3	N	0.148063167	0.038675224	0.228561671
4	C	0.247029776	0.036379954	1.686972267
5	C	0.740911544	–1.297773542	2.249214091
6	O	–2.110881636	0.591168912	0.244944675
7	C	1.348375713	0.261512818	–0.570431794
8	C	1.140878121	–0.222657564	–2.003569525
9	H	–1.129094265	1.461630496	–2.157007431
10	H	1.619730996	1.329955464	–0.559921739
11	H	2.18321224	–0.283025164	–0.115792321
12	H	0.909133601	0.855636959	2.005160301
13	H	–0.755794753	0.262408396	2.058846207
14	H	1.747034608	0.31819965	–2.733010379

15	H	1.293700395	–1.301834817	–2.100308239
16	H	0.032069513	–0.158383396	–2.362537392
17	H	0.797298084	–1.249050962	3.342628782
18	H	0.057818468	–2.107765513	1.974593453
19	H	1.740167344	–1.553680781	1.877075141

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –0.9118 y = –5.1408 z = 1.6024 Tot = 5.4614

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –365.2382649 Hartree

Zero-point correction = 0.160856 Hartree

Sum of electronic and zero-point energies = –365.0774089 Hartree

Zero-point vibrational energy = 422.3265 kJ/mol = 100.93846 kcal/mol

Enthalpy = -2.290835377×10^5 kcal/mol = -9.584855217×10^5 kJ/mol

Entropy = 90.354 cal/mol K = 378.041136 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.291104767×10^5 kcal/mol = -9.585982347×10^5 kJ/mol

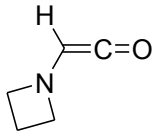
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	–303.1132	70.3525	33	–292
2	67.5832	1.9888	0	64
3	107.8105	1.0512	0	103
4	150.9228	1.8891	0	145
5	199.9196	0.717	0	192
6	218.5852	2.0362	0	210
7	325.9472	14.4051	6	313
8	345.0657	8.9109	4	331
9	383.1097	5.4105	2	368
10	440.849	14.8195	7	423
11	483.1876	3.2023	1	464
12	589.5387	32.948	15	566
13	617.9692	22.514	10	594
14	727.0438	7.0028	3	698
15	801.2986	3.6201	1	770

16	818.9117	11.8153	5	787
17	894.5976	12.7328	6	859
18	962.3659	4.0936	1	925
19	983.4292	13.7691	6	945
20	1042.408	43.5098	20	1002
21	1076.249	21.7371	10	1034
22	1104.402	6.0714	2	1061
23	1113.449	1.9197	0	1070
24	1146.407	3.8965	1	1102
25	1204.766	18.3893	8	1158
26	1260.565	31.0695	14	1211
27	1284.286	23.492	11	1234
28	1349.538	128.9632	61	1297
29	1366.385	31.3306	14	1313
30	1377.194	0.8967	0	1323
31	1411.938	12.6092	6	1357
32	1441.341	11.3365	5	1385
33	1471.038	25.7945	12	1414
34	1492.146	66.1186	31	1434
35	1517.47	10.163	4	1458
36	1522.481	7.6121	3	1463
37	1532.63	5.6242	2	1473
38	1546.809	7.1632	3	1486
39	1601.628	11.285	5	1539
40	1671.189	210.1293	100	1606
41	2110.648	144.7124	68	2028
42	2994.293	52.0309	24	2878
43	3018.948	51.2241	24	2902
44	3049.887	30.7647	14	2931
45	3051.335	10.7409	5	2933
46	3084.379	19.9392	9	2965
47	3099.235	14.6888	6	2979
48	3108.789	21.9698	10	2988
49	3128.647	20.0084	9	3007
50	3137.142	19.1354	9	3015
51	3171.714	11.3192	5	3048

[*] scaling factor = 0.9613, [#] rounded

AZETIDINYLKETENE (2c)



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_5H_7NO, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	z
1	C	–1.001582679	–0.000010489	1.802050023
2	O	–1.004822819	–1.74656E–05	2.97322491
3	C	–0.9932596	–0.000002626	0.476015212
4	N	0.257559902	1.1389E–06	–0.190017046
5	C	0.574701125	–1.058838731	–1.179999071
6	C	1.340478005	1.16557E–05	–2.010163316
7	C	0.574701355	1.058852494	–1.179986747
8	H	–1.952031574	6.122E–07	–0.051085903
9	H	–0.318317831	1.437760387	–1.703364488
10	H	1.134872434	1.908882118	–0.773994252
11	H	–0.318318144	–1.437740386	–1.703381182
12	H	1.134872102	–1.908873145	–0.774016486
13	H	2.414369928	0.000010351	–1.80859362
14	H	1.169987087	1.79917E–05	–3.088740634

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 2.2479 y = 0.0000 z = 1.2373 Tot = 2.5659

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –324.7506966 Hartree

Zero-point correction = 0.113645 Hartree

Sum of electronic and zero-point energies = –324.6370516 Hartree

Zero-point vibrational energy = 298.3758 kJ/mol = 71.31353 kcal/mol

Enthalpy = -2.037079795×10^5 kcal/mol = -8.523141863×10^5 kJ/mol

Entropy = 82.137 cal/mol K = 343.661208 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.037324686×10^5 kcal/mol = -8.524166488×10^5 kJ/mol

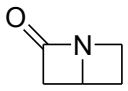
IR SPECTRUM

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	76.7229	0.0037	0	73
2	105.3818	0.3052	0	101
3	188.2805	0.7972	0	180
4	323.548	3.8763	0	311
5	327.0313	8.0171	1	314
6	535.8152	14.0726	2	515
7	551.7588	9.6999	1	530
8	630.149	34.4104	5	605
9	718.7881	0.0139	0	690
10	805.4125	10.0218	1	774
11	859.2924	0.0567	0	826
12	929.5343	11.5626	1	893
13	942.1527	1.884	0	905
14	1001.745	3.5331	0	962
15	1073.479	16.2367	2	1031
16	1126.008	1.9399	0	1082
17	1134.552	0.1566	0	1090
18	1156.524	8.3384	1	1111
19	1216.081	2.1192	0	1169
20	1229.057	4.7522	0	1181
21	1237.38	7.4526	1	1189
22	1279.895	4.4269	0	1230
23	1300.356	0.0024	0	1250
24	1352.623	14.035	2	1300
25	1431.619	15.7664	2	1376
26	1517.331	1.0818	0	1458
27	1534.696	2.5672	0	1475
28	1562.025	6.9037	1	1501
29	2219.529	660.7483	100	2133
30	2993.288	76.4259	11	2877
31	3000.958	61.7766	9	2884
32	3083.7	33.1154	5	2964
33	3085.521	53.8429	8	2966
34	3096.553	45.891	6	2976

35	3102.83	30.1745	4	2982
36	3154.92	29.0658	4	3032

* scaling factor = 0.9613, # rounded

1-AZA-BICYCLO[2.2.0]-HEXAN-2-ONE (3c)



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_5H_7NO, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	z
1	C	–0.66179216	0.96478657	–1.327658634
2	C	–0.662275538	0.964572869	0.228833569
3	C	0.680720227	0.964434953	0.99367993
4	C	0.671629071	–0.557634197	0.712430254
5	N	–0.666269751	–0.544457787	0.226792254
6	C	–0.821079319	–0.584761243	–1.267557676
7	O	1.484379308	–1.444388041	0.744804063
8	H	–0.055834917	–1.19077838	–1.761079994
9	H	–1.810871831	–0.95043583	–1.554038666
10	H	0.610758811	1.24320419	2.050074702
11	H	1.523023622	1.492904771	0.53762562
12	H	–1.512324182	1.452682239	0.712608388
13	H	–1.487827116	1.507676569	–1.794461625
14	H	0.278715726	1.302661565	–1.775071365

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 3.4460 y = 2.1178 z = 0.5443 Tot = 4.0812

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –324.7704564 Hartree

Zero-point correction = 0.115760 Hartree

Sum of electronic and zero-point energies = –324.6546964 Hartree

Zero-point vibrational energy = 303.9287 kJ/mol = 72.64071 kcal/mol

Enthalpy = -2.037197107×10^5 kcal/mol = -8.523632696×10^5 kJ/mol

Entropy = 76.294 cal/mol K = 319.214096 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.037424578×10^5 kcal/mol = -8.524584432×10^5 kJ/mol

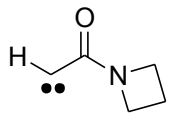
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	118.6447	2.7233	0	114
2	211.6745	5.6211	1	203
3	337.2433	1.9195	0	324
4	460.0735	2.0914	0	442
5	529.7006	7.2067	1	509
6	664.4126	1.8556	0	638
7	724.8255	2.2371	0	696
8	763.7138	4.9332	1	734
9	838.5562	2.5631	0	806
10	862.0252	13.2322	3	828
11	896.0475	5.8674	1	861
12	937.5436	6.3504	1	901
13	993.7074	14.8258	3	955
14	1000.157	2.431	0	961
15	1051.674	1.2908	0	1010
16	1080.278	20.1784	5	1038
17	1124.594	63.6845	15	1081
18	1155.685	54.4511	13	1110
19	1211.195	31.2264	7	1164
20	1218.744	5.5862	1	1171
21	1238.771	7.9337	1	1190
22	1251.175	41.6063	10	1202
23	1275.143	5.2296	1	1225
24	1319.796	7.0459	1	1268
25	1361.358	16.2098	4	1308
26	1471.914	7.6422	1	1414
27	1511.297	2.4829	0	1452

28	1538.022	2.2166	0	1478
29	1887.424	401.2004	100	1814
30	3079.201	27.077	6	2960
31	3085.408	53.6322	13	2966
32	3086.147	5.3593	1	2966
33	3110.373	27.1587	6	2990
34	3129.274	3.878	0	3008
35	3141.142	6.1139	1	3019
36	3145.966	45.1109	11	3024

* scaling factor = 0.9613, # rounded

AZETIDINYLCARBONYLCARBENE (5c)



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_5H_7NO, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	Z
1	C	0.774062664	0.106189818	–2.245518481
2	C	0.750877513	–0.154469169	–0.865246639
3	O	2.012645865	–0.070952733	–0.757974105
4	N	–0.142348773	–0.275626992	0.114878785
5	C	–1.586263382	0.022285176	0.090708585
6	C	0.023323119	0.050455387	1.546039523
7	H	0.97279875	–0.811837337	–2.816777792
8	H	–1.836784305	0.870811912	–0.555438731
9	C	–1.505378636	0.334175449	1.613086683
10	H	–2.205542152	–0.837567696	–0.185641385
11	H	0.678044262	0.911949412	1.712187887
12	H	0.379663384	–0.793367274	2.144653638
13	H	–1.765212268	1.36017715	1.879872603
14	H	–2.067420846	–0.354975327	2.24636709

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –4.9310 y = 0.8594 z = –1.3559 Tot = 5.1857

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –324.6749815 Hartree

Zero-point correction = 0.112365 Hartree

Sum of electronic and zero-point energies = –324.5626165 Hartree

Zero-point vibrational energy = 295.0146 kJ/mol = 70.51017 kcal/mol

Enthalpy = -2.036610988×10^5 kcal/mol = -8.521180375×10^5 kJ/mol

Entropy = 83.196 cal/mol K = 348.092064 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.036859037×10^5 kcal/mol = -8.52221821×10^5 kJ/mol

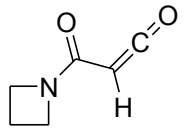
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	66.405	4.2606	0	63
2	149.7045	8.1379	1	143
3	155.8865	8.5581	1	149
4	169.3392	5.9153	1	162
5	306.9479	34.6905	6	295
6	495.0903	30.1301	5	475
7	553.8926	7.8277	1	532
8	602.1709	7.415	1	578
9	776.3612	2.1913	0	746
10	853.4209	3.2609	0	820
11	871.6917	13.1245	2	837
12	885.3974	7.594	1	851
13	934.5204	127.5106	24	898
14	948.0136	7.9614	1	911
15	975.825	7.8864	1	938
16	1135.084	18.6966	3	1091
17	1145.927	4.262	0	1101
18	1155.783	9.1773	1	1111
19	1207.397	2.2545	0	1160
20	1233.737	6.8627	1	1185
21	1243.786	0.5613	0	1195
22	1283.906	6.0036	1	1234

23	1305.915	0.0056	0	1255
24	1355.27	29.093	5	1302
25	1463.96	60.3488	11	1407
26	1519.168	6.6926	1	1460
27	1536.255	0.0297	0	1476
28	1558.725	23.1441	4	1498
29	1703.634	515.9755	100	1637
30	3065.049	46.8485	9	2946
31	3076.442	27.9448	5	2957
32	3077.208	21.2741	4	2958
33	3110.625	20.7471	4	2990
34	3111.992	28.0753	5	2991
35	3122.887	12.702	2	3002
36	3165.158	24.4505	4	3042

* scaling factor = 0.9613, # rounded

AZETIDINYLCARBONYLKETENE (13c), *s-cis* conformer



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_7NO_2$, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	Z
1	H	–1.747389757	0.729859166	–1.872458819
2	C	–1.575331647	1.039170497	–0.834324975
3	N	–0.180295293	0.898331626	–0.38542949
4	C	0.513763508	–0.145431647	0.159797843
5	C	–0.032928896	–1.485567012	–0.15804662
6	C	0.574625721	–2.553420883	0.342758419
7	O	1.097499442	–3.495748707	0.781117648
8	C	–0.030546895	2.310165002	–0.012209663
9	H	0.071586295	2.455597071	1.069263324
10	O	1.522511002	0.028659308	0.840347954
11	H	–0.893118134	–1.647711594	–0.797764096
12	H	–2.300893601	0.530954526	–0.185756543
13	H	0.801378431	2.814354543	–0.514765877

14	C	–1.449695838	2.570568851	–0.593476595
15	H	–2.17235969	2.987721698	0.11046236
16	H	–1.456535761	3.164709543	–1.509689203

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –3.4148 y = –3.7860 z = 0.0631 Tot = 5.0989

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –438.1605697 Hartree

Zero-point correction = 0.124236 Hartree

Sum of electronic and zero-point energies = –438.0363337 Hartree

Zero-point vibrational energy = 326.1816 kJ/mol = 77.95927 kcal/mol

Enthalpy = -2.748658513×10^5 kcal/mol = -1.150038722×10^6 kJ/mol

Entropy = 93.660 cal/mol K = 391.87344 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.74893776×10^5 kcal/mol = -1.150155559×10^6 kJ/mol

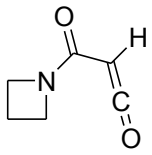
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	50.7003	0.6837	0	48
2	101.4593	0.3013	0	97
3	112.4309	1.0306	0	108
4	119.4075	2.6562	0	114
5	170.2551	8.9672	1	163
6	202.2998	5.8724	0	194
7	360.2774	7.4503	0	346
8	491.8905	0.2674	0	472
9	525.36	17.6534	1	505
10	553.2285	5.7992	0	531
11	555.2356	20.0968	2	533
12	741.6874	42.4384	4	712
13	776.2811	2.6828	0	746
14	828.7888	8.4991	0	796
15	860.3325	0.0732	0	827
16	903.5963	3.7631	0	868
17	945.0576	3.9983	0	908

18	969.0457	5.1949	0	931
19	1039.294	43.7203	4	999
20	1136.215	2.1174	0	1092
21	1145.935	1.5843	0	1101
22	1151.356	3.3748	0	1106
23	1193.169	32.5277	3	1146
24	1212.263	0.558	0	1165
25	1244.603	1.939	0	1196
26	1284.274	9.6932	1	1234
27	1307.022	1.8617	0	1256
28	1343.333	8.0242	0	1291
29	1368.846	127.9839	14	1315
30	1458.63	589.9675	66	1402
31	1520.51	3.5959	0	1461
32	1538.419	1.3038	0	1478
33	1562.256	8.9579	1	1501
34	1735.14	254.7949	28	1667
35	2240.128	891.3067	100	2153
36	3037.308	59.0603	6	2919
37	3065.774	33.9588	3	2947
38	3079.652	32.5219	3	2960
39	3106.112	23.2568	2	2985
40	3109.077	34.1248	3	2988
41	3160.122	26.8935	3	3037
42	3226.521	6.0894	0	3101

* scaling factor = 0.9613, # rounded

AZETIDINYLCARBONYLKETENE (13c), *s-trans* conformer



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry $C_6H_7NO_2$, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	Z
1	H	–1.584625253	0.24453968	–1.281405982
2	C	–1.122278246	0.842527795	–0.488581435

3	N	0.318697911	0.577444711	–0.285043257
4	C	0.713871238	1.980553566	–0.487989797
5	H	1.461763281	2.118437543	–1.275519791
6	C	0.965746553	–0.272949742	0.574816832
7	C	0.283713864	–1.557047042	0.901378235
8	C	–0.714844308	–2.082553758	0.212395642
9	O	–1.597731889	–2.536794469	–0.404342019
10	O	2.066043979	–0.006194885	1.042276749
11	H	–1.715973263	0.737913662	0.428448295
12	C	–0.757934254	2.304583029	–0.866578522
13	H	1.079236352	2.450603273	0.431583369
14	H	0.718711148	–2.150737329	1.697091071
15	H	–1.238245108	3.073228831	–0.258058862
16	H	–0.907898341	2.537133099	–1.92295887

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –0.8131 y = –2.9040 z = 0.7839 Tot = 3.1159

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –438.1587846 Hartree

Zero-point correction = 0.124401 Hartree

Sum of electronic and zero-point energies = –438.0343836 Hartree

Zero-point vibrational energy = 326.6159 kJ/mol = 78.06308 kcal/mol

Enthalpy = -2.748647155×10^5 kcal/mol = -1.150033969×10^6 kJ/mol

Entropy = 92.702 cal/mol K = 387.865168 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.748923545×10^5 kcal/mol = -1.150149611×10^6 kJ/mol

IR SPECTRUM

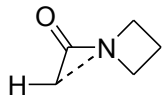
mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	57.5786	1.9006	0	55
2	97.3374	0.0704	0	93
3	111.7275	1.4317	0	107
4	146.3275	5.5195	0	140
5	186.558	8.4404	1	179
6	218.9458	9.2212	1	210

7	387.9441	4.6196	0	372
8	501.0402	5.2305	0	481
9	530.466	13.948	2	509
10	543.7767	23.9615	3	522
11	614.2268	1.6162	0	590
12	707.5199	12.2722	1	680
13	757.0105	41.1581	6	727
14	777.4551	1.2159	0	747
15	859.2487	0.2066	0	825
16	881.7099	5.1919	0	847
17	951.0909	3.2793	0	914
18	975.5901	2.9024	0	937
19	1084.607	39.6394	5	1042
20	1138.01	3.4446	0	1093
21	1146.002	3.4242	0	1101
22	1151.74	3.6259	0	1107
23	1179.585	21.8788	3	1133
24	1215.311	2.4372	0	1168
25	1244.488	2.1524	0	1196
26	1283.467	6.0716	0	1233
27	1306.564	0.9171	0	1255
28	1351.144	7.5917	1	1298
29	1379.339	28.8829	4	1325
30	1401.604	478.7665	71	1347
31	1519.595	1.8811	0	1460
32	1538.091	0.614	0	1478
33	1561.21	7.5251	1	1500
34	1754.934	399.1689	59	1687
35	2215.882	672.0465	100	2130
36	3047.345	42.9865	6	2929
37	3069.855	31.5003	4	2951
38	3095.878	22.1905	3	2976
39	3107.176	29.3364	4	2986
40	3112.571	21.2338	3	2992
41	3160.239	26.5602	3	3037
42	3235.718	17.5068	2	3110

[*] scaling factor = 0.9613, [#] rounded

TRANSITION STATE ^{1}5c→^{1}2c

GAUSSIAN 98; B3LYP/6-31g(d)



stoichiometry C_5H_7NO, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	Z
1	C	–1.466863536	0.283898698	–1.772418798
2	C	–1.213621132	0.045321184	–0.375233558
3	N	0.152533216	–0.204096001	–0.219909878
4	C	1.265356533	0.777770681	–0.301110786
5	O	–2.066788014	–0.150016177	0.484691181
6	C	0.731410142	–0.901402654	0.954430435
7	H	–1.118256523	1.284810739	–2.093364022
8	H	1.790156683	0.774625752	–1.261658369
9	H	0.951997173	1.802333412	–0.065578274
10	C	1.975403738	0.023132331	0.853304705
11	H	0.907744985	–1.967911965	0.78196498
12	H	0.118670953	–0.773646307	1.850885749
13	H	2.892184322	–0.488569983	0.553188053
14	H	2.173959545	0.624838329	1.74256959

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 4.5388 y = 2.1161 z = 0.8226 Tot = 5.0749

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –324.656607 Hartree

Zero-point correction = 0.110702 Hartree

Sum of electronic and zero-point energies = –324.545905 Hartree

Zero-point vibrational energy = 290.6468 kJ/mol = 69.46625 kcal/mol

Enthalpy = -2.036509266×10^5 kcal/mol = -8.520754769×10^5 kJ/mol

Entropy = 81.150 cal/mol K = 339.5316 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.036751215×10^5 kcal/mol = -8.521767082×10^5 kJ/mol

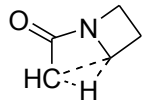
IR SPECTRUM

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	–236.4636	2.6701	1	–227
2	77.2709	0.2696	0	74
3	115.72	9.327	4	111
4	199.8694	4.1391	2	192
5	215.2097	5.8584	2	206
6	526.719	6.9111	3	506
7	576.2636	36.6055	18	553
8	648.1334	17.5174	8	623
9	685.1268	53.8568	26	658
10	777.6295	0.5143	0	747
11	850.1182	0.4066	0	817
12	873.4648	1.8459	0	839
13	952.4003	53.7861	26	915
14	959.3456	84.8961	42	922
15	978.5306	5.2937	2	940
16	1053.18	14.4346	7	1012
17	1119.183	11.0584	5	1075
18	1144.275	1.582	0	1099
19	1168.255	7.4958	3	1123
20	1212.56	0.4437	0	1165
21	1244.435	1.3516	0	1196
22	1277.642	35.1564	17	1228
23	1294.997	44.7355	22	1244
24	1324.286	176.662	87	1273
25	1348.392	1.0029	0	1296
26	1519.05	0.4405	0	1460
27	1532.322	0.3357	0	1473
28	1555.587	10.1649	5	1495
29	1719.71	202.0055	100	1653
30	3008.207	30.8982	15	2891
31	3053.161	47.4532	23	2935
32	3079.377	34.0038	16	2960
33	3103.198	20.2194	10	2983
34	3107.201	37.619	18	2986
35	3130.608	5.6122	2	3009

36	3160.915	27.0097	13	3038

[*] scaling factor = 0.9613, [#] rounded

TRANSITION STATE ^{1}5c→^{1}3c



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_5H_7NO, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	Z
1	C	–1.039371293	–0.315484673	–1.502161239
2	C	–1.172799329	–0.074765937	–0.070403087
3	N	–0.004886409	0.533464874	0.413489241
4	C	1.001722417	–0.18075018	1.252495157
5	O	–2.142074459	–0.472868392	0.559677113
6	C	0.894978519	0.633688127	–0.723229841
7	H	–1.530646746	0.403620293	–2.171552123
8	H	0.422729819	–0.030087471	–1.599565161
9	H	1.096700628	1.630156617	–1.123561515
10	H	0.668706498	–1.173161047	1.57020025
11	H	1.312377076	0.397495646	2.127139512
12	C	1.991324003	–0.141075236	0.043406779
13	H	2.919563461	0.415759479	0.194936112
14	H	2.226243903	–1.124763105	–0.370085286

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –4.8506 y = 1.8375 z = –0.7647 Tot = 5.2431

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –324.6543699 Hartree

Zero-point correction = 0.109553 Hartree

Sum of electronic and zero-point energies = –324.5448169 Hartree

Zero-point vibrational energy = 287.6315 kJ/mol = 68.74558 kcal/mol

Enthalpy = -2.03650604×10^5 kcal/mol = -8.520741271×10^5 kJ/mol

Entropy = 77.529 cal/mol K = 324.381336 J/mol K

Gibbs Free Energy (T = 298.15 K) = –2.036737193 × 10^5 kcal/mol = –8.521708414 × 10^5 kJ/mol

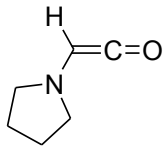
IR SPECTRUM

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	–416.3232	67.6495	24	–401
2	117.6967	1.71	0	113
3	201.6372	14.1933	5	193
4	236.2502	1.2796	0	227
5	437.7711	1.7158	0	420
6	507.0885	1.0092	0	487
7	611.021	28.6371	10	587
8	681.8457	3.2386	1	655
9	724.8409	7.1065	2	696
10	766.1337	1.8477	0	736
11	866.9859	10.6155	3	833
12	882.266	1.5534	0	848
13	919.5356	59.214	21	883
14	947.6408	69.0713	24	910
15	992.8888	11.543	4	954
16	1065.496	5.9454	2	1024
17	1113.797	28.0525	9	1070
18	1139.931	6.7046	2	1095
19	1184.719	2.4147	0	1138
20	1215.89	4.9542	1	1168
21	1262.422	0.2971	0	1213
22	1269.861	3.2691	1	1220
23	1281.515	30.5405	10	1231
24	1329.433	29.8704	10	1277
25	1379.941	198.7165	70	1326
26	1395.978	2.6541	0	1341
27	1505.708	3.1797	1	1447
28	1547.566	1.949	0	1487
29	1768.405	281.0881	100	1699
30	2036.018	135.6184	48	1957
31	3084.036	43.6028	15	2964
32	3098.854	23.1784	8	2978

33	3102.505	9.6068	3	2982
34	3124.381	23.7818	8	3003
35	3132.995	8.0338	2	3011
36	3155.173	20.0837	7	3033

* scaling factor = 0.9613, # rounded

PYRROLIDINYLKETENE (2d)



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_6H_9NO, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	Z
1	C	–1.489387549	–0.398428277	–1.621045925
2	C	–1.486781346	–0.391572288	–0.068723333
3	N	–0.070225114	–0.389820808	0.34742436
4	C	0.581859273	–1.273105564	–0.639696456
5	C	–0.102548851	–0.989419708	–2.003832714
6	C	0.510746637	0.915901845	0.436367182
7	C	0.994953254	1.291227181	1.611178831
8	O	1.42325311	1.623493362	2.649919473
9	H	0.580988626	1.619964214	–0.396154797
10	H	0.400093232	–2.312580806	–0.335568509
11	H	1.66136091	–1.106841563	–0.640333178
12	H	–1.950398925	–1.310939473	0.313198449
13	H	–2.011416607	0.458279839	0.373404611
14	H	0.479217188	–0.267985938	–2.587661529
15	H	–0.185834908	–1.897439266	–2.609701936
16	H	–2.32143395	–0.987367558	–2.020248776
17	H	–1.60007314	0.618090176	–2.013746147

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –2.5059 y = 0.0000 z = 0.9302 Tot = 2.6730

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –364.0999233 Hartree

Zero-point correction = 0.143691 Hartree

Sum of electronic and zero-point energies = –363.9562323 Hartree

Zero-point vibrational energy = 377.2619 kJ/mol = 90.16776 kcal/mol

Enthalpy = -2.283804813×10^5 kcal/mol = -9.555439338×10^5 kJ/mol

Entropy = 88.942 cal/mol K = 372.133328 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.284069993×10^5 kcal/mol = -9.556548852×10^5 kJ/mol

IR SPECTRUM

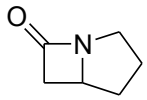
mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	62.4779	0.0286	0	60
2	67.1358	0.298	0	64
3	79.5347	0.2252	0	76
4	183.0038	0.6765	0	175
5	367.5686	8.7069	1	353
6	371.2162	4.9371	0	356
7	541.5388	7.6702	1	520
8	574.7144	17.667	2	552
9	619.8802	15.3988	2	595
10	661.8973	22.6599	3	636
11	678.2997	2.1346	0	652
12	817.1093	4.786	0	785
13	851.342	0.7212	0	818
14	876.0197	20.9255	3	842
15	892.8587	4.7129	0	858
16	926.6443	0.2705	0	890
17	952.3758	11.7617	1	915
18	1031.134	3.116	0	991
19	1076.585	6.9749	1	1034
20	1088.058	12.1573	1	1045
21	1153.527	1.5985	0	1108
22	1164.557	13.7418	2	1119
23	1220.266	4.464	0	1173
24	1241.994	2.7763	0	1193
25	1268.722	2.0955	0	1219
26	1296.975	0.3896	0	1246

27	1327.474	0.4906	0	1276
28	1356.813	9.7513	1	1304
29	1359.821	0.8223	0	1307
30	1380.156	29.6356	4	1326
31	1428.919	15.1566	2	1373
32	1515.347	0.8669	0	1456
33	1524.6	1.6548	0	1465
34	1526.445	2.2642	0	1467
35	1547.844	2.2269	0	1487
36	2221.119	632.2327	100	2135
37	3039.442	28.3489	4	2921
38	3044.173	66.0671	10	2926
39	3062.818	22.946	3	2944
40	3074.535	44.4378	7	2955
41	3097.872	8.7395	1	2977
42	3110.521	27.0245	4	2990
43	3117.381	42.8813	6	2996
44	3134.555	25.1565	3	3013
45	3137.989	39.4527	6	3016

* scaling factor = 0.9613, # rounded

1-AZA-BICYCLO[3.2.0]-HEPTAN-7-ONE (3d)

GAUSSIAN 98; B3LYP/6-31g(d)



stoichiometry C_6H_9NO, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	Z
1	C	–1.058422045	–0.407839451	–1.326426926
2	C	–1.058540603	–0.407710649	0.210119314
3	N	0.39143992	–0.407898469	0.53989829
4	C	1.23458143	–0.888596081	–0.56207621
5	C	0.201832111	–1.23835148	–1.671711089
6	C	0.35271102	0.902292837	1.023603948

7	O	1.236401364	1.686151351	1.273742216
8	C	–1.193560699	0.934201568	0.980754828
9	H	1.923702777	–0.089777945	–0.859450531
10	H	1.831437624	–1.758289829	–0.268652641
11	H	–1.681885323	0.875506586	1.957337872
12	H	–1.606649577	1.773569066	0.415077864
13	H	–1.604091221	–1.260374672	0.629875952
14	H	–0.034216973	–2.308352551	–1.632660893
15	H	0.585937765	–1.025788012	–2.674232733
16	H	–0.945310652	0.618845511	–1.698660452
17	H	–1.97182207	–0.823240142	–1.763443389

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 3.5761 y = 2.2086 z = –0.3459 Tot = 4.2173

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –364.141038 Hartree

Zero-point correction = 0.146277 Hartree

Sum of electronic and zero-point energies = –363.994761 Hartree

Zero-point vibrational energy = 384.0507 kJ/mol = 91.79032 kcal/mol

Enthalpy = -2.284054403×10^5 kcal/mol = -9.556483623×10^5 kJ/mol

Entropy = 80.825 cal/mol K = 338.1718 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.284295383×10^5 kcal/mol = -9.557491881×10^5 kJ/mol

IR SPECTRUM

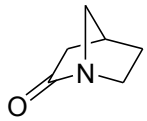
mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	106.5118	3.3549	0	102
2	180.8957	0.2958	0	173
3	213.3517	7.4768	1	205
4	346.6484	2.4636	0	333
5	455.6596	1.9055	0	438
6	560.2983	8.1013	1	538
7	574.4285	0.934	0	552
8	617.8186	6.8252	1	593
9	718.1262	3.2181	0	690

10	800.4219	0.8245	0	769
11	810.395	3.8806	0	779
12	875.2434	1.8376	0	841
13	882.5045	1.415	0	848
14	924.6512	4.5065	0	888
15	982.3722	2.6189	0	944
16	997.4987	0.5929	0	958
17	1028.415	14.1923	3	988
18	1042.796	10.6925	2	1002
19	1079.155	2.0525	0	1037
20	1099.656	22.0831	4	1057
21	1187.193	3.7457	0	1141
22	1197.932	8.8823	1	1151
23	1211.833	1.3097	0	1164
24	1240.642	16.7885	3	1192
25	1243.884	54.0971	11	1195
26	1259.323	0.529	0	1210
27	1322.275	2.3564	0	1271
28	1329.907	110.747	24	1278
29	1354.153	0.9244	0	1301
30	1369.557	7.4156	1	1316
31	1390.516	23.996	5	1336
32	1485.924	3.0185	0	1428
33	1516.876	3.749	0	1458
34	1526.398	2.5808	0	1467
35	1552.301	3.6528	0	1492
36	1879.837	459.0504	100	1807
37	3050.791	16.9655	3	2932
38	3063.024	12.5317	2	2944
39	3066.48	50.8262	11	2947
40	3073.059	36.223	7	2954
41	3097.852	14.1827	3	2977
42	3101.916	22.4859	4	2981
43	3114.904	26.1457	5	2994
44	3123.047	48.4668	10	3002
45	3151.785	10.3194	2	3029

[*] scaling factor = 0.9613, [#] rounded

1-AZA-BICYCLO[2.2.1]-HEPTAN-2-ONE (6d)

GAUSSIAN 98; B3LYP/6-31g(d)



stoichiometry C_6H_9NO, framework group C1

STANDARD ORIENTATION

center No.	atom type	coordinates [Å]		
		x	y	Z
1	C	–0.779239037	0.686248779	–1.085869216
2	N	–0.779571628	0.686660491	0.403800762
3	C	0.650021073	0.687040125	0.708965804
4	C	1.386301749	0.043211442	–0.48497568
5	C	0.191109983	–0.495672595	–1.295319027
6	C	–0.516192538	–1.589688835	–0.456163349
7	C	–1.190845709	–0.734780866	0.676103489
8	O	1.124714761	1.050123969	1.753622765
9	H	1.955280509	0.797450259	–1.044017502
10	H	2.09392292	–0.709697146	–0.123677419
11	H	0.416823394	–0.779411567	–2.326166571
12	H	0.18715553	–2.330613081	–0.062035012
13	H	–1.263699462	–2.124869338	–1.051108973
14	H	–2.282341294	–0.779094586	0.622160873
15	H	–0.889579334	–1.017327646	1.687080619
16	H	–0.412525095	1.642596355	–1.472587545
17	H	–1.792686984	0.515203258	–1.461688057

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –3.8618 y = 1.7864 z = –0.4028 Tot = 4.2740

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –364.1320873 Hartree

Zero-point correction = 0.146934 Hartree

Sum of electronic and zero-point energies = –363.9851533 Hartree

Zero-point vibrational energy = 385.7747 kJ/mol = 92.20237 kcal/mol

Enthalpy = -2.283997659×10^5 kcal/mol = -9.556246207×10^5 kJ/mol

Entropy = 77.835 cal/mol K = 325.66164 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.284229724×10^5 kcal/mol = -9.557217165×10^5 kJ/mol

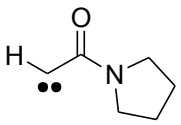
IR SPECTRUM

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	126.1081	2.5633	0	121
2	268.3623	0.9883	0	257
3	374.8244	0.2888	0	360
4	460.4856	0.2647	0	442
5	500.7336	0.999	0	481
6	565.5312	1.9182	0	543
7	609.1609	1.4319	0	585
8	708.7307	0.5872	0	681
9	774.4534	9.4777	3	744
10	796.5441	9.5634	3	765
11	832.8384	0.9902	0	800
12	870.3709	7.5073	2	836
13	898.81	19.7583	6	864
14	924.0697	20.6508	7	888
15	941.0754	2.7495	0	904
16	962.146	3.7435	1	924
17	970.1238	3.6864	1	932
18	1013.403	33.1443	11	974
19	1047.387	36.7793	12	1006
20	1093.668	53.178	18	1051
21	1115.112	14.3004	4	1071
22	1148.736	4.0831	1	1104
23	1172.413	4.6368	1	1127
24	1224.39	7.1681	2	1177
25	1266.729	0.6445	0	1217
26	1275.412	6.8041	2	1226
27	1300.397	13.8453	4	1250
28	1306.222	0.468	0	1255
29	1327.772	7.7272	2	1276
30	1351.344	8.7677	3	1299
31	1360.386	1.022	0	1307
32	1489.372	8.3852	2	1431

33	1524.067	2.5691	0	1465
34	1530.555	4.7721	1	1471
35	1550.348	0.63	0	1490
36	1877.821	289.5487	100	1805
37	3061.075	11.6679	4	2942
38	3071.149	30.4971	10	2952
39	3080.59	28.6795	9	2961
40	3090.795	29.226	10	2971
41	3111.413	12.1522	4	2991
42	3119.007	14.7048	5	2998
43	3123.801	36.871	12	3002
44	3130.529	22.679	7	3009
45	3148.222	20.9375	7	3026

* scaling factor = 0.9613, # rounded

PYRROLIDINYLCARBONYLCARBENE (5d)



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_6H_9NO, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	0.940350181	–0.897031708	–2.322377888
2	C	0.846653117	–0.713072608	–0.9325897
3	O	2.059944341	–1.047379873	–0.752956868
4	N	–0.007649907	–0.218035112	–0.040921838
5	C	–1.345244577	0.276835443	–0.408436136
6	C	0.399240001	0.176692481	1.318637785
7	H	0.777071913	–1.951607927	–2.58900108
8	H	–1.257500486	1.034075049	–1.197918825
9	C	–1.873143707	0.873614886	0.908381632
10	H	–1.97519191	–0.535773485	–0.785569373
11	H	1.445656535	0.492226539	1.3152864
12	C	–0.595703981	1.295414833	1.65915747
13	H	0.300766468	–0.672693993	2.006972571
14	H	–2.408071537	0.105534965	1.47926099

15	H	–2.565109709	1.702436161	0.735282267
16	H	–0.749251654	1.403506649	2.736656124
17	H	–0.227281194	2.252860844	1.272499759

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –5.2624 y = 0.8770 z = –1.4818 Tot = 5.5369

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –364.034363 Hartree

Zero-point correction = 0.142518 Hartree

Sum of electronic and zero-point energies = –363.891845 Hartree

Zero-point vibrational energy = 374.1807 kJ/mol = 89.43134 kcal/mol

Enthalpy = -2.283400607×10^5 kcal/mol = -9.553748141×10^5 kJ/mol

Entropy = 87.785 cal/mol K = 367.29244 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.283662338×10^5 kcal/mol = -9.554843222×10^5 kJ/mol

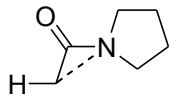
IR SPECTRUM

mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	40.0897	2.7758	0	38
2	147.8973	3.4942	0	142
3	162.8023	2.0941	0	156
4	189.7135	7.7184	1	182
5	255.3145	1.7992	0	245
6	305.1842	37.0541	7	293
7	493.1564	35.478	6	474
8	514.2795	12.4668	2	494
9	566.0616	2.0335	0	544
10	585.9152	2.0637	0	563
11	772.1275	0.6039	0	742
12	870.0176	3.6836	0	836
13	876.5131	12.619	2	842
14	883.9815	3.9778	0	849
15	919.9714	3.027	0	884
16	931.9386	54.3615	10	895
17	948.3096	82.4795	15	911

18	984.3876	4.5247	0	946
19	1036.929	3.5999	0	996
20	1131.213	21.5237	4	1087
21	1159.05	5.8507	1	1114
22	1192.491	6.521	1	1146
23	1209.666	8.3236	1	1162
24	1237.505	4.6654	0	1189
25	1265.694	1.696	0	1216
26	1290.575	8.0104	1	1240
27	1335.958	0.7202	0	1284
28	1365.738	0.13	0	1312
29	1373.728	5.7014	1	1320
30	1396.069	29.4016	5	1342
31	1468.55	55.1229	10	1411
32	1519.787	3.4337	0	1460
33	1526.263	12.5425	2	1467
34	1546.015	0.5357	0	1486
35	1557.33	16.2728	3	1497
36	1713.526	525.6228	100	1647
37	3047.779	54.0593	10	2929
38	3050.757	5.3101	1	2932
39	3065.308	15.1684	2	2946
40	3068.116	28.7607	5	2949
41	3071.158	20.8284	3	2952
42	3096.489	31.5602	6	2976
43	3123.164	20.8537	3	3002
44	3127.78	12.3574	2	3006
45	3133.825	37.1264	7	3012

* scaling factor = 0.9613, # rounded

TRANSITION STATE ^{1}5d→^{1}2d



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_6H_9NO, framework group C1

STANDARD ORIENTATION

centre No. **atom type** **coordinates [Å]**

		x	y	z
1	C	–1.627200955	0.23676658	–1.919711695
2	C	–1.494323929	0.07822777	–0.497155234
3	N	–0.130360595	–0.110879161	–0.232865849
4	C	0.953278066	0.824666464	–0.595237694
5	O	–2.393203981	–0.142375999	0.307606902
6	C	0.279075134	–1.026199026	0.85473426
7	H	–1.294068263	1.233329149	–2.267134324
8	H	1.476349978	0.493965463	–1.502471939
9	H	0.546659651	1.824016085	–0.783436565
10	C	1.892648755	0.759357484	0.617152155
11	C	1.769063543	–0.708761326	1.060083343
12	H	–0.319541035	–0.810803868	1.745428289
13	H	0.09623554	–2.068061999	0.570475712
14	H	2.917061372	1.051623758	0.367447546
15	H	1.529790372	1.427204826	1.407204728
16	H	2.083912515	–0.872731721	2.094817813
17	H	2.386512204	–1.347727247	0.417683656

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 4.8395 y = 2.2065 z = 0.3097 Tot = 5.3278

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –364.0135108 Hartree

Zero-point correction = 0.140982 Hartree

Sum of electronic and zero-point energies = –363.8725288 Hartree

Zero-point vibrational energy = 370.1479 kJ/mol = 88.46748 kcal/mol

Enthalpy = -2.283283004×10^5 kcal/mol = -9.55325609×10^5 kJ/mol

Entropy = 84.783 cal/mol K = 354.732072 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.283535784×10^5 kcal/mol = -9.55431372×10^5 kJ/mol

IR SPECTRUM

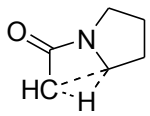
mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	–233.0424	1.3811	0	–225
2	62.7006	1.0478	0	60

3	139.8162	1.6361	0	134
4	203.8764	4.6835	2	195
5	234.2683	4.3632	1	225
6	267.6757	1.6331	0	257
7	461.9476	9.9091	4	444
8	577.0401	0.8062	0	554
9	579.2788	8.3847	3	556
10	644.4765	13.3854	5	619
11	681.4564	77.3253	34	655
12	773.4613	5.3768	2	743
13	867.7168	2.3718	1	834
14	888.1711	5.8354	2	853
15	923.7537	3.2023	1	888
16	933.6929	13.9327	6	897
17	956.5312	94.0771	41	919
18	983.3606	26.7331	11	945
19	1030.02	9.0759	4	990
20	1073.94	4.5994	2	1032
21	1139.866	43.3717	19	1095
22	1151.802	1.6592	0	1107
23	1200.233	2.1928	0	1153
24	1212.72	8.746	3	1165
25	1259.063	28.5373	12	1210
26	1265.426	20.6075	9	1216
27	1325.547	122.1032	53	1274
28	1335.726	3.8141	1	1284
29	1366.646	0.3132	0	1313
30	1379.524	1.9731	0	1326
31	1389.969	40.3033	17	1336
32	1519.12	3.5438	1	1460
33	1525.625	3.6973	1	1466
34	1541.667	0.9273	0	1482
35	1553.456	3.8479	1	1493
36	1725.01	226.7975	100	1658
37	3012.972	28.8024	12	2896
38	3034.489	47.6545	21	2917
39	3063.767	17.0627	7	2945

40	3068.832	15.8812	7	2950
41	3072.253	30.0758	13	2953
42	3098.407	21.1741	9	2978
43	3108.206	11.8892	5	2987
44	3121.024	24.3965	10	3000
45	3129.358	44.3899	19	3008

* scaling factor = 0.9613, # rounded

TRANSITION STATE ^{1}5d→^{1}3d



GAUSSIAN 98; B3LYP/6-31g(d)

stoichiometry C_6H_9NO, framework group C1

STANDARD ORIENTATION

centre No.	atom type			coordinates [Å]
		x	y	z
1	C	–1.568970305	–0.091877181	–1.450163186
2	C	–1.392214478	0.314556599	–0.063563753
3	N	–0.065971006	0.616955179	0.207968391
4	C	0.64702624	0.098092889	1.380426478
5	O	–2.337783846	0.267698401	0.718469004
6	C	0.695458031	0.412911146	–1.009783846
7	H	–1.960888681	0.699771466	–2.106725947
8	H	–0.036212112	–0.171173917	–1.725852307
9	C	1.888930497	–0.489622493	–0.62741975
10	H	0.967621983	1.338539059	–1.524874356
11	H	–0.082122353	–0.251744181	2.115288066
12	H	1.25166158	0.889897912	1.839293118
13	C	1.529955489	–1.01557083	0.780887035
14	H	0.947694058	–1.940120531	0.700568304
15	H	2.41713467	–1.225816528	1.385900099
16	H	2.799278469	0.121444895	–0.598542435
17	H	2.058787357	–1.292012416	–1.350883169

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = –4.7691 y = 1.7093 z = –1.4087 Tot = 5.2584

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –364.0206896 Hartree

Zero-point correction = 0.140226 Hartree

Sum of electronic and zero-point energies = –363.8804636 Hartree

Zero-point vibrational energy = 368.1635 kJ/mol = 87.99318 kcal/mol

Enthalpy = -2.283335852×10^5 kcal/mol = -9.553477204×10^5 kJ/mol

Entropy = 81.882 cal/mol K = 342.594288 J/mol K

Gibbs Free Energy (T = 298.15 K) = -2.283579983×10^5 kcal/mol = -9.554498649×10^5 kJ/mol

IR SPECTRUM

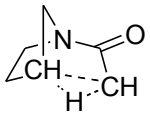
mode No.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	–334.8684	47.0013	17	–322
2	117.2707	2.5806	0	112
3	129.0684	5.4555	2	124
4	245.796	1.9139	0	236
5	272.6169	10.7099	4	262
6	422.8297	2.4267	0	406
7	559.2875	2.7945	1	537
8	573.2767	21.7668	8	551
9	593.6683	9.8879	3	570
10	655.5706	4.4666	1	630
11	742.675	7.4114	2	713
12	803.1969	1.6586	0	772
13	836.4333	1.0467	0	804
14	894.0526	2.6877	1	859
15	915.1037	4.9705	1	879
16	943.3891	8.9681	3	906
17	968.8411	26.0845	9	931
18	972.6824	67.2912	25	935
19	1017.939	6.0506	2	978
20	1079.969	3.3517	1	1038
21	1124.161	11.6416	4	1080
22	1175.991	8.7236	3	1130
23	1206.775	4.466	1	1160
24	1233.919	5.1713	1	1186

25	1274.158	17.8903	6	1224
26	1295.161	21.511	8	1245
27	1320.889	8.2474	3	1269
28	1336.249	1.1441	0	1284
29	1360.088	5.0575	1	1307
30	1384.253	12.4938	4	1330
31	1422.082	203.7243	76	1367
32	1445.26	25.4826	9	1389
33	1511.004	4.4993	1	1452
34	1522.646	5.0036	1	1463
35	1542.331	3.333	1	1482
36	1744.019	265.4863	100	1676
37	2140.338	170.3867	64	2057
38	3057.9	45.2883	17	2939
39	3063.663	13.9452	5	2945
40	3074.826	18.4262	6	2955
41	3078.935	18.987	7	2959
42	3105.038	33.4413	12	2984
43	3118.982	14.8112	5	2998
44	3128.337	23.8329	8	3007
45	3141.446	10.6003	3	3019

* scaling factor = 0.9613, # rounded

TRANSITION STATE ^{1}5d→^{1}6d

GAUSSIAN 98; B3LYP/6-31g(d)



stoichiometry C_6H_9NO, framework group C1

STANDARD ORIENTATION

centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–1.331283096	–0.308644109	–0.926129381
2	C	–1.383989758	–0.189210014	0.597637639
3	N	0.044185048	–0.232863262	0.960160226
4	C	0.540102445	–1.402878628	0.178342241
5	C	–0.250193795	–1.377504657	–1.174298855
6	C	0.708322801	0.940328796	0.437472383
7	O	1.74711359	1.384944653	0.915668524
8	C	0.11594782	1.678452953	–0.646232648
9	H	0.739059905	1.645069444	–1.549529035
10	H	1.62363234	–1.337374344	0.062187599
11	H	0.314164503	–2.310335436	0.746665411
12	H	–1.848551047	0.733932611	0.94973573
13	H	–1.893203789	–1.045198198	1.056317475
14	H	–0.719620495	–2.347298555	–1.373865309
15	H	0.38222156	–1.143244322	–2.035419761
16	H	–2.275158633	–0.449941391	–1.463491237
17	H	–1.002186901	0.761609751	–1.239818916

DIPOLE MOMENT [DEBYE] [B3LYP/6-311+g(3df,2p)]

x = 5.5102 y = –0.3579 z = –1.0869 Tot = 5.6278

THERMOCHEMICAL DATA [B3LYP/6-311+g(3df,2p)]

HF = –363.9989984 Hartree

Zero-point correction = 0.140274 Hartree

Sum of electronic and zero-point energies = –363.8587244 Hartree

Zero-point vibrational energy = 368.2898 kJ/mol = 88.02338 kcal/mol

Enthalpy = $–2.283201269 \times 10^5$ kcal/mol = $–9.552914109 \times 10^5$ kJ/mol

Entropy = 80.018 cal/mol K = 334.795312 J/mol K

Gibbs Free Energy (T = 298.15 K) = –2.283439843 × 10^5 kcal/mol = –9.553912301 × 10^5 kJ/mol

IR SPECTRUM

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	–279.8442	82.2728	22	–270
2	113.7125	0.728	0	109
3	224.4248	7.0086	1	215
4	270.8127	1.4965	0	260
5	380.5261	7.7353	2	365
6	423.8581	2.1784	0	407
7	493.7633	2.5505	0	474
8	605.0907	45.972	12	581
9	625.751	16.9324	4	601
10	712.2846	12.5034	3	684
11	769.568	35.0043	9	739
12	800.2241	1.2037	0	769
13	853.1895	0.6381	0	820
14	889.1608	6.2253	1	854
15	905.4063	12.3231	3	870
16	925.4483	11.8235	3	889
17	942.273	20.7631	5	905
18	959.1977	34.5957	9	922
19	986.1487	31.783	8	947
20	1015.023	10.9462	3	975
21	1071.711	20.6939	5	1030
22	1139.682	8.8565	2	1095
23	1148.498	1.4837	0	1104
24	1216.384	13.7297	3	1169
25	1243.231	24.5482	6	1195
26	1250.959	11.4117	3	1202
27	1265.059	3.2659	0	1216
28	1316.536	2.6251	0	1265
29	1335.235	9.3749	2	1283
30	1351.291	34.209	9	1298
31	1371.975	6.2784	1	1318
32	1517.094	6.0527	1	1458

33	1518.373	6.5424	1	1459
34	1531.274	24.2601	6	1472
35	1543.931	1.8052	0	1484
36	1712.722	218.5537	61	1646
37	2277.239	358.0989	100	2189
38	3072.083	22.554	6	2953
39	3072.788	16.7229	4	2953
40	3087.532	38.681	10	2968
41	3102.959	4.3587	1	2982
42	3108.432	19.2556	5	2988
43	3117.85	13.6731	3	2997
44	3151.843	13.1324	3	3029
45	3152.696	5.9895	1	3030

* scaling factor = 0.9613, # rounded