Supplementary Material

^{13}C NMR Spectroscopic Studies of Intra- and Intermolecular Interactions of Amino Acid Derivatives and Peptide Derivatives in Solutions

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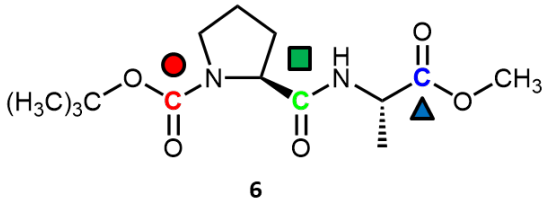
Index

Table S1. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in the gas phase for *N*-Boc-L-proline-L-alanine-OMe **6**



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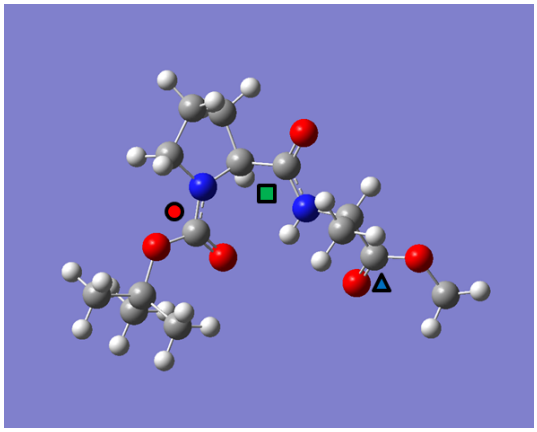

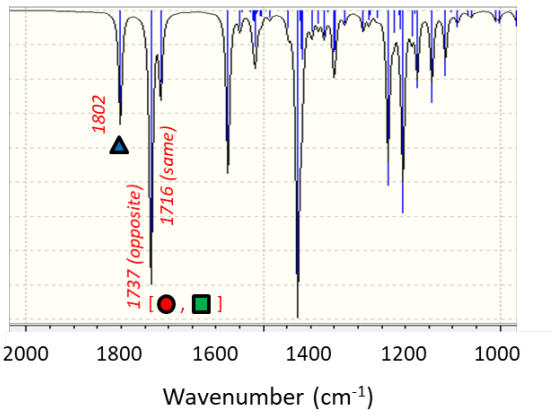


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Zero-point correction = 0.384068 (Hartree/Particle)
Thermal correction to Energy = 0.407394
Thermal correction to Enthalpy = 0.408338
Thermal correction to Gibbs Free Energy = 0.329378
Sum of electronic and zero-point Energies = -1033.287776
Sum of electronic and thermal Energies = -1033.264451
Sum of electronic and thermal Enthalpies = -1033.263507
Sum of electronic and thermal Free Energies = -1033.342466
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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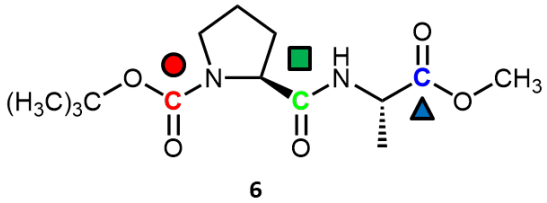
2	6	0	-0.387335	1.908191	-0.876161
3	6	0	-0.908407	3.351692	-0.933320
4	6	0	-1.775370	3.479359	0.331506
5	6	0	-2.446569	2.103291	0.455176
6	6	0	-1.669510	-0.139603	-0.374097
7	8	0	-0.885173	-0.857294	-0.997075
8	8	0	-2.823455	-0.552196	0.198358
9	6	0	-3.241598	-1.969487	0.161184
10	6	0	-4.559908	-1.943104	0.940157
11	6	0	-3.476584	-2.411156	-1.287292
12	6	0	-2.207391	-2.844423	0.878020
13	6	0	0.959696	1.796932	-0.115667
14	8	0	1.462535	2.757099	0.471892

15	7	0	1.536967	0.570468	-0.164533
16	1	0	1.041208	-0.195117	-0.622408
17	6	0	2.787157	0.294133	0.522787
18	6	0	2.578961	-0.069004	2.009096
19	1	0	3.404146	1.196623	0.472288
20	6	0	3.509657	-0.832165	-0.206066
21	8	0	2.993122	-1.605383	-0.986066
22	8	0	4.806925	-0.886605	0.157083
23	6	0	5.583695	-1.950446	-0.428471
24	1	0	-0.259858	1.466291	-1.870505
25	1	0	-0.090634	4.074213	-0.958904
26	1	0	-1.521193	3.477016	-1.834543
27	1	0	-1.132860	3.670836	1.197023
28	1	0	-2.511070	4.287320	0.266101
29	1	0	-2.640199	1.808357	1.490581
30	1	0	-3.398568	2.062149	-0.090156
31	1	0	-4.400065	-1.584178	1.962651
32	1	0	-5.286924	-1.284994	0.452165
33	1	0	-4.984568	-2.951784	0.989385
34	1	0	-4.185756	-1.737310	-1.782001
35	1	0	-2.544303	-2.424026	-1.854881
36	1	0	-3.906844	-3.419730	-1.294323
37	1	0	-2.596907	-3.865324	0.969108
38	1	0	-2.018787	-2.463355	1.888486
39	1	0	-1.264086	-2.879355	0.329558
40	1	0	2.070260	0.760533	2.508423
41	1	0	1.963437	-0.970567	2.105139
42	1	0	3.540287	-0.239779	2.504127
43	1	0	5.602482	-1.850081	-1.516737
44	1	0	6.585039	-1.837466	-0.012632
45	1	0	5.159353	-2.921793	-0.161231

Frequencies --	1716.3783			1736.7926			1801.5732		
Red. masses --	10.8151			8.6924			11.0425		
Frc consts --	18.7719			15.4485			21.1165		
IR Inten --	139.5033			474.8374			195.4426		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	0.04	-0.13	-0.04	0.01	-0.07	-0.02	0.00	-0.01	0.00
2 6	-0.02	0.03	0.03	-0.01	-0.04	-0.02	0.00	0.01	0.00
3 6	0.01	-0.01	-0.01	0.01	0.02	0.00	0.00	0.00	0.00
4 6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
5 6	-0.01	-0.02	-0.01	-0.01	0.00	0.00	0.00	0.00	0.00
6 6	-0.37	0.45	0.32	-0.20	0.23	0.17	-0.01	0.02	0.01
7 8	0.23	-0.22	-0.19	0.12	-0.11	-0.09	0.01	-0.01	-0.01
8 8	0.04	-0.03	-0.03	0.03	-0.01	-0.02	0.00	0.00	0.00
9 6	-0.02	0.04	0.02	-0.01	0.02	0.01	0.00	0.00	0.00
10 6	0.00	-0.01	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
12 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13 6	-0.15	-0.30	-0.19	0.21	0.48	0.27	-0.03	-0.05	-0.03

14	8	0.10	0.17	0.11	−0.14	−0.27	−0.16	0.01	0.02	0.01
15	7	0.02	0.05	0.02	−0.02	−0.06	−0.03	0.01	0.01	0.01
16	1	0.01	0.03	−0.05	0.33	−0.34	0.05	−0.13	0.10	−0.01
17	6	−0.01	−0.01	−0.01	0.02	−0.01	0.01	0.01	−0.05	−0.03
18	6	0.01	0.00	0.00	−0.01	0.00	0.00	0.00	0.00	−0.01
19	1	−0.01	−0.02	0.00	−0.08	0.08	−0.05	0.12	−0.12	−0.12
20	6	−0.02	−0.04	−0.04	0.01	0.02	0.02	0.29	0.50	0.49
21	8	0.02	0.02	0.03	−0.01	−0.02	−0.02	−0.20	−0.31	−0.31
22	8	0.00	0.00	0.00	−0.01	0.00	0.00	−0.03	−0.03	−0.03
23	6	0.00	0.00	0.00	0.00	0.00	0.00	−0.01	0.02	0.02
24	1	0.17	0.02	0.07	−0.19	0.11	−0.08	0.01	0.00	0.01
25	1	−0.07	0.06	−0.05	0.05	0.00	0.07	0.00	0.00	0.00
26	1	0.02	0.09	0.00	−0.03	−0.12	0.01	0.00	0.01	0.00
27	1	−0.04	0.02	0.02	0.05	−0.03	−0.02	0.00	0.00	0.00
28	1	0.02	0.03	0.03	−0.01	−0.01	−0.05	0.00	0.00	0.00
29	1	−0.07	0.07	0.00	0.00	0.02	0.01	0.00	0.00	0.00
30	1	−0.06	0.09	0.10	−0.01	0.02	0.01	0.00	0.00	0.00
31	1	0.02	0.00	−0.01	0.01	0.00	0.00	0.00	0.00	0.00
32	1	0.02	0.00	−0.01	0.01	0.00	−0.01	0.00	0.00	0.00
33	1	−0.04	0.02	0.03	−0.02	0.01	0.01	0.00	0.00	0.00
34	1	0.01	0.03	0.02	0.01	0.02	0.01	0.00	0.00	0.00
35	1	−0.05	−0.12	−0.07	−0.03	−0.06	−0.04	0.00	0.00	0.00
36	1	0.09	−0.04	−0.09	0.05	−0.02	−0.04	0.00	0.00	0.00
37	1	0.11	−0.05	−0.05	0.06	−0.02	−0.03	0.00	0.00	0.00
38	1	0.00	0.04	−0.01	0.00	0.02	0.00	0.00	0.00	0.00
39	1	0.01	−0.14	0.04	0.01	−0.08	0.02	0.00	0.00	0.00
40	1	0.00	−0.02	0.02	0.00	0.03	−0.04	−0.03	−0.06	0.04
41	1	−0.01	0.01	−0.01	0.02	−0.02	0.01	−0.02	0.03	0.06
42	1	−0.01	0.01	0.04	0.02	−0.02	−0.06	0.00	−0.01	−0.01
43	1	−0.01	0.01	0.00	0.01	0.00	0.00	0.13	−0.07	0.03
44	1	0.00	0.01	0.01	0.00	−0.01	0.00	0.07	−0.18	−0.12
45	1	−0.01	0.00	0.00	0.01	0.00	0.00	0.14	−0.03	−0.02

Table S2. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in chloroform for *N*-Boc-L-proline-L-alanine-OMe **6**



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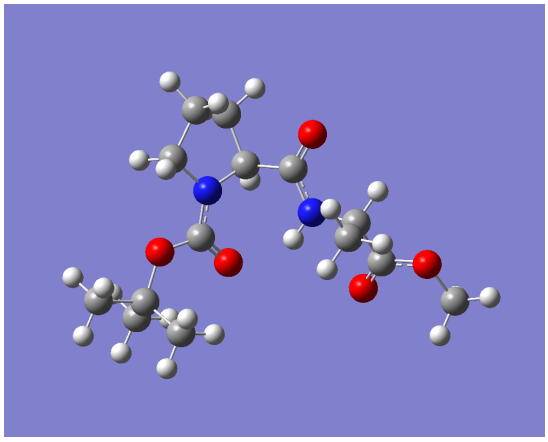
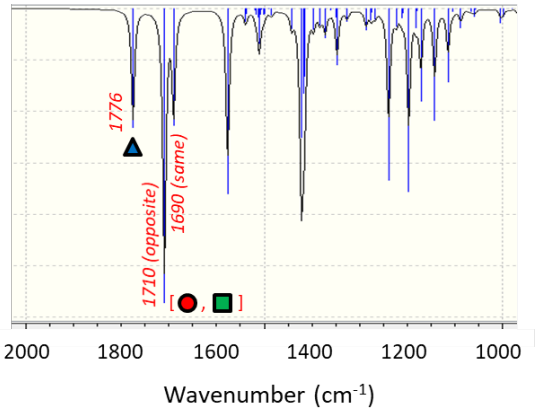





```
Zero-point correction = 0.383573 (Hartree/Particle)
Thermal correction to Energy = 0.406921
Thermal correction to Enthalpy = 0.407865
Thermal correction to Gibbs Free Energy = 0.328702
Sum of electronic and zero-point Energies = -1033.298307
Sum of electronic and thermal Energies = -1033.274960
Sum of electronic and thermal Enthalpies = -1033.274016
Sum of electronic and thermal Free Energies = -1033.353179
```

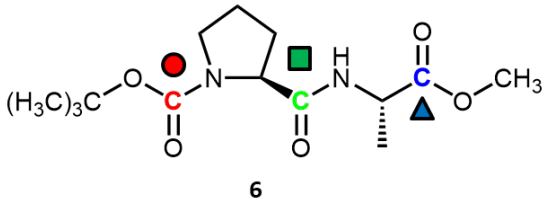
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.453357	1.193111	-0.160987
2	6	0	-0.377630	1.924913	-0.864034
3	6	0	-0.914037	3.362582	-0.915250
4	6	0	-1.781531	3.478617	0.349740
5	6	0	-2.440793	2.097373	0.465864
6	6	0	-1.655486	-0.133929	-0.376639
7	8	0	-0.863852	-0.849698	-1.000742
8	8	0	-2.810729	-0.549910	0.181541
9	6	0	-3.236564	-1.969524	0.149182
10	6	0	-4.558639	-1.932038	0.920708
11	6	0	-3.467408	-2.415647	-1.297859
12	6	0	-2.211269	-2.843393	0.878377
13	6	0	0.978811	1.814389	-0.118202
14	8	0	1.525151	2.790453	0.408646

15	7	0	1.516125	0.572014	-0.115117
16	1	0	0.984828	-0.188335	-0.541669
17	6	0	2.766313	0.269295	0.561636
18	6	0	2.555006	-0.143304	2.034368
19	1	0	3.385069	1.170712	0.536926
20	6	0	3.490598	-0.833412	-0.203737
21	8	0	2.969436	-1.579393	-1.011688
22	8	0	4.781523	-0.900808	0.157216
23	6	0	5.571926	-1.945762	-0.454496
24	1	0	-0.248040	1.492888	-1.862245
25	1	0	-0.105787	4.095194	-0.946759
26	1	0	-1.530429	3.480913	-1.814110
27	1	0	-1.146944	3.672972	1.220922
28	1	0	-2.524489	4.279213	0.285095
29	1	0	-2.635218	1.797067	1.499067
30	1	0	-3.387729	2.051679	-0.086180
31	1	0	-4.402653	-1.569887	1.942639
32	1	0	-5.280738	-1.274655	0.424536
33	1	0	-4.986209	-2.939050	0.971973
34	1	0	-4.166360	-1.737277	-1.800501
35	1	0	-2.532944	-2.444092	-1.861363
36	1	0	-3.908457	-3.419199	-1.300118
37	1	0	-2.608990	-3.860154	0.975376
38	1	0	-2.025317	-2.455272	1.886443
39	1	0	-1.265101	-2.891468	0.335813
40	1	0	2.041876	0.665992	2.562037
41	1	0	1.942041	-1.048907	2.100427
42	1	0	3.515027	-0.327718	2.526279
43	1	0	5.604761	-1.805869	-1.537425
44	1	0	6.566540	-1.841915	-0.022336
45	1	0	5.147878	-2.924835	-0.219832

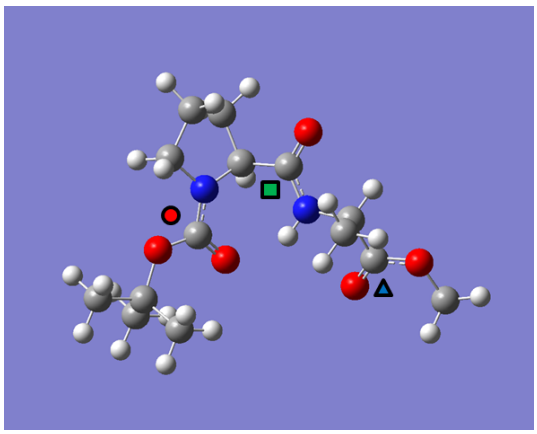
Frequencies --	1690.1274			1709.5899			1775.5564		
Red. masses --	10.6197			7.8521			10.9987		
Frc consts --	17.8732			13.5213			20.4296		
IR Inten --	289.0707			735.9207			308.7897		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	0.05	-0.14	-0.04	0.01	-0.05	-0.01	0.00	0.00	0.00
2 6	-0.02	0.03	0.02	-0.01	-0.04	-0.02	0.00	0.01	0.00
3 6	0.01	-0.01	-0.01	0.01	0.02	0.00	0.00	0.00	0.00
4 6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5 6	0.00	-0.02	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
6 6	-0.40	0.48	0.34	-0.15	0.16	0.12	-0.01	0.01	0.01
7 8	0.24	-0.23	-0.19	0.09	-0.08	-0.07	0.00	-0.01	0.00
8 8	0.05	-0.03	-0.03	0.02	-0.01	-0.01	0.00	0.00	0.00
9 6	-0.02	0.04	0.02	-0.01	0.01	0.01	0.00	0.00	0.00
10 6	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
12 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13 6	-0.12	-0.24	-0.13	0.24	0.48	0.25	-0.04	-0.07	-0.04

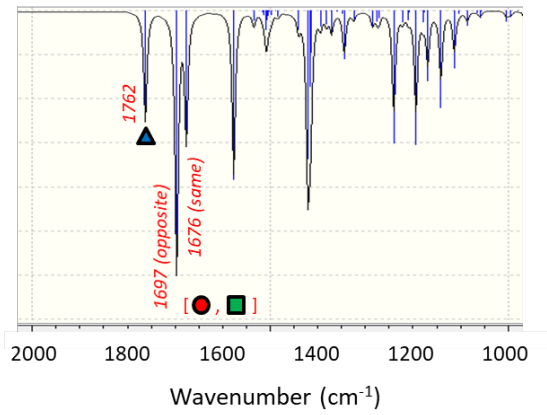
14	8	0.08	0.14	0.08	−0.15	−0.27	−0.15	0.02	0.03	0.02
15	7	0.01	0.05	0.02	−0.04	−0.05	−0.03	0.00	0.02	0.01
16	1	0.08	−0.05	−0.02	0.38	−0.41	0.10	−0.11	0.10	0.00
17	6	−0.01	−0.01	−0.01	0.03	−0.01	0.01	0.01	−0.06	−0.04
18	6	0.01	0.00	0.00	−0.01	0.00	0.00	0.00	0.00	−0.01
19	1	−0.04	0.00	−0.01	−0.08	0.08	−0.06	0.12	−0.12	−0.13
20	6	−0.02	−0.03	−0.03	0.02	0.04	0.04	0.29	0.49	0.51
21	8	0.01	0.02	0.02	−0.02	−0.03	−0.03	−0.20	−0.30	−0.32
22	8	0.00	0.00	0.00	−0.01	0.00	0.00	−0.03	−0.03	−0.03
23	6	0.00	0.00	0.00	0.00	0.00	0.00	−0.01	0.03	0.02
24	1	0.14	0.03	0.06	−0.19	0.10	−0.08	0.02	−0.01	0.01
25	1	−0.06	0.06	−0.03	0.04	0.00	0.06	−0.01	0.00	0.00
26	1	0.01	0.07	0.00	−0.02	−0.13	0.00	0.00	0.02	0.00
27	1	−0.02	0.02	0.01	0.04	−0.02	−0.01	0.00	0.00	0.00
28	1	0.02	0.03	0.02	−0.01	−0.01	−0.04	0.00	0.00	0.00
29	1	−0.10	0.08	0.00	0.00	0.02	0.00	0.00	0.00	0.00
30	1	−0.08	0.10	0.13	−0.01	0.02	0.01	0.00	0.00	0.00
31	1	0.02	−0.01	−0.01	0.01	0.00	0.00	0.00	0.00	0.00
32	1	0.01	−0.01	−0.02	0.00	0.00	0.00	0.00	0.00	0.00
33	1	−0.05	0.02	0.04	−0.02	0.01	0.01	0.00	0.00	0.00
34	1	0.01	0.03	0.03	0.01	0.01	0.01	0.00	0.00	0.00
35	1	−0.05	−0.12	−0.07	−0.02	−0.05	−0.03	0.00	0.00	0.00
36	1	0.10	−0.04	−0.09	0.04	−0.02	−0.03	0.00	0.00	0.00
37	1	0.12	−0.05	−0.05	0.04	−0.02	−0.02	0.00	0.00	0.00
38	1	−0.01	0.04	−0.01	0.00	0.01	0.00	0.00	0.00	0.00
39	1	0.01	−0.14	0.04	0.00	−0.06	0.02	0.00	0.00	0.00
40	1	0.00	−0.01	0.01	−0.01	0.01	−0.01	−0.02	−0.06	0.04
41	1	0.00	0.01	−0.01	0.01	−0.01	0.01	−0.02	0.03	0.06
42	1	−0.01	0.00	0.03	0.03	0.00	−0.06	0.00	0.00	−0.01
43	1	−0.01	0.01	0.00	0.01	0.00	0.00	0.12	−0.08	0.03
44	1	0.00	0.01	0.01	0.01	−0.01	−0.01	0.07	−0.18	−0.13
45	1	−0.01	0.00	0.00	0.01	0.00	0.00	0.15	−0.03	−0.03

Table S3. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in acetonitrile for *N*-Boc-L-proline-L-alanine-OMe **6**



6






```
Zero-point correction = 0.383286 (Hartree/Particle)
Thermal correction to Energy = 0.406658
Thermal correction to Enthalpy = 0.407602
Thermal correction to Gibbs Free Energy = 0.328430
Sum of electronic and zero-point Energies = -1033.302954
Sum of electronic and thermal Energies = -1033.279582
Sum of electronic and thermal Enthalpies = -1033.278638
Sum of electronic and thermal Free Energies = -1033.357809
```

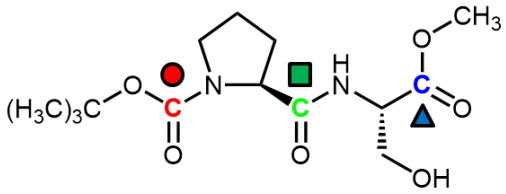
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.446722	1.191808	-0.160388
2	6	0	-0.386728	1.941985	-0.868400
3	6	0	-0.944140	3.371806	-0.909326
4	6	0	-1.800495	3.471027	0.364377
5	6	0	-2.441552	2.081616	0.478236
6	6	0	-1.638588	-0.135144	-0.380205
7	8	0	-0.839551	-0.842974	-1.008518
8	8	0	-2.787340	-0.563343	0.177196
9	6	0	-3.201846	-1.988409	0.154880
10	6	0	-4.523683	-1.955662	0.926697
11	6	0	-3.430268	-2.445777	-1.288669
12	6	0	-2.168935	-2.846941	0.890745
13	6	0	0.981342	1.845292	-0.140817
14	8	0	1.547868	2.835414	0.340058

15	7	0	1.507573	0.600466	-0.104759
16	1	0	0.962096	-0.165648	-0.502575
17	6	0	2.770204	0.300193	0.550520
18	6	0	2.590658	-0.056543	2.041834
19	1	0	3.406774	1.186322	0.475749
20	6	0	3.451558	-0.843278	-0.194930
21	8	0	2.890661	-1.602345	-0.965807
22	8	0	4.746670	-0.928868	0.134147
23	6	0	5.502193	-2.011633	-0.459607
24	1	0	-0.259688	1.518162	-1.870494
25	1	0	-0.147365	4.116470	-0.949298
26	1	0	-1.571841	3.482916	-1.800837
27	1	0	-1.162235	3.668070	1.232624
28	1	0	-2.553835	4.262287	0.310318
29	1	0	-2.624350	1.773807	1.511156
30	1	0	-3.390491	2.027462	-0.068765
31	1	0	-4.369976	-1.585273	1.945989
32	1	0	-5.251459	-1.308420	0.425531
33	1	0	-4.942290	-2.965846	0.985260
34	1	0	-4.131674	-1.774058	-1.796568
35	1	0	-2.495739	-2.475332	-1.852099
36	1	0	-3.867200	-3.450915	-1.282908
37	1	0	-2.557837	-3.866205	0.995218
38	1	0	-1.986411	-2.449567	1.895690
39	1	0	-1.221968	-2.891329	0.349052
40	1	0	2.108640	0.780762	2.554924
41	1	0	1.961518	-0.945946	2.155753
42	1	0	3.559663	-0.244533	2.514037
43	1	0	5.512343	-1.907915	-1.546850
44	1	0	6.508233	-1.913294	-0.054211
45	1	0	5.064333	-2.972157	-0.179294

Frequencies --		1676.2982			1696.5465			1762.3547		
Red. masses --		10.1388			7.4439			10.8888		
Frc consts --		16.7856			12.6236			19.9259		
IR Inten --		414.2857			866.7151			364.1131		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	7	0.05	-0.15	-0.04	0.00	-0.03	-0.01	0.00	0.00	0.00
2	6	-0.02	0.03	0.02	-0.02	-0.04	-0.02	0.00	0.01	0.00
3	6	0.01	-0.01	-0.01	0.01	0.02	0.00	0.00	0.00	0.00
4	6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	-0.02	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
6	6	-0.40	0.48	0.34	-0.12	0.12	0.09	0.00	0.00	0.00
7	8	0.24	-0.23	-0.19	0.07	-0.06	-0.05	0.00	0.00	0.00
8	8	0.05	-0.03	-0.03	0.02	0.00	-0.01	0.00	0.00	0.00
9	6	-0.02	0.04	0.02	-0.01	0.01	0.01	0.00	0.00	0.00
10	6	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	-0.09	-0.19	-0.09	0.26	0.48	0.23	-0.04	-0.08	-0.04

14	8	0.06	0.11	0.06	−0.16	−0.27	−0.13	0.02	0.04	0.02
15	7	0.00	0.06	0.01	−0.05	−0.04	−0.03	0.00	0.02	0.01
16	1	0.16	−0.13	0.01	0.41	−0.43	0.12	−0.12	0.11	−0.01
17	6	−0.01	−0.02	−0.01	0.03	−0.02	0.01	0.00	−0.06	−0.03
18	6	0.00	0.00	0.00	−0.01	0.00	0.00	0.00	0.00	−0.01
19	1	−0.06	0.01	−0.01	−0.07	0.07	−0.06	0.11	−0.12	−0.13
20	6	−0.01	−0.02	−0.02	0.03	0.05	0.05	0.31	0.49	0.48
21	8	0.01	0.01	0.01	−0.02	−0.03	−0.04	−0.21	−0.30	−0.30
22	8	0.00	0.00	0.00	−0.01	0.00	0.00	−0.03	−0.03	−0.03
23	6	0.00	0.00	0.00	0.00	0.00	0.00	−0.01	0.03	0.02
24	1	0.11	0.03	0.05	−0.18	0.09	−0.08	0.02	−0.01	0.01
25	1	−0.06	0.06	−0.02	0.04	0.00	0.06	−0.01	0.00	−0.01
26	1	0.01	0.06	0.00	−0.02	−0.13	0.00	0.00	0.02	0.00
27	1	−0.01	0.01	0.00	0.03	−0.02	−0.01	0.00	0.00	0.00
28	1	0.02	0.03	0.02	−0.01	−0.01	−0.04	0.00	0.00	0.01
29	1	−0.12	0.09	0.00	0.00	0.01	0.00	0.00	0.00	0.00
30	1	−0.09	0.10	0.15	−0.01	0.01	0.01	0.00	0.00	0.00
31	1	0.02	−0.02	−0.01	0.00	0.00	0.00	0.00	0.00	0.00
32	1	0.01	−0.02	−0.02	0.00	0.00	0.00	0.00	0.00	0.00
33	1	−0.06	0.02	0.04	−0.01	0.00	0.01	0.00	0.00	0.00
34	1	0.02	0.04	0.02	0.01	0.01	0.00	0.00	0.00	0.00
35	1	−0.06	−0.12	−0.07	−0.02	−0.03	−0.02	0.00	0.00	0.00
36	1	0.10	−0.04	−0.09	0.03	−0.01	−0.02	0.00	0.00	0.00
37	1	0.12	−0.05	−0.05	0.03	−0.01	−0.02	0.00	0.00	0.00
38	1	−0.01	0.04	−0.02	0.00	0.01	0.00	0.00	0.00	0.00
39	1	0.01	−0.14	0.05	0.00	−0.04	0.01	0.00	0.00	0.00
40	1	0.01	−0.01	0.02	−0.01	0.01	−0.01	−0.02	−0.06	0.05
41	1	−0.01	0.01	−0.02	0.00	−0.01	0.01	−0.01	0.03	0.05
42	1	−0.01	0.01	0.03	0.03	0.00	−0.07	−0.01	0.00	0.00
43	1	−0.01	0.00	0.00	0.01	−0.01	0.00	0.12	−0.10	0.02
44	1	0.00	0.01	0.00	0.01	−0.02	−0.01	0.07	−0.19	−0.12
45	1	−0.01	0.00	0.00	0.02	−0.01	0.00	0.15	−0.04	−0.04

Table S4. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in the gas phase for *N*-Boc-L-proline-L-serine-OMe **7**



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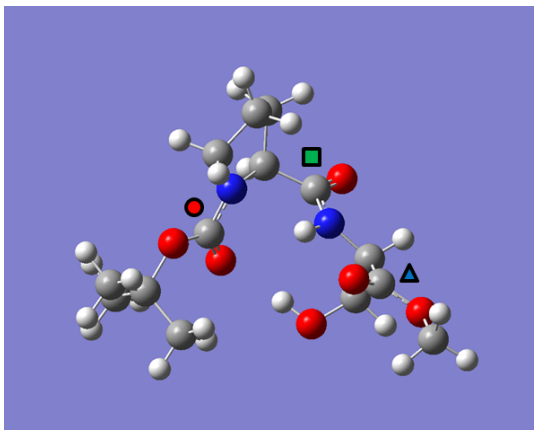
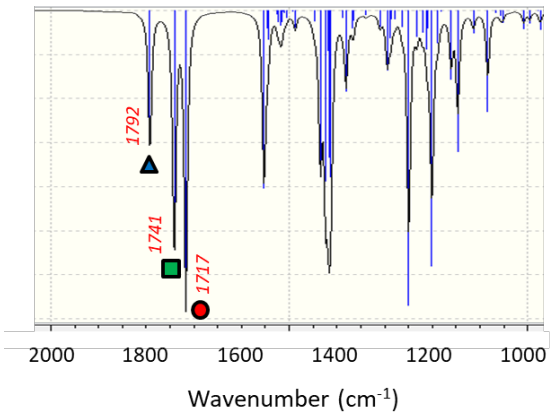





```
Zero-point correction = 0.389713 (Hartree/Particle)
Thermal correction to Energy = 0.413685
Thermal correction to Enthalpy = 0.414629
Thermal correction to Gibbs Free Energy = 0.335087
Sum of electronic and zero-point Energies = -1108.498909
Sum of electronic and thermal Energies = -1108.474937
Sum of electronic and thermal Enthalpies = -1108.473993
Sum of electronic and thermal Free Energies = -1108.553535
```

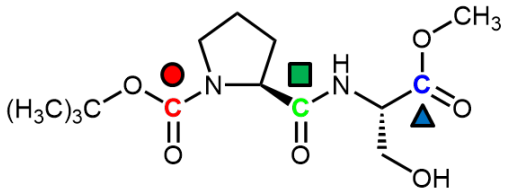
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.299835	1.330791	-0.248856
2	6	0	0.530788	2.325203	0.518267
3	6	0	0.692452	3.619577	-0.312937
4	6	0	0.961423	3.114702	-1.741323
5	6	0	1.824424	1.865685	-1.520003
6	6	0	1.712711	0.170642	0.342792
7	8	0	1.277672	-0.222196	1.427209
8	8	0	2.622643	-0.466982	-0.418636
9	6	0	3.160057	-1.800158	-0.051128
10	6	0	4.124308	-2.088475	-1.204965
11	6	0	3.914802	-1.713455	1.279116
12	6	0	2.028037	-2.831067	-0.019149
13	6	0	-0.940178	1.949888	0.772698

14	8	0	-1.599267	2.593128	1.588665
15	7	0	-1.429477	0.896724	0.073016
16	1	0	-0.814241	0.397207	-0.558074
17	6	0	-2.648409	0.205094	0.453201
18	6	0	-2.453337	-0.560975	1.792066
19	1	0	-3.458412	0.930661	0.590377
20	6	0	-3.013447	-0.744031	-0.679684
21	8	0	-2.298567	-0.994458	-1.630259
22	8	0	-4.226092	-1.288315	-0.485249
23	6	0	-4.652658	-2.256330	-1.465498
24	8	0	-1.389124	-1.491101	1.726352
25	1	0	-0.536254	-1.012430	1.730434
26	1	0	0.957039	2.437495	1.520070
27	1	0	-0.185894	4.264413	-0.228434
28	1	0	1.557049	4.182506	0.058001
29	1	0	0.021015	2.839479	-2.233761
30	1	0	1.463648	3.857898	-2.368325
31	1	0	1.730505	1.122551	-2.315879
32	1	0	2.888329	2.120123	-1.418047
33	1	0	3.591414	-2.108256	-2.161677
34	1	0	4.906557	-1.323624	-1.259225
35	1	0	4.602640	-3.062561	-1.055376
36	1	0	4.414990	-2.669647	1.472855
37	1	0	4.683130	-0.932893	1.234658
38	1	0	3.239157	-1.498664	2.108978
39	1	0	1.470416	-2.821575	-0.962319
40	1	0	1.332887	-2.646953	0.801782
41	1	0	2.456412	-3.831938	0.110437
42	1	0	-2.294342	0.183557	2.581589
43	1	0	-3.361766	-1.125279	2.019960
44	1	0	-5.637479	-2.585104	-1.133746
45	1	0	-3.952519	-3.094901	-1.494991
46	1	0	-4.710751	-1.793079	-2.453792

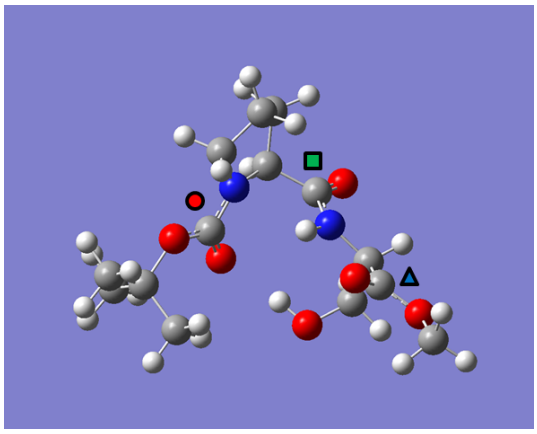
Frequencies --	1716.7591			1741.0289			1792.0968		
Red. masses --	10.4190			10.2892			10.9351		
Frc consts --	18.0924			18.3757			20.6916		
IR Inten --	386.7178			330.8984			190.4276		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	0.01	0.10	-0.10	0.01	0.01	-0.02	0.00	0.00	0.00
2 6	-0.02	0.01	0.03	0.04	-0.02	-0.03	-0.01	0.00	0.01
3 6	0.01	-0.01	-0.01	-0.01	0.01	-0.01	0.00	0.00	0.00
4 6	0.00	0.00	0.01	0.00	-0.01	0.00	0.00	0.00	0.00
5 6	-0.01	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
6 6	-0.23	-0.30	0.66	0.00	-0.02	0.02	-0.01	0.00	0.01
7 8	0.14	0.14	-0.37	0.00	0.01	-0.01	0.00	0.00	-0.01
8 8	0.03	0.01	-0.06	0.00	0.00	0.00	0.00	0.00	0.00
9 6	-0.01	-0.03	0.04	0.00	0.00	0.00	0.00	0.00	0.00
10 6	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
12 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

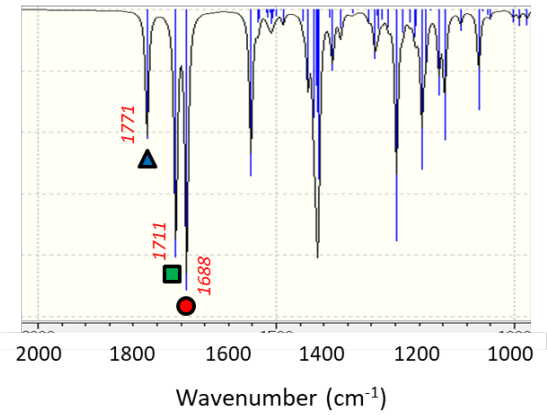
13	6	−0.01	−0.04	−0.02	−0.36	0.41	0.50	0.05	−0.04	−0.06
14	8	0.00	0.01	0.01	0.24	−0.23	−0.29	−0.03	0.02	0.03
15	7	0.02	0.04	0.01	0.03	−0.06	−0.06	−0.01	0.01	0.02
16	1	−0.11	−0.15	0.02	−0.20	−0.24	−0.13	0.14	0.12	0.07
17	6	−0.01	−0.01	0.00	−0.02	−0.01	0.01	0.01	−0.04	−0.04
18	6	0.01	−0.01	0.00	0.01	0.00	0.01	−0.01	0.01	−0.01
19	1	0.03	0.02	−0.02	0.03	0.08	0.00	−0.06	−0.08	−0.14
20	6	0.01	0.00	−0.01	−0.05	0.02	0.07	−0.42	0.17	0.60
21	8	−0.01	0.00	0.01	0.03	−0.01	−0.05	0.27	−0.10	−0.38
22	8	0.00	0.00	0.00	0.01	0.00	0.00	0.04	0.00	−0.04
23	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.02
24	8	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	1	0.00	−0.09	−0.05	0.01	−0.02	0.04	0.00	0.01	0.01
26	1	0.09	−0.09	0.01	−0.24	0.00	0.11	0.03	0.00	−0.01
27	1	−0.01	−0.04	0.03	−0.04	−0.03	0.03	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.02	−0.07	0.05	0.00	0.01	−0.01
29	1	0.00	0.00	0.00	0.01	0.02	−0.01	0.00	0.00	0.00
30	1	0.01	−0.02	−0.01	−0.02	0.01	0.00	0.00	0.00	0.00
31	1	−0.04	−0.05	0.05	0.00	−0.01	0.01	0.01	0.00	0.00
32	1	−0.01	−0.04	0.14	0.00	−0.01	0.01	0.00	0.00	−0.01
33	1	0.02	0.00	−0.02	0.00	0.00	0.00	0.00	0.00	0.00
34	1	0.01	0.00	−0.02	0.00	0.00	0.00	0.00	0.00	0.00
35	1	−0.03	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00
36	1	0.06	0.00	−0.14	0.00	0.00	0.00	0.00	0.00	0.00
37	1	0.02	−0.02	0.03	0.00	0.00	0.00	0.00	0.00	0.00
38	1	−0.10	0.11	−0.10	0.00	0.00	0.00	0.00	0.00	0.00
39	1	−0.01	−0.04	0.01	0.01	−0.01	0.00	0.01	−0.01	0.00
40	1	0.01	0.16	−0.02	0.00	0.00	0.00	0.01	0.00	0.01
41	1	0.10	0.03	−0.11	0.00	0.00	0.00	0.00	0.00	−0.01
42	1	−0.02	0.00	−0.01	0.04	0.07	−0.05	0.02	−0.06	0.03
43	1	−0.04	0.06	−0.01	−0.03	0.00	−0.11	0.00	0.00	0.01
44	1	0.00	0.00	0.00	0.00	−0.02	−0.02	−0.02	−0.14	−0.18
45	1	0.00	0.00	0.00	−0.02	−0.01	0.00	−0.13	−0.07	−0.04
46	1	0.00	0.00	0.00	−0.02	−0.01	0.00	−0.11	−0.11	−0.01

Table S5. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in chloroform for *N*-Boc-L-proline-L-serine-OMe **7**



7



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Zero-point correction = 0.389152 (Hartree/Particle)
Thermal correction to Energy = 0.413188
Thermal correction to Enthalpy = 0.414132
Thermal correction to Gibbs Free Energy = 0.334384
Sum of electronic and zero-point Energies = -1108.512193
Sum of electronic and thermal Energies = -1108.488157
Sum of electronic and thermal Enthalpies = -1108.487213
Sum of electronic and thermal Free Energies = -1108.566961
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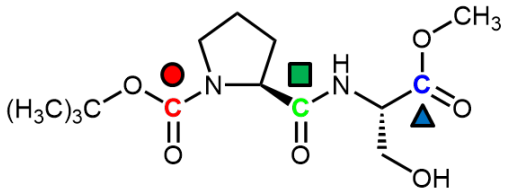
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.280411	1.327419	-0.250215
2	6	0	0.516009	2.313395	0.530863
3	6	0	0.645253	3.611875	-0.303131
4	6	0	0.916897	3.115253	-1.733348
5	6	0	1.798633	1.879693	-1.519539
6	6	0	1.712622	0.171250	0.331517
7	8	0	1.281274	-0.236355	1.416631
8	8	0	2.629581	-0.447062	-0.431343
9	6	0	3.213036	-1.766342	-0.072443
10	6	0	4.172127	-2.022556	-1.237626
11	6	0	3.979572	-1.657035	1.248557
12	6	0	2.114509	-2.831709	-0.030567
13	6	0	-0.941038	1.915053	0.815685

14	8	0	-1.586667	2.527833	1.672352
15	7	0	-1.440898	0.879076	0.104119
16	1	0	-0.837926	0.413312	-0.564447
17	6	0	-2.649204	0.169109	0.486966
18	6	0	-2.416307	-0.647355	1.788241
19	1	0	-3.456400	0.885219	0.675724
20	6	0	-3.053009	-0.733181	-0.672136
21	8	0	-2.361128	-0.949194	-1.650803
22	8	0	-4.259090	-1.274160	-0.465089
23	6	0	-4.738676	-2.197152	-1.470889
24	8	0	-1.337226	-1.559969	1.665711
25	1	0	-0.491921	-1.064988	1.646774
26	1	0	0.962933	2.434340	1.522596
27	1	0	-0.244974	4.240088	-0.217808
28	1	0	1.499456	4.190245	0.065759
29	1	0	-0.019822	2.829297	-2.226163
30	1	0	1.408421	3.868475	-2.355848
31	1	0	1.714704	1.140107	-2.319044
32	1	0	2.856942	2.150737	-1.411869
33	1	0	3.629128	-2.058532	-2.188165
34	1	0	4.930270	-1.234379	-1.298419
35	1	0	4.680849	-2.981586	-1.093340
36	1	0	4.516434	-2.595119	1.430425
37	1	0	4.718052	-0.848747	1.198795
38	1	0	3.307029	-1.472516	2.088380
39	1	0	1.542378	-2.832852	-0.964990
40	1	0	1.428977	-2.675238	0.804270
41	1	0	2.576928	-3.818713	0.084387
42	1	0	-2.246991	0.064064	2.604956
43	1	0	-3.311011	-1.232750	2.014393
44	1	0	-5.715472	-2.522930	-1.115753
45	1	0	-4.054847	-3.044445	-1.556664
46	1	0	-4.826219	-1.689070	-2.433846

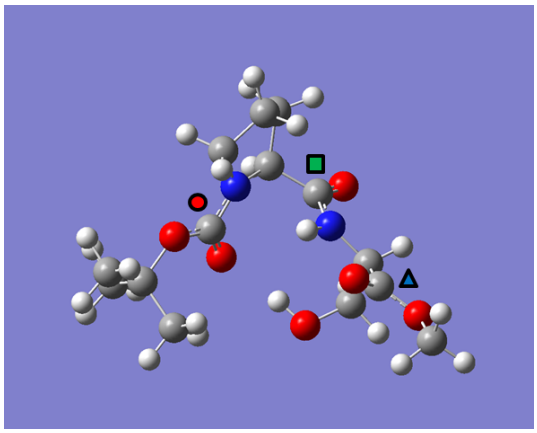
Frequencies --	1688.1055			1710.7314			1771.0112		
Red. masses --	10.0755			9.6671			10.9113		
Frc consts --	16.9167			16.6689			20.1637		
IR Inten --	618.9953			553.2475			298.7386		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	0.01	0.11	-0.10	0.01	0.01	-0.02	0.00	0.00	0.00
2 6	-0.03	0.01	0.03	0.04	-0.02	-0.03	-0.01	0.00	0.01
3 6	0.01	0.00	-0.01	-0.01	0.01	-0.01	0.00	0.00	0.00
4 6	0.00	0.00	0.01	0.00	-0.01	0.00	0.00	0.00	0.00
5 6	-0.01	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
6 6	-0.22	-0.31	0.64	0.00	-0.03	0.04	0.00	0.00	0.01
7 8	0.14	0.14	-0.36	0.01	0.01	-0.02	0.00	0.00	0.00
8 8	0.03	0.01	-0.06	0.00	0.01	0.00	0.00	0.00	0.00
9 6	-0.01	-0.04	0.04	0.00	0.00	0.00	0.00	0.00	0.00
10 6	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
12 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

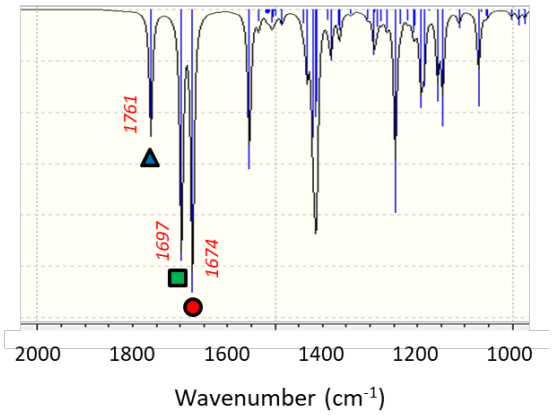
13	6	0.00	−0.05	−0.04	−0.34	0.37	0.50	0.05	−0.05	−0.07
14	8	−0.01	0.01	0.01	0.22	−0.21	−0.29	−0.03	0.02	0.04
15	7	0.02	0.04	0.01	0.04	−0.05	−0.06	−0.01	0.01	0.02
16	1	−0.12	−0.15	0.01	−0.25	−0.28	−0.14	0.13	0.12	0.07
17	6	0.00	−0.01	0.00	−0.03	−0.01	0.01	0.01	−0.04	−0.05
18	6	0.01	−0.01	0.00	0.01	0.00	0.01	−0.01	0.01	−0.01
19	1	0.03	0.02	−0.02	0.02	0.08	−0.01	−0.06	−0.08	−0.15
20	6	0.01	0.00	0.00	−0.05	0.02	0.08	−0.41	0.15	0.62
21	8	0.00	0.00	0.00	0.04	−0.01	−0.05	0.26	−0.09	−0.39
22	8	0.00	0.00	0.00	0.01	0.01	0.00	0.04	0.00	−0.04
23	6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.03
24	8	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	1	0.00	−0.09	−0.06	0.03	−0.04	0.03	0.00	0.01	0.00
26	1	0.12	−0.08	0.00	−0.25	−0.01	0.12	0.04	0.00	−0.02
27	1	−0.02	−0.05	0.03	−0.04	−0.02	0.01	0.00	0.00	0.00
28	1	0.00	0.00	0.01	0.02	−0.07	0.06	0.00	0.01	−0.01
29	1	0.00	0.00	0.00	0.00	0.02	−0.02	0.00	0.00	0.00
30	1	0.02	−0.02	0.00	−0.02	0.01	0.01	0.00	0.00	0.00
31	1	−0.07	−0.07	0.06	−0.01	−0.01	0.01	0.01	0.00	0.00
32	1	−0.01	−0.04	0.18	0.00	0.00	0.02	0.00	0.00	−0.01
33	1	0.02	0.01	−0.02	0.00	0.00	0.00	0.00	0.00	0.00
34	1	0.01	0.00	−0.03	0.00	0.00	0.00	0.00	0.00	0.00
35	1	−0.04	−0.01	0.06	0.00	0.00	0.00	0.00	0.00	0.00
36	1	0.05	0.00	−0.14	0.00	0.00	−0.01	0.00	0.00	0.00
37	1	0.03	−0.03	0.03	0.00	0.00	0.00	0.00	0.00	0.00
38	1	−0.10	0.09	−0.09	0.00	0.00	0.00	0.00	0.00	0.00
39	1	−0.01	−0.05	0.01	0.00	−0.01	0.00	0.01	0.00	0.00
40	1	0.00	0.16	−0.02	0.00	0.00	0.00	0.00	0.00	0.00
41	1	0.10	0.03	−0.11	0.00	0.00	0.00	0.00	0.00	0.00
42	1	−0.02	−0.01	0.00	0.03	0.06	−0.04	0.02	−0.07	0.03
43	1	−0.04	0.06	0.00	−0.04	0.02	−0.11	0.01	−0.01	0.01
44	1	0.00	0.00	0.00	0.00	−0.02	−0.02	−0.02	−0.14	−0.20
45	1	0.00	0.00	0.00	−0.02	−0.01	0.00	−0.13	−0.06	−0.06
46	1	0.00	0.00	0.00	−0.02	−0.01	0.00	−0.10	−0.12	−0.02

Table S6. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in acetonitrile for *N*-Boc-L-proline-L-serine-OMe **7**



7






```
Zero-point correction = 0.388894 (Hartree/Particle)
Thermal correction to Energy = 0.412963
Thermal correction to Enthalpy = 0.413907
Thermal correction to Gibbs Free Energy = 0.333811
Sum of electronic and zero-point Energies = -1108.517566
Sum of electronic and thermal Energies = -1108.493497
Sum of electronic and thermal Enthalpies = -1108.492553
Sum of electronic and thermal Free Energies= -1108.572650
```

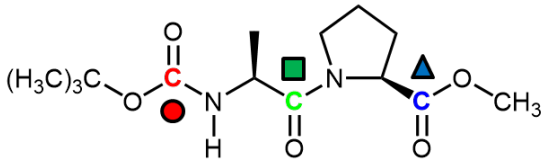
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.272506	1.329984	-0.252399
2	6	0	0.508607	2.310048	0.535349
3	6	0	0.606150	3.607121	-0.307498
4	6	0	0.881851	3.110427	-1.736897
5	6	0	1.782719	1.889531	-1.522607
6	6	0	1.712719	0.175647	0.323663
7	8	0	1.286264	-0.236358	1.411520
8	8	0	2.627688	-0.438064	-0.442575
9	6	0	3.234840	-1.747814	-0.083409
10	6	0	4.179999	-1.998596	-1.260887
11	6	0	4.018979	-1.616750	1.224960
12	6	0	2.152966	-2.828753	-0.017917
13	6	0	-0.936025	1.890946	0.846768

14	8	0	-1.564844	2.475363	1.738229
15	7	0	-1.447496	0.872296	0.121611
16	1	0	-0.860796	0.433143	-0.579282
17	6	0	-2.648882	0.150474	0.505668
18	6	0	-2.395050	-0.693828	1.784699
19	1	0	-3.456594	0.858025	0.721181
20	6	0	-3.067756	-0.729043	-0.665861
21	8	0	-2.380772	-0.934585	-1.651402
22	8	0	-4.274602	-1.263331	-0.460032
23	6	0	-4.775130	-2.162833	-1.479159
24	8	0	-1.304182	-1.590193	1.631615
25	1	0	-0.466243	-1.081764	1.601751
26	1	0	0.971351	2.444484	1.518104
27	1	0	-0.296964	4.217080	-0.223376
28	1	0	1.449313	4.204551	0.055323
29	1	0	-0.051019	2.809370	-2.227751
30	1	0	1.361380	3.869912	-2.360745
31	1	0	1.708807	1.148086	-2.321004
32	1	0	2.836134	2.177384	-1.413553
33	1	0	3.623089	-2.052227	-2.202506
34	1	0	4.924141	-1.198823	-1.339618
35	1	0	4.706303	-2.947797	-1.115729
36	1	0	4.570503	-2.546102	1.406997
37	1	0	4.745646	-0.799259	1.157535
38	1	0	3.356521	-1.434243	2.073428
39	1	0	1.563376	-2.840317	-0.941370
40	1	0	1.482332	-2.679965	0.830470
41	1	0	2.632608	-3.808136	0.089906
42	1	0	-2.226240	-0.001701	2.617639
43	1	0	-3.280107	-1.295441	2.005077
44	1	0	-5.750160	-2.486797	-1.118396
45	1	0	-4.100249	-3.014266	-1.589178
46	1	0	-4.870534	-1.633278	-2.429447

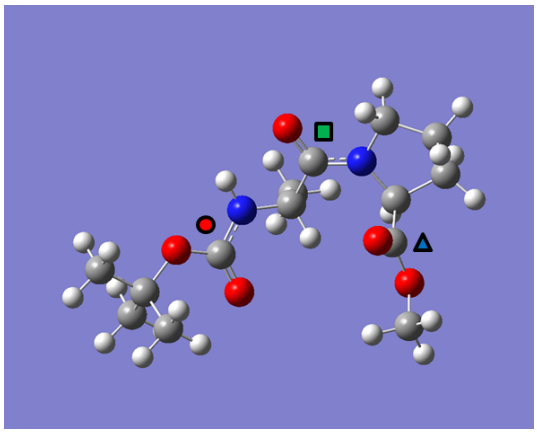
Frequencies --	1673.7049			1696.8674			1761.3669		
Red. masses --	9.7713			9.2867			10.8457		
Frc consts --	16.1272			15.7546			19.8247		
IR Inten --	769.5763			693.4302			353.9204		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	0.01	0.11	-0.10	0.00	0.01	-0.02	0.00	0.00	0.00
2 6	-0.03	0.01	0.03	0.05	-0.02	-0.04	-0.01	0.00	0.01
3 6	0.01	0.00	-0.01	-0.01	0.01	-0.01	0.00	0.00	0.00
4 6	0.00	0.00	0.01	0.00	-0.01	0.00	0.00	0.00	0.00
5 6	-0.01	0.02	-0.02	0.00	0.00	0.00	0.00	0.00	0.00
6 6	-0.21	-0.31	0.63	0.00	-0.03	0.03	0.00	0.00	0.00
7 8	0.13	0.14	-0.35	0.00	0.01	-0.02	0.00	0.00	0.00
8 8	0.03	0.01	-0.06	0.00	0.01	0.00	0.00	0.00	0.00
9 6	-0.01	-0.04	0.04	0.00	0.00	0.00	0.00	0.00	0.00
10 6	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
12 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

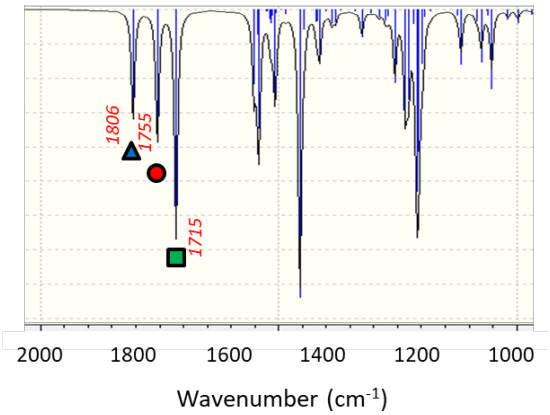
13	6	−0.01	−0.05	−0.04	−0.33	0.35	0.51	0.06	−0.05	−0.08
14	8	−0.01	0.01	0.01	0.21	−0.19	−0.29	−0.03	0.03	0.04
15	7	0.02	0.04	0.01	0.04	−0.04	−0.06	−0.01	0.01	0.02
16	1	−0.13	−0.16	0.00	−0.27	−0.29	−0.14	0.13	0.12	0.07
17	6	0.00	−0.01	−0.01	−0.03	−0.02	0.01	0.01	−0.04	−0.05
18	6	0.00	−0.01	0.00	0.01	0.00	0.01	−0.01	0.01	−0.01
19	1	0.03	0.02	−0.02	0.03	0.08	−0.02	−0.07	−0.08	−0.15
20	6	0.01	0.00	0.00	−0.06	0.02	0.08	−0.40	0.15	0.62
21	8	0.00	0.00	0.00	0.04	−0.01	−0.06	0.26	−0.09	−0.39
22	8	0.00	0.00	0.00	0.01	0.01	0.00	0.04	0.00	−0.04
23	6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.03
24	8	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	1	0.00	−0.09	−0.06	0.03	−0.05	0.03	0.00	0.01	−0.01
26	1	0.13	−0.07	−0.01	−0.26	−0.01	0.13	0.05	0.00	−0.02
27	1	−0.02	−0.05	0.04	−0.04	−0.02	0.01	0.01	0.00	0.00
28	1	0.00	−0.01	0.01	0.03	−0.07	0.07	0.00	0.01	−0.01
29	1	0.00	0.01	−0.01	0.00	0.02	−0.02	0.00	0.00	0.00
30	1	0.02	−0.02	0.00	−0.01	0.01	0.01	0.00	0.00	0.00
31	1	−0.08	−0.08	0.07	−0.02	−0.01	0.01	0.00	0.00	0.00
32	1	−0.01	−0.04	0.21	0.00	0.00	0.03	0.00	0.00	−0.01
33	1	0.01	0.02	−0.02	0.00	0.00	0.00	0.00	0.00	0.00
34	1	0.00	0.01	−0.03	0.00	0.00	0.00	0.00	0.00	0.00
35	1	−0.04	−0.01	0.07	0.00	0.00	0.01	0.00	0.00	0.00
36	1	0.05	0.00	−0.14	0.00	0.00	−0.01	0.00	0.00	0.00
37	1	0.03	−0.02	0.03	0.00	0.00	0.00	0.00	0.00	0.00
38	1	−0.10	0.09	−0.09	0.00	0.00	0.00	0.00	0.00	0.00
39	1	−0.01	−0.05	0.01	0.00	0.00	0.00	0.00	0.00	0.00
40	1	−0.01	0.16	−0.02	0.00	0.00	0.00	0.00	0.00	0.00
41	1	0.10	0.04	−0.12	0.00	0.00	0.00	0.00	0.00	0.00
42	1	−0.02	−0.01	0.00	0.03	0.05	−0.04	0.02	−0.07	0.03
43	1	−0.04	0.07	0.01	−0.05	0.03	−0.11	0.01	−0.01	0.02
44	1	0.00	0.00	0.00	0.00	−0.02	−0.03	−0.03	−0.14	−0.20
45	1	0.00	0.00	0.00	−0.02	−0.01	−0.01	−0.13	−0.06	−0.07
46	1	0.00	0.00	0.00	−0.02	−0.02	0.00	−0.09	−0.13	−0.02

Table S7. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in the gas phase for *N*-Boc-L-alanine-L-proline-OMe **9**



9






```
Zero-point correction = 0.383927 (Hartree/Particle)
Thermal correction to Energy = 0.407410
Thermal correction to Enthalpy = 0.408354
Thermal correction to Gibbs Free Energy = 0.328750
Sum of electronic and zero-point Energies = -1033.282259
Sum of electronic and thermal Energies = -1033.258776
Sum of electronic and thermal Enthalpies = -1033.257832
Sum of electronic and thermal Free Energies = -1033.337436
```

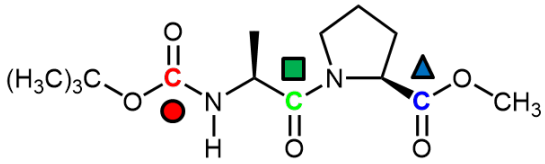
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.428189	-1.096411	-0.132740
2	6	0	2.913168	0.125628	0.505031
3	6	0	4.451715	-0.013191	0.381001
4	6	0	4.634697	-0.774115	-0.943421
5	6	0	3.449826	-1.751052	-0.973930
6	6	0	-2.161772	-0.201131	0.368830
7	8	0	-2.071994	0.837551	1.014689
8	8	0	-3.246265	-0.610333	-0.336890
9	6	0	-4.481183	0.190918	-0.388409
10	6	0	-5.390941	-0.661691	-1.278119
11	6	0	-5.078346	0.334205	1.016327
12	6	0	-4.204051	1.548994	-1.043722
13	6	0	2.423558	1.391740	-0.211278
14	8	0	2.100881	1.457880	-1.377689

15	7	0	-1.169891	-1.126786	0.265159
16	1	0	-1.279485	-1.922909	-0.352891
17	6	0	0.144938	-0.911839	0.840029
18	6	0	0.247496	-1.493307	2.266362
19	1	0	0.305218	0.168663	0.885101
20	6	0	1.164398	-1.597408	-0.085211
21	8	0	0.845181	-2.606695	-0.718304
22	8	0	2.435419	2.439840	0.635349
23	6	0	2.019519	3.708255	0.084876
24	1	0	2.609001	0.185935	1.552828
25	1	0	4.960780	0.954654	0.408789
26	1	0	4.817187	-0.609505	1.225297
27	1	0	4.574008	-0.081235	-1.789340
28	1	0	5.597950	-1.290358	-0.998533
29	1	0	3.052004	-1.921010	-1.977673
30	1	0	3.700754	-2.729270	-0.545027
31	1	0	-6.362966	-0.170895	-1.400153
32	1	0	-4.944408	-0.799872	-2.268721
33	1	0	-5.553705	-1.649058	-0.832576
34	1	0	-5.216203	-0.651922	1.474786
35	1	0	-4.436874	0.937848	1.661505
36	1	0	-6.060975	0.816442	0.948026
37	1	0	-3.730266	1.410735	-2.022396
38	1	0	-5.151230	2.080282	-1.196848
39	1	0	-3.553704	2.165349	-0.419886
40	1	0	1.237133	-1.318053	2.705622
41	1	0	-0.502444	-1.016648	2.904854
42	1	0	0.063720	-2.572729	2.246794
43	1	0	2.676288	3.996164	-0.740071
44	1	0	0.989308	3.640322	-0.272639
45	1	0	2.096900	4.417473	0.908779

Frequencies --	1715.4737			1754.6591			1805.8503		
Red. masses --	10.6411			10.2399			11.0093		
Frc consts --	18.4504			18.5752			21.1531		
IR Inten --	384.2178			227.5007			190.6316		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	-0.06	-0.08	-0.03	0.00	0.01	0.01	0.00	-0.01	0.00
2 6	-0.02	-0.01	0.00	0.00	0.00	0.00	-0.01	0.02	-0.05
3 6	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00
4 6	0.00	-0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.01
5 6	-0.01	0.02	0.02	0.00	0.00	0.00	0.00	0.00	0.00
6 6	-0.02	0.09	0.05	-0.03	0.65	0.37	0.00	0.00	0.00
7 8	0.00	-0.05	-0.03	-0.02	-0.36	-0.22	0.00	0.00	0.00
8 8	0.00	-0.01	-0.01	-0.01	-0.05	-0.04	0.00	0.00	0.00
9 6	0.00	0.01	0.00	-0.01	0.04	0.02	0.00	0.00	0.00
10 6	0.00	0.00	0.00	0.01	-0.01	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
12 6	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
13 6	0.00	0.00	-0.03	0.00	0.01	0.00	0.21	-0.07	0.73

14	8	0.00	0.00	0.02	0.00	0.00	0.00	−0.13	0.03	−0.47
15	7	0.03	−0.01	0.01	0.05	−0.10	−0.04	0.00	0.00	0.00
16	1	−0.21	0.04	−0.02	0.27	−0.19	0.04	−0.01	0.00	0.00
17	6	−0.01	−0.03	−0.01	0.02	0.02	0.02	0.00	0.00	0.00
18	6	0.00	0.00	−0.01	−0.01	−0.01	0.00	0.00	0.00	0.00
19	1	0.24	−0.05	−0.20	−0.14	0.06	0.00	0.03	−0.01	0.02
20	6	0.23	0.61	0.37	−0.03	−0.08	−0.05	0.02	0.02	0.02
21	8	−0.11	−0.37	−0.23	0.01	0.04	0.03	−0.01	−0.02	−0.01
22	8	0.00	0.01	0.00	0.00	0.00	0.00	−0.01	−0.01	−0.05
23	6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	−0.02	0.02
24	1	0.06	0.07	0.01	−0.01	−0.01	0.00	−0.12	0.22	−0.07
25	1	0.01	0.00	−0.01	0.00	0.00	0.00	0.00	−0.01	0.02
26	1	0.00	−0.01	0.00	0.00	0.00	0.00	0.05	0.01	−0.03
27	1	−0.01	0.00	0.00	0.00	0.00	0.00	0.05	−0.02	−0.01
28	1	0.03	0.04	0.01	−0.01	−0.01	0.00	0.01	0.01	−0.06
29	1	0.11	0.00	−0.01	−0.02	0.00	0.00	0.01	−0.04	0.00
30	1	0.09	0.02	−0.08	−0.01	0.00	0.01	0.01	−0.01	−0.03
31	1	0.00	0.00	0.00	0.02	0.04	0.03	0.00	0.00	0.00
32	1	0.00	0.00	0.00	−0.01	−0.01	−0.01	0.00	0.00	0.00
33	1	0.00	0.00	0.00	−0.01	−0.01	−0.01	0.00	0.00	0.00
34	1	−0.01	0.00	0.00	−0.03	0.01	0.02	0.00	0.00	0.00
35	1	0.02	−0.01	−0.01	0.12	−0.05	−0.06	0.00	0.00	0.00
36	1	−0.01	−0.01	−0.01	−0.03	−0.08	−0.09	0.00	0.00	0.00
37	1	0.00	0.01	0.00	−0.02	0.03	−0.01	0.00	0.00	0.00
38	1	−0.01	−0.01	−0.01	−0.05	−0.11	−0.05	0.00	0.00	0.00
39	1	0.01	−0.02	0.01	0.08	−0.12	0.05	0.00	0.00	0.00
40	1	0.01	−0.01	−0.01	0.02	0.00	−0.06	0.00	0.00	0.00
41	1	−0.01	−0.07	0.02	−0.01	0.05	−0.04	0.00	0.00	0.00
42	1	−0.03	0.01	0.09	0.04	−0.01	0.00	0.00	0.00	0.00
43	1	0.00	0.00	0.00	0.01	−0.01	0.01	−0.04	0.13	0.05
44	1	0.00	0.00	0.00	−0.01	−0.01	0.02	0.01	0.14	0.04
45	1	0.00	0.00	0.00	0.00	0.00	0.00	−0.07	0.16	−0.13

Table S8. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in chloroform for *N*-Boc-L-alanine-L-proline-OMe **9**



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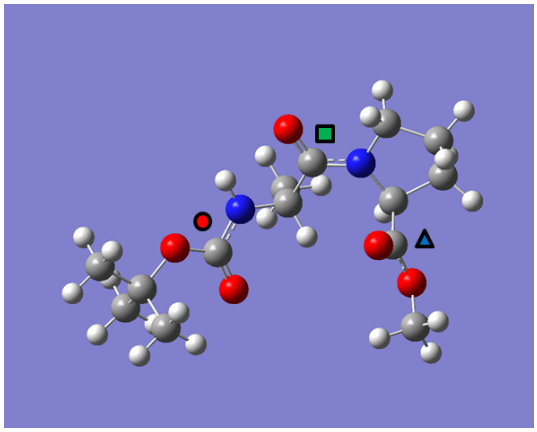
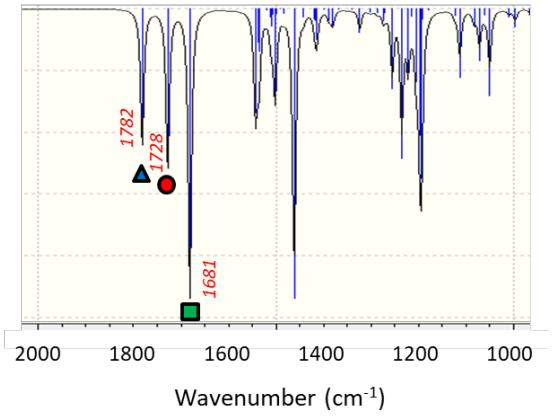





```
Zero-point correction = 0.383450 (Hartree/Particle)
Thermal correction to Energy = 0.406957
Thermal correction to Enthalpy = 0.407901
Thermal correction to Gibbs Free Energy = 0.328493
Sum of electronic and zero-point Energies = -1033.294669
Sum of electronic and thermal Energies = -1033.271162
Sum of electronic and thermal Enthalpies = -1033.270218
Sum of electronic and thermal Free Energies = -1033.349626
```

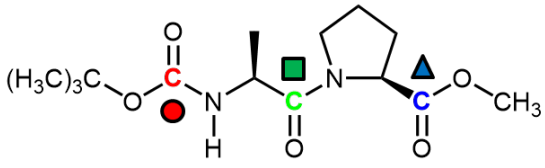
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.398096	-1.111179	-0.153795
2	6	0	2.909708	0.090564	0.507123
3	6	0	4.445814	-0.100796	0.425556
4	6	0	4.640004	-0.860171	-0.896979
5	6	0	3.427031	-1.798538	-0.964262
6	6	0	-2.192336	-0.161909	0.360403
7	8	0	-2.102339	0.868609	1.024736
8	8	0	-3.282148	-0.566065	-0.336232
9	6	0	-4.531099	0.223336	-0.371206
10	6	0	-5.435296	-0.630868	-1.264630
11	6	0	-5.121553	0.341830	1.037776
12	6	0	-4.273568	1.590047	-1.014469
13	6	0	2.477650	1.375849	-0.211461
14	8	0	2.078752	1.441316	-1.357302

15	7	0	-1.194182	-1.073090	0.222972
16	1	0	-1.326990	-1.880824	-0.374596
17	6	0	0.119053	-0.895946	0.818242
18	6	0	0.194114	-1.499829	2.236876
19	1	0	0.306155	0.178717	0.875802
20	6	0	1.133987	-1.593360	-0.103309
21	8	0	0.796981	-2.605164	-0.734258
22	8	0	2.630216	2.434459	0.599741
23	6	0	2.302921	3.730477	0.045269
24	1	0	2.581650	0.152867	1.547147
25	1	0	4.985538	0.848570	0.472592
26	1	0	4.764563	-0.713574	1.276004
27	1	0	4.627154	-0.163246	-1.741813
28	1	0	5.585519	-1.408824	-0.928040
29	1	0	3.057652	-1.957554	-1.980491
30	1	0	3.635479	-2.780872	-0.523601
31	1	0	-6.411993	-0.147731	-1.376317
32	1	0	-4.993458	-0.753486	-2.259390
33	1	0	-5.587791	-1.623628	-0.827351
34	1	0	-5.239109	-0.650411	1.488243
35	1	0	-4.490828	0.953072	1.686405
36	1	0	-6.112784	0.806165	0.977017
37	1	0	-3.802763	1.468206	-1.996611
38	1	0	-5.228590	2.109093	-1.157672
39	1	0	-3.630243	2.211179	-0.388131
40	1	0	1.183027	-1.353302	2.686330
41	1	0	-0.549685	-1.016117	2.877170
42	1	0	-0.014778	-2.574216	2.201074
43	1	0	2.944448	3.944116	-0.812746
44	1	0	1.254316	3.751950	-0.259287
45	1	0	2.485837	4.440362	0.850965

Frequencies --	1681.2657			1727.9523			1781.5804		
Red. masses --	10.3575			10.3106			11.0547		
Frc consts --	17.2496			18.1383			20.6731		
IR Inten --	680.5317			389.1041			331.6460		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	-0.08	-0.08	-0.03	0.00	0.01	0.01	-0.01	-0.01	0.00
2 6	-0.02	-0.01	0.00	0.00	0.00	0.00	-0.01	0.03	-0.05
3 6	0.00	0.01	0.00	0.00	0.00	0.00	-0.01	0.00	0.00
4 6	0.00	-0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
5 6	-0.01	0.02	0.02	0.00	0.00	0.00	0.00	0.00	0.00
6 6	-0.02	0.11	0.06	-0.03	0.65	0.38	0.00	-0.01	0.00
7 8	0.00	-0.06	-0.04	-0.02	-0.35	-0.22	0.00	0.00	0.00
8 8	0.00	-0.01	-0.01	-0.01	-0.05	-0.03	0.00	0.00	0.00
9 6	0.00	0.01	0.00	-0.01	0.04	0.02	0.00	0.00	0.00
10 6	0.00	0.00	0.00	0.01	-0.01	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
12 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13 6	-0.01	0.00	-0.03	0.00	0.00	0.01	0.25	-0.07	0.72

14	8	0.01	0.00	0.02	0.00	0.00	−0.01	−0.16	0.03	−0.46
15	7	0.02	−0.02	0.01	0.05	−0.10	−0.04	0.00	0.00	0.00
16	1	−0.18	0.03	−0.02	0.29	−0.18	0.02	−0.01	0.00	0.00
17	6	−0.02	−0.04	−0.01	0.02	0.02	0.02	0.00	0.00	0.00
18	6	0.00	0.00	−0.01	−0.01	−0.01	0.00	0.00	0.00	0.00
19	1	0.27	−0.07	−0.21	−0.13	0.07	0.01	0.03	−0.01	0.02
20	6	0.25	0.60	0.35	−0.04	−0.10	−0.06	0.02	0.02	0.01
21	8	−0.12	−0.35	−0.22	0.02	0.05	0.03	−0.01	−0.02	−0.01
22	8	0.00	0.01	0.00	0.00	0.00	0.00	−0.01	−0.01	−0.05
23	6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	−0.03	0.02
24	1	0.06	0.09	0.01	−0.01	−0.02	0.00	−0.11	0.21	−0.07
25	1	0.03	−0.01	−0.01	−0.01	0.00	0.00	0.00	−0.01	0.02
26	1	0.00	−0.01	0.00	0.00	0.00	0.00	0.05	0.01	−0.03
27	1	0.01	0.00	0.00	0.00	0.00	0.00	0.03	−0.01	0.00
28	1	0.04	0.05	0.00	−0.01	−0.01	0.00	0.00	0.01	−0.05
29	1	0.12	−0.04	0.00	−0.02	0.01	0.00	0.01	−0.03	0.00
30	1	0.09	0.00	−0.12	−0.01	0.00	0.02	0.01	−0.01	−0.02
31	1	0.00	0.01	0.00	0.02	0.05	0.04	0.00	0.00	0.00
32	1	0.00	0.00	0.00	−0.01	−0.02	−0.01	0.00	0.00	0.00
33	1	0.00	0.00	0.00	0.00	−0.01	−0.01	0.00	0.00	0.00
34	1	−0.01	0.00	0.00	−0.03	0.01	0.01	0.00	0.00	0.00
35	1	0.02	−0.01	−0.01	0.11	−0.04	−0.06	0.00	0.00	0.00
36	1	−0.01	−0.02	−0.01	−0.03	−0.08	−0.09	0.00	0.00	0.00
37	1	−0.01	0.01	0.00	−0.02	0.03	−0.01	0.00	0.00	0.00
38	1	−0.01	−0.02	−0.01	−0.05	−0.10	−0.05	0.00	0.00	0.00
39	1	0.02	−0.02	0.01	0.07	−0.11	0.05	0.00	0.00	0.00
40	1	0.00	−0.01	−0.01	0.02	0.01	−0.07	0.00	0.00	0.00
41	1	−0.01	−0.07	0.03	−0.01	0.04	−0.03	0.00	0.00	0.00
42	1	−0.02	0.01	0.08	0.03	−0.02	0.00	0.00	0.00	0.00
43	1	0.00	0.00	0.00	0.01	0.00	0.00	−0.04	0.14	0.04
44	1	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.15	0.02
45	1	0.00	0.00	0.00	0.00	0.00	0.00	−0.07	0.17	−0.14

Table S9. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in acetonitrile for *N*-Boc-L-alanine-L-proline-OMe **9**



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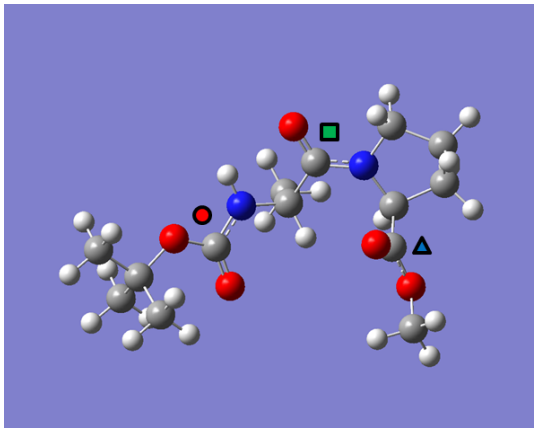
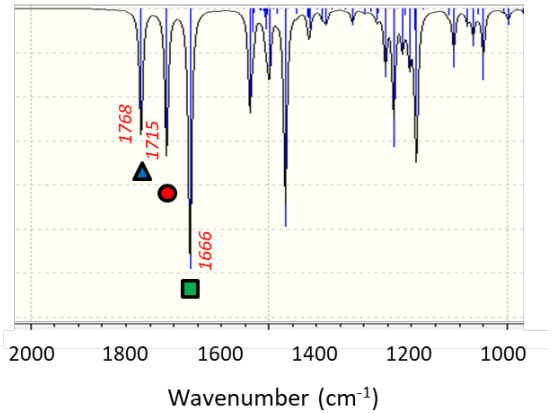





```
Zero-point correction = 0.383113 (Hartree/Particle)
Thermal correction to Energy = 0.406675
Thermal correction to Enthalpy = 0.407619
Thermal correction to Gibbs Free Energy = 0.328105
Sum of electronic and zero-point Energies = -1033.300055
Sum of electronic and thermal Energies = -1033.276492
Sum of electronic and thermal Enthalpies = -1033.275548
Sum of electronic and thermal Free Energies = -1033.355062
```

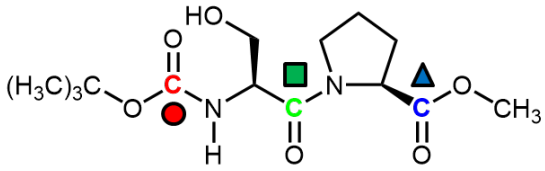
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.386655	-1.115566	-0.164023
2	6	0	2.907243	0.076446	0.510024
3	6	0	4.441664	-0.131822	0.440916
4	6	0	4.638669	-0.883188	-0.885152
5	6	0	3.418625	-1.810437	-0.966244
6	6	0	-2.199832	-0.144656	0.352798
7	8	0	-2.103902	0.886952	1.016890
8	8	0	-3.295255	-0.548061	-0.333403
9	6	0	-4.548609	0.239604	-0.361361
10	6	0	-5.455594	-0.618713	-1.247642
11	6	0	-5.129746	0.357398	1.051096
12	6	0	-4.298146	1.605099	-1.009112
13	6	0	2.489909	1.369807	-0.202620
14	8	0	2.031730	1.437748	-1.327735

15	7	0	-1.201322	-1.052383	0.201650
16	1	0	-1.352706	-1.874118	-0.371660
17	6	0	0.109319	-0.899472	0.811457
18	6	0	0.167995	-1.527592	2.220106
19	1	0	0.307285	0.171685	0.886220
20	6	0	1.123751	-1.593150	-0.113336
21	8	0	0.780778	-2.602300	-0.750388
22	8	0	2.721600	2.428598	0.584879
23	6	0	2.423499	3.733725	0.032815
24	1	0	2.571944	0.134807	1.547873
25	1	0	4.991004	0.810872	0.499314
26	1	0	4.744460	-0.755120	1.289044
27	1	0	4.638556	-0.180725	-1.725723
28	1	0	5.578722	-1.440742	-0.913224
29	1	0	3.058840	-1.964980	-1.986692
30	1	0	3.614819	-2.794034	-0.523355
31	1	0	-6.433813	-0.137939	-1.353712
32	1	0	-5.020278	-0.741170	-2.245376
33	1	0	-5.603599	-1.610792	-0.807281
34	1	0	-5.241704	-0.634581	1.503399
35	1	0	-4.497782	0.971767	1.695595
36	1	0	-6.122434	0.818725	0.995480
37	1	0	-3.833571	1.482556	-1.994147
38	1	0	-5.255596	2.120484	-1.147456
39	1	0	-3.653497	2.230725	-0.388486
40	1	0	1.155165	-1.398700	2.677847
41	1	0	-0.574892	-1.047420	2.864202
42	1	0	-0.051914	-2.598986	2.165459
43	1	0	3.029306	3.909848	-0.858739
44	1	0	1.362154	3.799901	-0.215851
45	1	0	2.680110	4.441777	0.819479

Frequencies --	1665.4993			1714.6954			1768.1388		
Red. masses --	10.1152			10.3079			11.0834		
Frc consts --	16.5315			17.8564			20.4153		
IR Inten --	879.5226			491.5088			437.2905		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	-0.08	-0.08	-0.03	0.01	0.02	0.01	-0.01	-0.01	0.00
2 6	-0.02	-0.02	0.00	0.01	0.00	0.00	-0.01	0.03	-0.05
3 6	0.00	0.01	0.00	0.00	0.00	0.00	-0.01	0.00	0.00
4 6	0.00	-0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
5 6	-0.01	0.02	0.02	0.00	-0.01	-0.01	0.00	0.00	0.00
6 6	-0.02	0.12	0.07	-0.03	0.64	0.38	0.00	-0.01	-0.01
7 8	0.00	-0.07	-0.05	-0.02	-0.35	-0.22	0.00	0.01	0.00
8 8	0.00	-0.01	-0.01	-0.01	-0.05	-0.03	0.00	0.00	0.00
9 6	0.00	0.01	0.00	-0.01	0.04	0.02	0.00	0.00	0.00
10 6	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13 6	-0.01	0.00	-0.03	0.01	0.00	0.02	0.29	-0.08	0.71

14	8	0.01	0.00	0.02	0.00	0.00	−0.01	−0.18	0.04	−0.45
15	7	0.02	−0.02	0.00	0.05	−0.10	−0.04	0.00	0.00	0.00
16	1	−0.16	0.03	−0.02	0.29	−0.18	0.01	−0.01	0.00	0.00
17	6	−0.02	−0.03	−0.01	0.02	0.02	0.02	0.00	0.00	0.00
18	6	0.00	0.00	−0.01	−0.01	−0.01	0.00	0.00	0.00	0.00
19	1	0.28	−0.07	−0.21	−0.13	0.07	0.01	0.03	−0.01	0.01
20	6	0.26	0.59	0.35	−0.05	−0.11	−0.07	0.02	0.02	0.01
21	8	−0.11	−0.34	−0.22	0.02	0.06	0.04	−0.01	−0.02	−0.01
22	8	0.00	0.01	0.00	0.00	0.00	0.00	−0.02	−0.01	−0.05
23	6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	−0.03	0.02
24	1	0.07	0.10	0.01	−0.01	−0.02	0.00	−0.11	0.20	−0.07
25	1	0.03	−0.01	0.00	−0.01	0.00	0.00	0.00	−0.01	0.01
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.00	−0.03
27	1	0.01	0.00	0.01	0.00	0.00	0.00	0.03	−0.01	0.00
28	1	0.04	0.06	0.00	−0.01	−0.01	0.00	0.00	0.00	−0.04
29	1	0.12	−0.06	0.01	−0.02	0.01	0.00	0.01	−0.02	0.00
30	1	0.09	−0.01	−0.14	−0.02	0.00	0.03	0.01	−0.01	−0.02
31	1	0.00	0.01	0.01	0.02	0.05	0.04	0.00	0.00	0.00
32	1	0.00	0.00	0.00	0.00	−0.02	−0.01	0.00	0.00	0.00
33	1	0.00	0.00	0.00	0.00	−0.02	−0.01	0.00	0.00	0.00
34	1	−0.01	0.00	0.00	−0.03	0.01	0.01	0.00	0.00	0.00
35	1	0.03	−0.01	−0.01	0.11	−0.04	−0.06	0.00	0.00	0.00
36	1	−0.01	−0.02	−0.02	−0.03	−0.07	−0.09	0.00	0.00	0.00
37	1	−0.01	0.01	0.00	−0.02	0.03	−0.01	0.00	0.00	0.00
38	1	−0.01	−0.02	−0.02	−0.05	−0.10	−0.05	0.00	0.00	0.00
39	1	0.02	−0.03	0.01	0.07	−0.10	0.05	0.00	0.00	0.00
40	1	0.00	−0.01	−0.01	0.03	0.01	−0.07	0.00	0.00	0.00
41	1	−0.01	−0.07	0.03	−0.02	0.03	−0.02	0.00	0.00	0.00
42	1	−0.02	0.01	0.08	0.02	−0.02	0.01	0.00	0.00	0.00
43	1	−0.01	0.00	0.00	0.00	0.00	0.00	−0.04	0.15	0.04
44	1	0.00	0.00	−0.01	0.00	0.00	0.00	0.04	0.15	0.01
45	1	0.00	0.00	0.00	0.00	0.00	0.00	−0.07	0.18	−0.14

Table S10. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in the gas phase for *N*-Boc-L-serine-L-proline-OMe **10**



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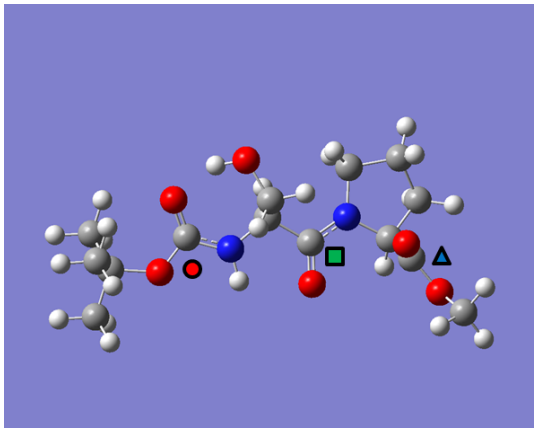
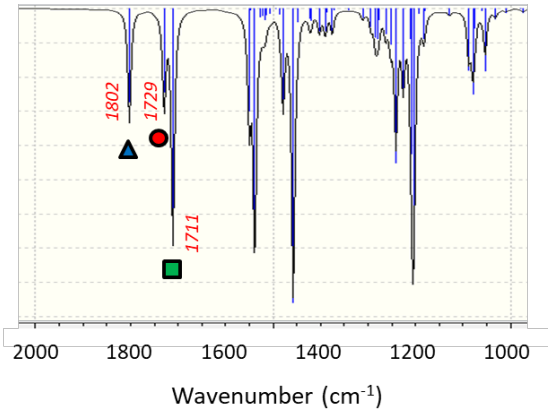





```
Zero-point correction = 0.389722 (Hartree/Particle)
Thermal correction to Energy = 0.413794
Thermal correction to Enthalpy = 0.414738
Thermal correction to Gibbs Free Energy = 0.334033
Sum of electronic and zero-point Energies = -1108.494680
Sum of electronic and thermal Energies = -1108.470608
Sum of electronic and thermal Enthalpies = -1108.469663
Sum of electronic and thermal Free Energies = -1108.550368
```

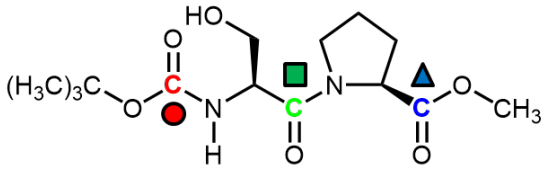
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.061296	0.554991	-0.627909
2	6	0	3.298797	-0.143380	-0.976054
3	6	0	4.198516	0.987202	-1.530189
4	6	0	3.716625	2.234897	-0.770721
5	6	0	2.199516	2.025554	-0.657867
6	6	0	-2.725791	0.158632	-0.020824
7	8	0	-3.056368	1.272088	0.395853
8	8	0	-3.575818	-0.824508	-0.385097
9	6	0	-5.040746	-0.678897	-0.256696
10	6	0	-5.424302	-0.463704	1.211405
11	6	0	-5.536929	0.452795	-1.163004
12	6	0	-5.548216	-2.035055	-0.754934
13	6	0	3.922403	-0.803159	0.257891

14	8	0	3.779441	-0.424353	1.401199
15	7	0	-1.441247	-0.240751	-0.184183
16	1	0	-1.234195	-1.205310	-0.423371
17	6	0	-0.299218	0.617598	0.087001
18	6	0	-0.191753	1.055791	1.582650
19	1	0	-0.388829	1.534986	-0.507360
20	8	0	-0.853186	2.280322	1.831527
21	6	0	0.945896	-0.165580	-0.346020
22	8	0	0.930989	-1.399060	-0.411901
23	8	0	4.704497	-1.836638	-0.105672
24	6	0	5.381160	-2.526756	0.964531
25	1	0	3.103536	-0.923645	-1.715319
26	1	0	5.263407	0.778266	-1.393739
27	1	0	4.013898	1.092486	-2.605804
28	1	0	4.162465	2.266087	0.229022
29	1	0	3.965328	3.168433	-1.284503
30	1	0	1.779935	2.486583	0.239225
31	1	0	1.673464	2.434904	-1.531769
32	1	0	-6.515741	-0.499768	1.309646
33	1	0	-5.002041	-1.257981	1.837661
34	1	0	-5.074939	0.502455	1.581015
35	1	0	-6.633294	0.469332	-1.156438
36	1	0	-5.170830	1.423968	-0.824384
37	1	0	-5.206555	0.288246	-2.195070
38	1	0	-5.232311	-2.211167	-1.788773
39	1	0	-5.159589	-2.847843	-0.132062
40	1	0	-6.642792	-2.061014	-0.716831
41	1	0	-0.589763	0.237991	2.201560
42	1	0	0.853902	1.205611	1.866528
43	1	0	-1.764032	2.184892	1.484303
44	1	0	5.942565	-3.326513	0.481392
45	1	0	6.053031	-1.844270	1.491883
46	1	0	4.650872	-2.934837	1.667540

Frequencies --	1710.6395			1729.1347			1802.3532		
Red. masses --	10.6825			8.8962			10.9353		
Frc consts --	18.4179			15.6716			20.9296		
IR Inten --	394.0436			165.0304			191.8545		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	-0.05	-0.12	0.01	0.01	0.04	0.00	0.01	0.00	0.00
2 6	-0.02	0.03	0.00	0.01	-0.01	0.00	-0.02	-0.01	-0.06
3 6	0.01	-0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.00
4 6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5 6	-0.02	-0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00
6 6	-0.11	0.20	0.08	-0.26	0.58	0.22	0.00	0.01	0.00
7 8	0.04	-0.12	-0.05	0.10	-0.32	-0.12	0.00	0.00	0.00
8 8	0.00	-0.02	-0.01	0.01	-0.06	-0.02	0.00	0.00	0.00
9 6	-0.01	0.01	0.01	-0.03	0.03	0.02	0.00	0.00	0.00
10 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
12 6	0.00	0.00	0.00	0.01	-0.01	0.00	0.00	0.00	0.00

13	6	0.00	0.02	0.03	0.00	−0.01	−0.01	−0.07	0.22	0.72
14	8	0.00	−0.01	−0.02	0.00	0.00	0.01	0.05	−0.14	−0.46
15	7	0.06	−0.01	0.00	0.08	−0.08	−0.03	0.00	0.00	0.00
16	1	−0.19	−0.06	−0.02	0.39	0.00	−0.04	0.01	0.00	0.00
17	6	−0.01	−0.04	0.01	0.02	0.02	0.00	0.00	0.00	0.00
18	6	0.00	−0.01	−0.01	−0.03	0.02	0.01	0.00	0.00	0.00
19	1	0.23	−0.09	−0.14	−0.19	0.03	0.01	−0.01	0.00	0.00
20	8	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
21	6	0.06	0.72	0.02	−0.02	−0.21	−0.01	0.00	−0.04	0.00
22	8	0.00	−0.42	−0.02	0.00	0.12	0.01	0.00	0.02	0.00
23	8	0.00	−0.01	0.00	0.00	0.00	0.00	0.02	−0.03	−0.04
24	6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	−0.01	0.03
25	1	0.09	0.03	−0.01	−0.03	−0.01	0.00	−0.10	0.17	−0.18
26	1	0.02	0.05	−0.02	−0.01	−0.02	0.01	0.00	0.00	0.03
27	1	−0.01	0.00	0.00	0.00	0.00	0.00	−0.05	−0.04	0.00
28	1	0.00	−0.01	0.00	0.00	0.00	0.00	−0.01	−0.05	0.02
29	1	0.01	0.00	−0.01	−0.01	0.00	0.00	−0.01	−0.03	−0.05
30	1	0.02	0.11	−0.04	−0.01	−0.03	0.01	0.02	−0.02	0.02
31	1	0.04	0.15	0.05	−0.01	−0.05	−0.02	0.00	−0.03	−0.01
32	1	0.00	−0.04	−0.02	0.00	−0.10	−0.07	0.00	0.00	0.00
33	1	−0.01	0.00	0.01	−0.03	0.00	0.02	0.00	0.00	0.00
34	1	0.05	0.00	−0.03	0.12	−0.01	−0.07	0.00	0.00	0.00
35	1	0.00	−0.04	−0.01	0.00	−0.12	−0.02	0.00	0.00	0.00
36	1	0.05	−0.02	0.01	0.13	−0.05	0.04	0.00	0.00	0.00
37	1	−0.01	0.01	0.00	−0.03	0.02	−0.01	0.00	0.00	0.00
38	1	0.00	0.00	0.00	0.00	−0.02	0.00	0.00	0.00	0.00
39	1	0.00	−0.01	0.00	0.00	−0.02	−0.01	0.00	0.00	0.00
40	1	0.00	0.01	0.01	0.00	0.05	0.02	0.00	0.00	0.00
41	1	−0.01	0.03	0.03	0.04	−0.03	−0.01	0.00	0.00	0.00
42	1	0.00	0.00	−0.02	−0.01	−0.04	−0.05	0.01	−0.02	0.00
43	1	0.03	−0.07	−0.02	0.11	−0.21	−0.07	0.00	0.01	0.00
44	1	0.00	0.00	−0.01	0.00	0.00	0.00	−0.08	0.07	−0.20
45	1	−0.01	0.00	0.01	0.00	0.00	0.00	−0.07	0.13	−0.02
46	1	0.01	0.01	0.01	0.00	0.00	0.00	−0.11	0.10	−0.01

Table S11. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in chloroform for *N*-Boc-L-serine-L-proline-OMe **10**



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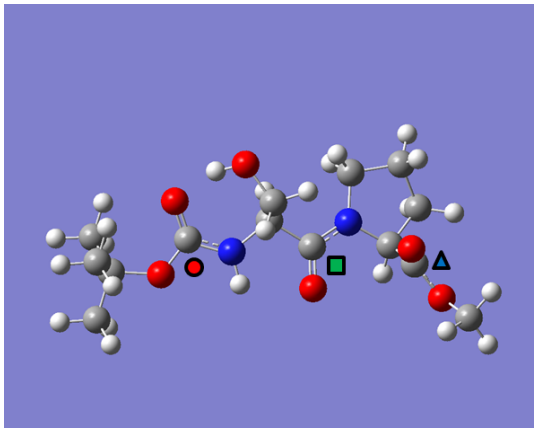

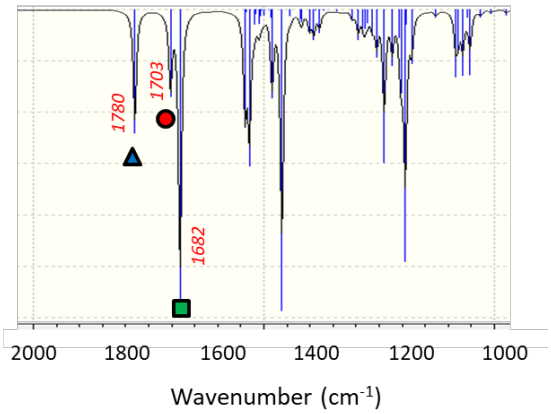


```
Zero-point correction = 0.389060 (Hartree/Particle)
Thermal correction to Energy = 0.413192
Thermal correction to Enthalpy = 0.414136
Thermal correction to Gibbs Free Energy = 0.333342
Sum of electronic and zero-point Energies = -1108.508158
Sum of electronic and thermal Energies = -1108.484026
Sum of electronic and thermal Enthalpies = -1108.483082
Sum of electronic and thermal Free Energies = -1108.563877
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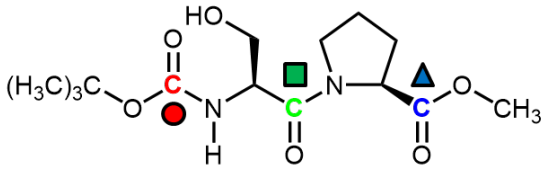
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.050107	-0.544779	-0.587138
2	6	0	-3.273946	0.166937	-0.965050
3	6	0	-4.146076	-0.938109	-1.610890
4	6	0	-3.682387	-2.223930	-0.907852
5	6	0	-2.173170	-2.013218	-0.729600
6	6	0	2.733004	-0.167295	-0.006001
7	8	0	3.086324	-1.300764	0.342266
8	8	0	3.559565	0.828916	-0.374482
9	6	0	5.036002	0.707484	-0.294149
10	6	0	5.463538	0.447442	1.153468
11	6	0	5.523374	-0.378686	-1.257664
12	6	0	5.501720	2.090646	-0.755828
13	6	0	-3.958250	0.785891	0.256359

14	8	0	-3.856715	0.383827	1.399080
15	7	0	1.441668	0.235504	-0.073868
16	1	0	1.228589	1.207624	-0.273012
17	6	0	0.301146	-0.639209	0.162550
18	6	0	0.191199	-1.117460	1.639516
19	1	0	0.395673	-1.531434	-0.467095
20	8	0	0.985632	-2.266245	1.895203
21	6	0	-0.947678	0.158181	-0.244245
22	8	0	-0.933988	1.397785	-0.232487
23	8	0	-4.736556	1.814265	-0.116274
24	6	0	-5.497631	2.462967	0.927701
25	1	0	-3.044778	0.971963	-1.666841
26	1	0	-5.216077	-0.743374	-1.499297
27	1	0	-3.923098	-0.980585	-2.682713
28	1	0	-4.164107	-2.319731	0.070973
29	1	0	-3.902685	-3.125591	-1.486089
30	1	0	-1.780731	-2.531818	0.147615
31	1	0	-1.615119	-2.350276	-1.612862
32	1	0	6.555952	0.504132	1.221821
33	1	0	5.042788	1.208615	1.820302
34	1	0	5.147257	-0.539482	1.497396
35	1	0	6.619242	-0.373146	-1.283166
36	1	0	5.187456	-1.369680	-0.946371
37	1	0	5.159462	-0.181552	-2.272471
38	1	0	5.153183	2.297978	-1.773255
39	1	0	5.119589	2.872232	-0.090477
40	1	0	6.596035	2.134053	-0.748857
41	1	0	0.472114	-0.277376	2.290786
42	1	0	-0.839322	-1.395959	1.877153
43	1	0	1.863465	-2.107357	1.485235
44	1	0	-6.046957	3.260361	0.428391
45	1	0	-6.185086	1.750928	1.390680
46	1	0	-4.822921	2.872271	1.682864

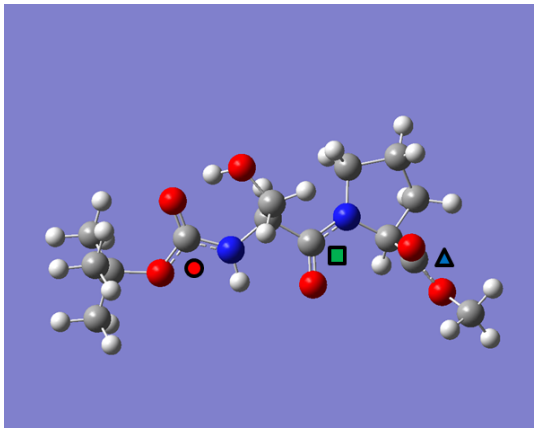
Frequencies --		1681.8910			1702.5880			1779.7434		
Red. masses --		10.3009			8.5131			10.9462		
Frc consts --		17.1681			14.5398			20.4281		
IR Inten --		742.6573			216.3966			322.6177		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	7	-0.06	-0.12	-0.03	0.02	0.05	0.01	-0.01	0.00	0.00
2	6	-0.02	0.03	0.00	0.01	-0.01	0.00	0.02	0.01	-0.06
3	6	0.01	-0.01	0.00	0.00	0.01	0.00	-0.01	-0.01	0.00
4	6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	-0.02	-0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00
6	6	-0.14	0.27	-0.08	-0.25	0.55	-0.17	0.00	-0.01	0.00
7	8	0.06	-0.16	0.05	0.10	-0.30	0.09	0.00	0.00	0.00
8	8	0.00	-0.03	0.01	0.01	-0.05	0.02	0.00	0.00	0.00
9	6	-0.01	0.02	-0.01	-0.03	0.03	-0.01	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.01	-0.01	0.00	0.00	0.00	0.00

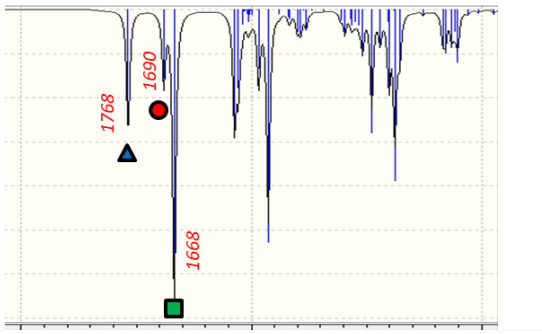
13	6	0.00	0.02	−0.03	0.00	−0.01	0.02	0.04	−0.23	0.72
14	8	0.00	−0.01	0.02	0.00	0.01	−0.01	−0.04	0.15	−0.45
15	7	0.06	−0.02	0.00	0.08	−0.07	0.02	0.00	0.00	0.00
16	1	−0.13	−0.06	0.02	0.41	0.00	0.02	−0.01	0.00	0.00
17	6	−0.01	−0.03	−0.02	0.02	0.03	0.00	0.00	0.00	0.00
18	6	−0.01	−0.01	0.01	−0.03	0.01	−0.01	0.00	0.00	0.00
19	1	0.23	−0.10	0.15	−0.22	0.03	−0.02	0.01	−0.01	0.01
20	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	6	0.08	0.67	0.03	−0.03	−0.28	−0.01	0.01	0.04	0.00
22	8	0.00	−0.39	0.00	0.00	0.15	0.00	0.00	−0.02	0.00
23	8	0.00	−0.01	0.00	0.00	0.00	0.00	−0.01	0.02	−0.04
24	6	0.00	0.00	0.00	0.00	0.00	0.00	−0.01	0.01	0.03
25	1	0.09	0.02	0.00	−0.04	−0.01	0.00	0.10	−0.16	−0.19
26	1	0.02	0.05	0.03	−0.01	−0.02	−0.01	−0.01	0.00	0.02
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.05	0.00
28	1	0.00	−0.01	0.00	0.00	0.00	0.00	0.01	0.03	0.02
29	1	0.02	0.00	0.00	−0.01	0.00	0.00	0.01	0.03	−0.04
30	1	0.01	0.13	0.08	0.00	−0.05	−0.03	−0.01	0.02	0.02
31	1	0.03	0.20	−0.06	−0.01	−0.08	0.03	0.00	0.02	−0.01
32	1	0.00	−0.06	0.03	0.00	−0.10	0.06	0.00	0.00	0.00
33	1	−0.02	0.00	−0.01	−0.03	0.00	−0.02	0.00	0.00	0.00
34	1	0.06	0.00	0.04	0.11	0.00	0.06	0.00	0.00	0.00
35	1	0.00	−0.06	0.01	0.00	−0.12	0.01	0.00	0.00	0.00
36	1	0.06	−0.03	−0.02	0.11	−0.04	−0.04	0.00	0.00	0.00
37	1	−0.02	0.01	0.01	−0.03	0.01	0.01	0.00	0.00	0.00
38	1	0.00	−0.01	0.00	0.00	−0.02	0.00	0.00	0.00	0.00
39	1	0.00	−0.01	0.00	0.00	−0.02	0.01	0.00	0.00	0.00
40	1	0.00	0.02	−0.01	0.00	0.06	−0.02	0.00	0.00	0.00
41	1	0.02	0.03	−0.03	0.06	−0.03	0.01	0.00	0.00	0.00
42	1	−0.01	−0.02	0.01	0.00	−0.05	0.04	−0.01	0.01	0.00
43	1	0.07	−0.11	0.04	0.14	−0.20	0.08	0.00	0.00	0.00
44	1	0.00	0.00	0.01	0.00	0.00	0.00	0.09	−0.06	−0.20
45	1	−0.01	0.00	0.00	0.00	0.00	0.00	0.06	−0.13	−0.03
46	1	0.00	0.01	−0.01	0.00	0.00	0.00	0.13	−0.08	−0.02

Table S12. B3LYP/6-31+G(d) Optimized cartesian coordinates, energies, and calculated frequencies of carbonyl groups in acetonitrile for *N*-Boc-L-serine-L-proline-OMe **10**



10






```
Zero-point correction = 0.388764 (Hartree/Particle)
Thermal correction to Energy = 0.412936
Thermal correction to Enthalpy = 0.413880
Thermal correction to Gibbs Free Energy = 0.332963
Sum of electronic and zero-point Energies = -1108.513725
Sum of electronic and thermal Energies = -1108.489553
Sum of electronic and thermal Enthalpies = -1108.488608
Sum of electronic and thermal Free Energies = -1108.569525
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.042660	-0.540769	-0.571914
2	6	0	-3.261133	0.175677	-0.961109
3	6	0	-4.121856	-0.918322	-1.642057
4	6	0	-3.657704	-2.219959	-0.969923
5	6	0	-2.152552	-2.005215	-0.769372
6	6	0	2.732792	-0.164485	0.009880
7	8	0	3.092359	-1.306286	0.328652
8	8	0	3.550734	0.835925	-0.359708
9	6	0	5.031496	0.718158	-0.313366
10	6	0	5.489875	0.434503	1.119956
11	6	0	5.500044	-0.348554	-1.306860
12	6	0	5.481810	2.110909	-0.760350
13	6	0	-3.967910	0.779877	0.253872

14	8	0	-3.879307	0.371966	1.397069
15	7	0	1.440691	0.239856	-0.014635
16	1	0	1.224929	1.212801	-0.205830
17	6	0	0.301969	-0.644953	0.197083
18	6	0	0.188228	-1.149133	1.662873
19	1	0	0.403038	-1.522022	-0.451981
20	8	0	1.028916	-2.267967	1.916217
21	6	0	-0.949853	0.155678	-0.196479
22	8	0	-0.942983	1.396250	-0.141896
23	8	0	-4.746797	1.804288	-0.122665
24	6	0	-5.543596	2.433617	0.908294
25	1	0	-3.019456	0.989533	-1.648511
26	1	0	-5.193586	-0.732224	-1.534090
27	1	0	-3.889047	-0.931336	-2.712131
28	1	0	-4.150472	-2.348676	-0.000282
29	1	0	-3.864461	-3.105140	-1.577410
30	1	0	-1.764596	-2.551010	0.092986
31	1	0	-1.583690	-2.303795	-1.658803
32	1	0	6.582949	0.496958	1.166108
33	1	0	5.078789	1.180627	1.809366
34	1	0	5.187531	-0.560802	1.452355
35	1	0	6.594802	-0.337113	-1.357201
36	1	0	5.176264	-1.346651	-1.005399
37	1	0	5.112092	-0.135570	-2.309395
38	1	0	5.110857	2.334560	-1.766320
39	1	0	5.112753	2.879004	-0.072266
40	1	0	6.575738	2.157368	-0.776592
41	1	0	0.424689	-0.309859	2.332226
42	1	0	-0.833183	-1.475694	1.877802
43	1	0	1.892770	-2.086120	1.484556
44	1	0	-6.093281	3.225655	0.401438
45	1	0	-6.230849	1.706861	1.347447
46	1	0	-4.893821	2.848833	1.681769

Frequencies --	1667.6702	1690.3679	1767.8528
Red. masses --	9.9841	8.3376	10.9270
Frc consts --	16.3599	14.0363	20.1208
IR Inten --	983.2084	235.9609	415.9510

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	7	-0.06	-0.12	-0.04	0.02	0.06	0.01	-0.01	0.00	0.00
2	6	-0.02	0.03	0.00	0.01	-0.01	0.00	0.02	0.01	-0.06
3	6	0.01	-0.01	0.00	0.00	0.01	0.00	-0.01	-0.01	-0.01
4	6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	-0.02	-0.02	0.00	0.01	0.01	0.00	0.00	0.00	0.00
6	6	-0.15	0.30	-0.08	-0.24	0.54	-0.14	0.00	-0.01	0.00
7	8	0.06	-0.17	0.05	0.10	-0.29	0.08	0.00	0.00	0.00
8	8	0.00	-0.03	0.01	0.01	-0.05	0.02	0.00	0.00	0.00
9	6	-0.01	0.02	-0.01	-0.03	0.03	-0.01	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.01	-0.01	0.00	0.00	0.00	0.00

13	6	0.00	0.01	−0.03	0.00	−0.01	0.02	0.03	−0.23	0.72
14	8	0.00	−0.01	0.02	0.00	0.01	−0.01	−0.03	0.15	−0.45
15	7	0.07	−0.03	0.00	0.07	−0.07	0.02	0.00	0.00	0.00
16	1	−0.09	−0.05	0.02	0.42	0.00	0.00	−0.01	0.00	0.00
17	6	−0.02	−0.03	−0.02	0.02	0.03	0.00	0.00	0.00	0.00
18	6	−0.01	−0.01	0.01	−0.03	0.01	−0.01	0.00	0.00	0.00
19	1	0.22	−0.10	0.14	−0.23	0.03	−0.02	0.02	−0.01	0.01
20	8	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	6	0.08	0.64	0.06	−0.04	−0.31	−0.02	0.01	0.04	0.00
22	8	0.00	−0.37	−0.02	0.00	0.17	0.01	0.00	−0.02	0.00
23	8	0.00	−0.01	0.00	0.00	0.00	0.00	−0.01	0.02	−0.04
24	6	0.00	0.00	0.00	0.00	0.00	0.00	−0.02	0.01	0.03
25	1	0.10	0.01	0.00	−0.05	−0.01	0.00	0.10	−0.15	−0.19
26	1	0.02	0.06	0.03	−0.01	−0.03	−0.02	−0.01	0.00	0.02
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.06	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.02
29	1	0.03	0.00	0.00	−0.01	0.00	0.00	0.00	0.03	−0.03
30	1	0.00	0.14	0.09	0.01	−0.06	−0.04	−0.01	0.02	0.02
31	1	0.03	0.23	−0.06	−0.01	−0.10	0.03	0.00	0.02	−0.01
32	1	0.00	−0.06	0.03	0.00	−0.10	0.06	0.00	0.00	0.00
33	1	−0.02	0.00	−0.01	−0.03	0.00	−0.02	0.00	0.00	0.00
34	1	0.07	0.00	0.04	0.10	0.00	0.06	0.00	0.00	0.00
35	1	0.00	−0.07	0.01	0.00	−0.11	0.01	0.00	0.00	0.00
36	1	0.07	−0.03	−0.03	0.10	−0.04	−0.05	0.00	0.00	0.00
37	1	−0.02	0.01	0.01	−0.03	0.01	0.01	0.00	0.00	0.00
38	1	0.00	−0.01	0.00	0.01	−0.02	0.00	0.00	0.00	0.00
39	1	0.00	−0.01	0.01	0.01	−0.01	0.01	0.00	0.00	0.00
40	1	0.00	0.03	−0.01	0.00	0.06	−0.02	0.00	0.00	0.00
41	1	0.03	0.02	−0.04	0.06	−0.03	0.01	0.00	0.00	0.00
42	1	−0.01	−0.02	0.00	0.00	−0.05	0.04	0.00	0.01	0.00
43	1	0.09	−0.14	0.06	0.15	−0.20	0.08	0.00	0.00	0.00
44	1	0.00	0.00	0.01	0.00	0.00	0.00	0.10	−0.06	−0.20
45	1	−0.01	0.00	0.00	0.00	0.00	0.00	0.06	−0.13	−0.04
46	1	0.00	0.00	0.00	0.00	0.00	0.00	0.13	−0.08	−0.02

Table S13. ^{13}C NMR chemical shifts of carbonyl carbons in **1a**, **1b**, **2**, and **3a**

Solvent	E_T^N	**1a**		**1b**		**2**		**3a**	
		COOH	COO^{t}Bu	COOMe	COO^{t}Bu	COOH	COO^{t}Bu	COOH	COO^{t}Bu
THF (no-D)	0.207	173.2	154.4	173.7	154.9	173.7	156.5	173.6 (172.9)[1]	152.9 (153.6)[1]
$CDCl_3$	0.259	176.9	155.6	174.2	155.4	176.0	155.9	174.1	156.9
Acetone-d_6	0.355	174.5	156.1	174.8	156.7	174.1	157.1	175.1 (174.5)[1]	154.7 (154.3)[1]
DMSO-d_6	0.444	174.7	155.3	173.6	155.3	173.5	155.8	174.4 (174.0)[1]	153.1 (153.5)[1]
Acetonitrile-d_3	0.460	174.8	156.5	174.7	156.3	173.7	154.9	174.7 (174.1)[1]	156.0 (154.5)[1]
Ethanol (no-D)	0.654	175.6	156.0	174.3	156.4	175.5	157.7	175.9 (175.6)[1]	155.9 (155.2)[1]
Methanol-d_4	0.762	177.7	158.7	176.3	158.7	176.5	159.1	177.6	156.8
D_2O	1.000	178.2	158.0	———	———	177.0	158.4	178.7	156.2

1. Chemical shift in parentheses is minor amide rotational isomer.

Table S14. ^{13}C NMR chemical shifts of carbonyl carbons in **3b**, **4a**, **4b**, and **5**

Solvent	E_T^N	**3b**		**4a**		**4b**		**5**	
		COOMe	COO^{t}Bu	COOH	COO^{t}Bu	COOMe	COO^{t}Bu	COOH	COO^{t}Bu
THF (no-D)	0.207	173.2 (172.7)[1]	153.0 (153.7)[1]	172.6	156.4	170.9	155.1	171.7	155.6
$CDCl_3$	0.259	173.8	154.4	173.5	156.5	171.2	155.7	173.8	156.8
Acetone-d_6	0.355	174.7 (174.3)[1]	154.5	172.9	156.5	172.6	156.8	173.2	157.3
DMSO-d_6	0.444	173.3 (173.0)[1]	152.9	172.4	155.3	171.5	155.3	172.5	155.7
Acetonitrile-d_3	0.460	174.7 (174.4)[1]	154.4 (153.4)[1]	172.5	156.6	172.3	156.5	172.7	156.7
Ethanol (no-D)	0.654	173.7 (173.4)[1]	153.9 (154.4)[1]	174.3	156.4	171.1	155.8	174.4	157.8
Methanol-d_4	0.762	176.2 (175.9)[1]	156.6 (157.1)[1]	174.9	158.7	173.8	158.7	174.5	158.3
D_2O	1.000	———	———	175.0	158.3	———	———	175.2	158.4

1. Chemical shift in parentheses is minor amide rotational isomer.

Table S15. ^{13}C NMR chemical shifts of carbonyl carbons in **6** and **7**

Solvent	E_T^N	**6**			**7**		
		COOMe	CONH	COO^{t}Bu	COOMe	CONH	COO^{t}Bu
THF (no-D)	0.207	173.1	172.1 (171.7)[1]	155.6 (154.6)[1]	170.9	172.4 (171.9)[1]	154.6 (153.7)[1]
$CDCl_3$	0.259	173.1	171.7 (172.1)[1]	155.6 (154.6)[1]	170.8	172.6 (173.2)[1]	155.2 (154.6)[1]
Acetone-d_6	0.355	174.3	173.7 (173.1)[1]	155.1 (156.0)[1]	172.1	174.0 (173.5)[1]	155.2 (156.0)[1]
DMSO-d_6	0.444	173.0 (173.1)[1]	172.4 (172.2)[1]	153.3 (153.5)[1]	171.1	172.7 (172.4)[1]	153.4 (153.6)[1]
Acetonitrile-d_3	0.460	174.0	173.6 (173.2)[1]	154.9 (156.0)[1]	171.8	174.0 (173.6)[1]	155.0 (155.8)[1]
Ethanol (no-D)	0.654	173.8	173.0 (173.3)[1]	154.3 (154.6)[1]	170.7	174.1 (173.6)[1]	154.6 (154.8)
Methanol-d_4	0.762	175.6 (175.2)[1]	174.4 (174.7)[1]	156.0 (156.3)[1]	172.1	175.8 (175.4)[1]	156.1 (156.4)

1. Chemical shift in parentheses is minor amide rotational isomer.

Table S16. ^{13}C NMR chemical shifts of carbonyl carbons in **8** and **9**

Solvent	E_T^N	**8**			**9**		
		COOMe	CON	COO^{t}Bu	COOMe	CON	COO^{t}Bu
THF (no-D)	0.207	171.0	154.9 (153.4)[1]	153.7 (153.0)[1]	171.9	170.7	154.8
$CDCl_3$	0.259	171.5 (171.0)[1]	154.9 (154.3)[1]	154.1 (153.7)[1]	172.4	171.7	155.2
Acetone-d_6	0.355	172.0	155.7 (154.2)[1]	154.5 (154.1)[1]	173.1	172.0	155.8
DMSO-d_6	0.444	170.4	153.0 (153.2)[1]	152.8 (152.9)[1]	172.4	171.3	155.1
Acetonitrile-d_3	0.460	172.4	155.9 (154.6)[1]	154.8 (154.3)[1]	173.6	172.5	156.1
Ethanol (no-D)	0.654	171.0	154.7 (154.1)[1]	153.8 (153.3)[1]	172.9	172.5	156.0
Methanol-d_4	0.762	172.9	156.4 (155.8)[1]	155.3 (154.9)[1]	174.2	174.1	157.7

1. Chemical shift in parentheses is minor amide rotational isomer.

Table S17. ^{13}C NMR chemical shifts of carbonyl carbons in **10**

Solvent	E_T^N	**10**		
		COOMe	CON	COO^{t}Bu
THF (no-D)	0.207	172.3	169.6	155.3
$CDCl_3$	0.259	172.6 (172.1)[1]	169.9	155.4 (157.0)[1]
Acetone-d_6	0.355	173.5	170.3	156.3
DMSO-d_6	0.444	172.4	169.2	155.4 (156.7)[1]
Acetonitrile-d_3	0.460	173.9	170.5	156.5
Ethanol (no-D)	0.654	172.4	170.1	156.0 (158.0)[1]
Methanol-d_4	0.762	174.2	171.9	157.9

1. Chemical shift in parentheses is minor amide rotational isomer.