Optimized Geometry for Mixed Nitronic Anhydride *syn* 7
Theory: B3LYP/6-31G*

Energy with zero-point correction (Hartrees): -926.438658595

Cartesian Coordinates:

Atom	X	Y	Z
C	1.24977	-1.05075	.12486
C	2.27255	-.16639	.01929
C	2.09084	1.26390	.05169
C	.83514	1.74856	-.05887
C	-.34110	.87814	-.19838
C	-.09281	-.56840	-.26316
C	.31218	3.16207	-.04703
C	-1.22600	2.94122	-.10276
N	-1.47887	1.49928	-.22017
N	-1.04314	-1.50236	-.44275
N	3.63655	-.69534	.14276
O	-2.35383	-1.01807	-.72186
O	-.91177	-2.71908	-.47833
O	-2.69980	-.97907	1.53866
C	-3.11326	-.77021	.43545
C	-4.44984	-.23360	.01324
O	3.79420	-1.91532	.11400
O	4.54613	.12757	.26819
H	1.43905	-2.11524	-.14772
H	2.96285	1.89531	.16865
H	.67638	3.73097	-.91069
H	.62426	3.70752	.85019
H	-1.69723	3.45105	-.95187
H	-1.73325	3.30572	.79966
H	-5.10189	-.17749	.88567
H	-4.89734	-.86882	-.75649
H	-4.29886	.76433	-.40927

Calculated Frequencies (unscaled) for Mixed Nitronic Anhydride *syn* 7

Frequency (cm^{-1})	Intensity	Frequency (cm^{-1})	Intensity
41	0.45	1053	2.48
50	0.20	1068	14.5
57	1.12	1072	13.5
71	0.44	1087	86.7
90	2.68	1188	265
109	0.19	1196	1.28
122	0.46	1222	5.43
146	2.38	1248	1.40
165	2.76	1277	18.6
185	0.42	1291	3.32
234	1.56	1336	25.5
255	7.87	1364	157
293	0.99	1383	354
327	0.74	1415	50.7
348	2.76	1422	19.0
370	1.39	1427	35.4
412	4.61	1497	0.56
461	4.93	1498	8.90
475	3.67	1503	11.1
535	0.46	1517	3.96
545	7.64	1599	11.8
557	0.29	1624	81.3
587	0.05	1637	637
620	4.97	1650	121
659	12.6	1703	30.7
707	2.78	1896	193
734	7.24	3051	29.7
751	66.3	3064	14.0
752	20.9	3079	10.3
791	60.4	3081	0.53
824	5.96	3104	16.4
837	0.99	3153	1.16
850	253	3187	3.77
882	27.2	3250	3.45
908	7.45	3276	20.9
944	15.1		
952	50.9		
971	58.2		
1007	48.4		
1024	20.3		

Optimized Geometry for Mixed Nitronic Anhydride *anti* 7
Theory: B3LYP/6-31G*

Energy with zero-point correction (Hartrees): -926.436895569

Cartesian Coordinates:

Atom	X	Y	Z
C	-.04584	.90954	-.25853
C	1.17790	1.47009	-.05051
C	2.38885	.71218	.14913
C	2.30389	-.63608	.12196
C	1.03387	-1.33618	-.10149
C	-.16884	-.51470	-.28485
C	3.34552	-1.71350	.28638
C	2.50095	-3.01124	.11548
N	1.10191	-2.62843	-.11311
N	-1.34961	-1.11690	-.46996
N	1.26505	2.93478	-.03247
O	-2.47619	-.18570	-.71397
O	-1.62250	-2.29650	-.52424
O	-3.04661	-.53241	1.47138
C	-3.31697	-.07832	.39569
C	-4.55527	.67968	-.00678
O	.23222	3.58474	-.20385
O	2.37845	3.42860	.15528
H	-.90494	1.54477	-.41071
H	3.31572	1.24847	.31014
H	3.83010	-1.66095	1.26812
H	4.13801	-1.63074	-.46616
H	2.53987	-3.66057	.99869
H	2.83340	-3.62294	-.73239
H	-5.14991	.88150	.88477
H	-5.13795	.07851	-.71279
H	-4.29301	1.61703	-.50646

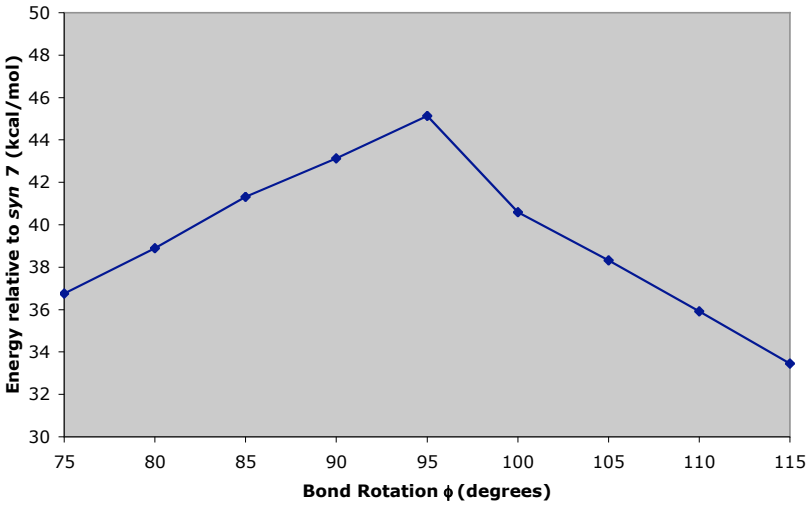
Calculated Frequencies (unscaled) for Mixed Nitronic Anhydride *anti* 7

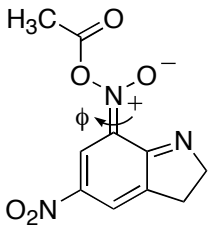
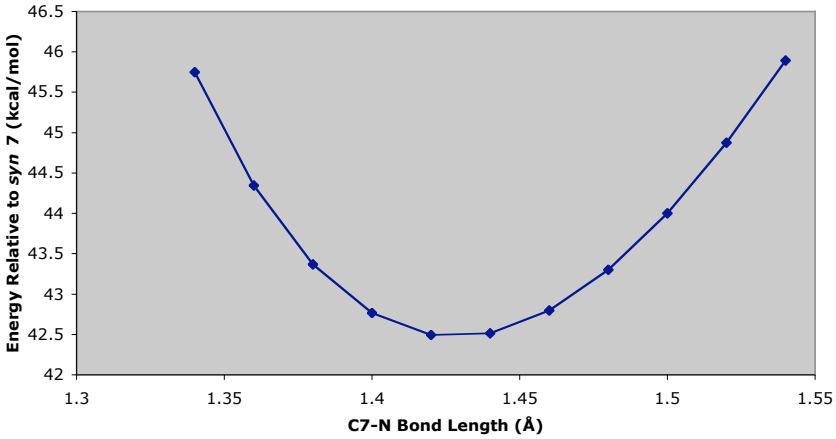
Frequency (cm^{-1})	Intensity	Frequency (cm^{-1})	Intensity
34	0.97	1051	2.73
45	2.82	1067	27.8
54	2.01	1074	8.02
57	2.53	1095	122
67	0.57	1194	0.54
88	0.66	1197	317
120	1.17	1219	3.04
156	1.45	1244	0.19
163	3.20	1281	5.81
185	0.30	1294	7.96
217	0.57	1339	12.1
257	7.60	1371	41.7
271	5.87	1381	520
325	0.08	1420	31.0
345	0.03	1425	15.8
369	1.11	1446	15.5
419	23.5	1495	1.06
452	5.01	1496	14.8
473	3.08	1500	10.0
532	14.3	1514	4.32
536	0.86	1592	43.4
558	0.63	1623	73.6
578	1.30	1644	166
601	7.11	1692	439
675	1.95	1699	24.4
712	121	1883	212
729	62.0	3055	26.7
741	17.3	3066	17.3
751	17.5	3076	0.27
758	169	3081	4.13
802	92.6	3102	18.1
820	0.48	3141	1.56
838	59.7	3187	3.66
867	99.6	3251	3.23
902	4.24	3295	11.2
928	14.2		
943	23.5		
962	7.16		
1002	77.9		
1016	1.13		

Plots of Single-Point Energies vs. Bond Rotation and Bond Length

Energies were calculated at the B3LYP/6-31G* level of theory starting with the calculated geometry of *anti* **7** and setting the rotation about the C7-N bond (ϕ below) to a value ranging from 75º to 105º. A maximum was observed along this reaction coordinate at ϕ=95º. Energies were then calculated at ϕ=95º varying the C7-N bond length from 1.34 to 1.54 Å. A minimum was observed along this reaction coordinate at a bond length of approximately 1.43 Å. This unoptimized energy was approximately 42 kcal/mol above the calculated energy of *syn* **7**, and approximately 40 kcal/mol above the calculated energy of *anti* **7**

Single-Point Energies for C7-N Bond Rotation





Single-Point Energies for C7-N Bond Lengthening at ϕ=95º