10.1071/CH13536_AC

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Supplementary Material

Sydnone Photochemistry. Direct Observation of Earl's Bicyclic Lactone Valence Isomers (Oxadiazabicyclo[2.1.0]pentanones), Formation of Carbodiimides, Reaction Mechanism, and Photochromism

Rakesh Naduvile Veedu, David Kvaskoff and Curt Wentrup*

School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Qld 4072, Australia. Email: wentrup@uq.edu.au

Contents:

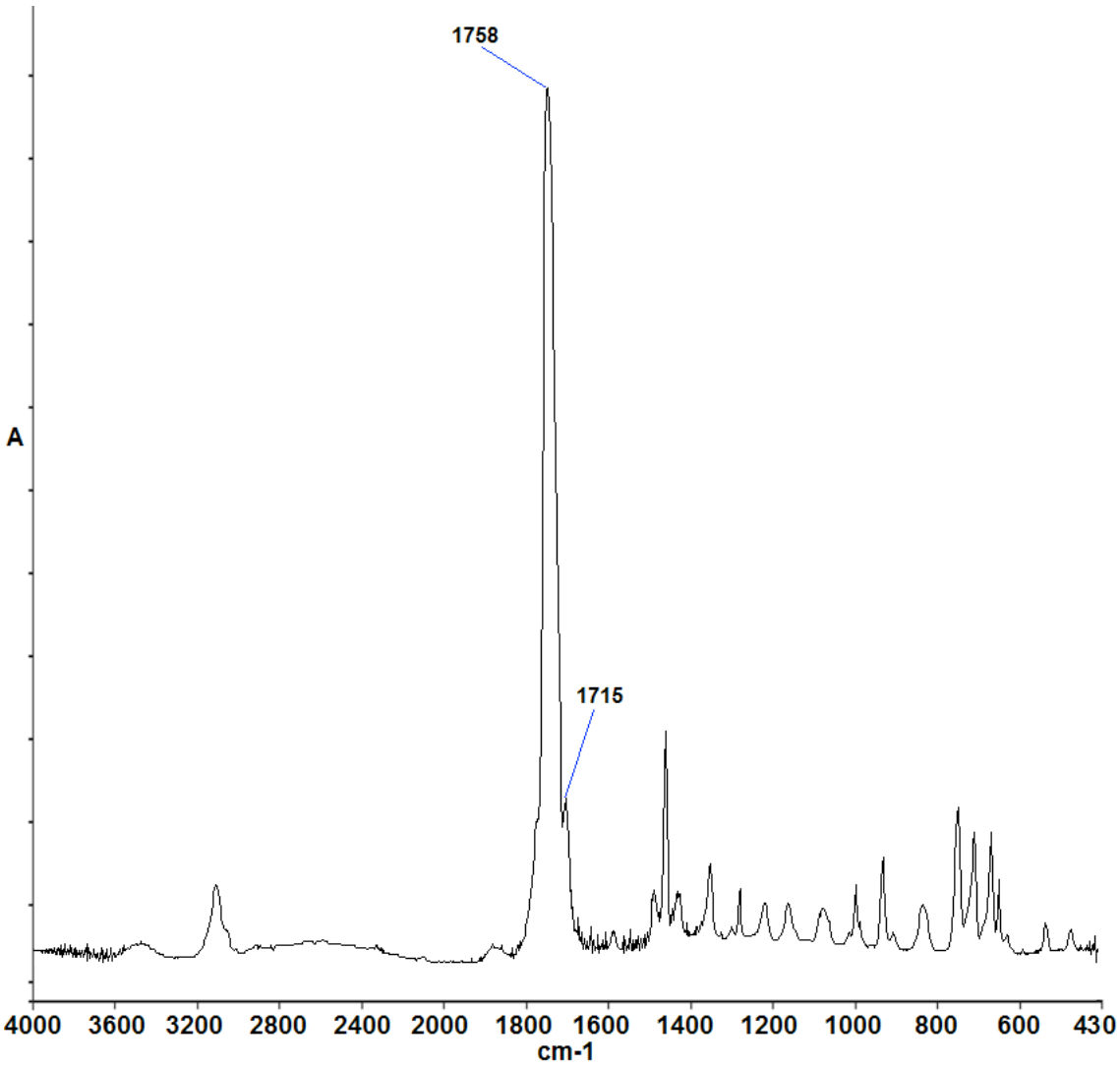


Figure S1. IR spectrum of 3-phenylsydnone depostited as a neat solid at 50 K.

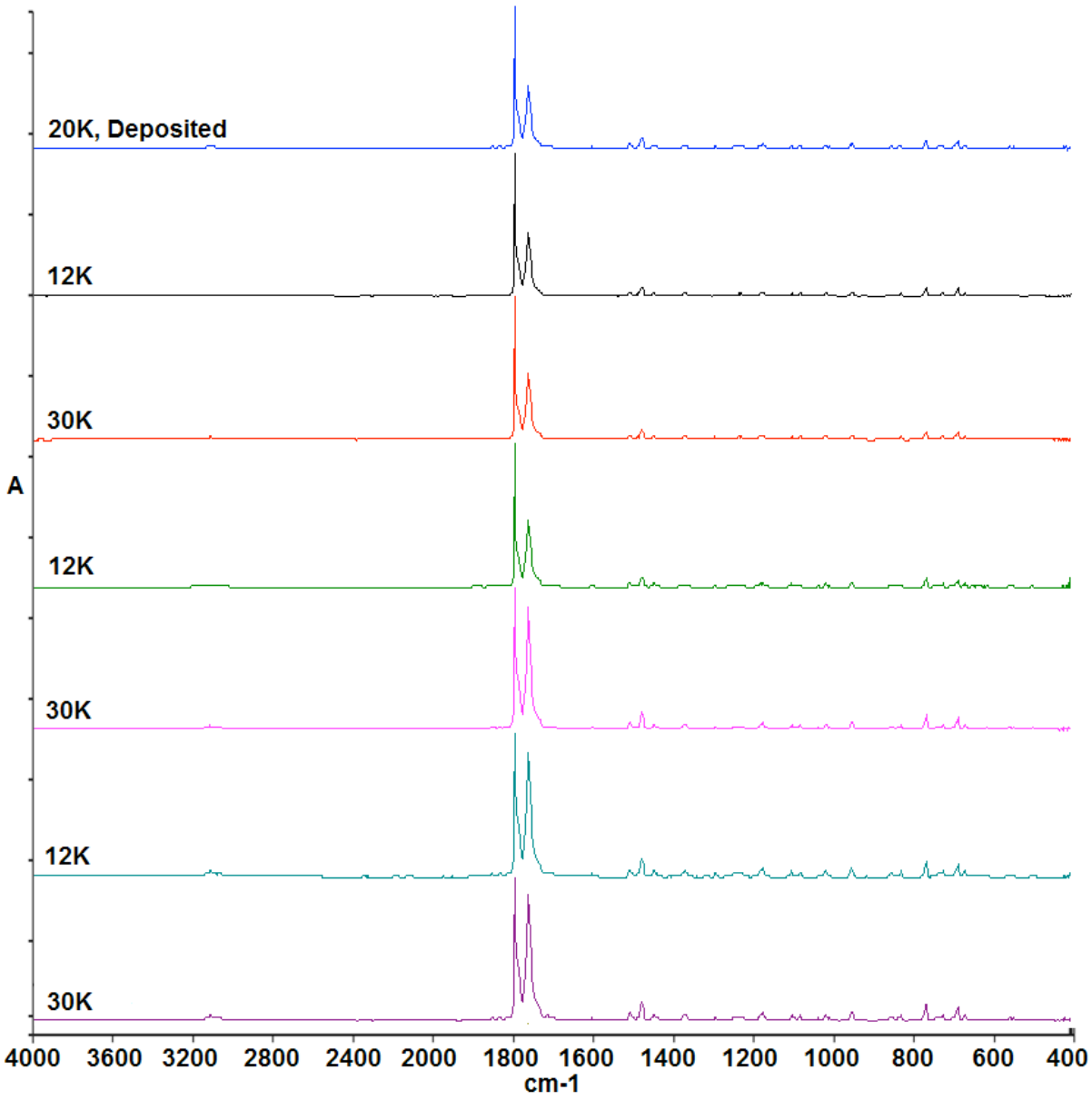


Figure S2. Annealing of 3-phenylsydnone in Ar matrix (12 – 30 K) [the less active site at 1757 cm^{-1} is increasing, probably due to aggregation].

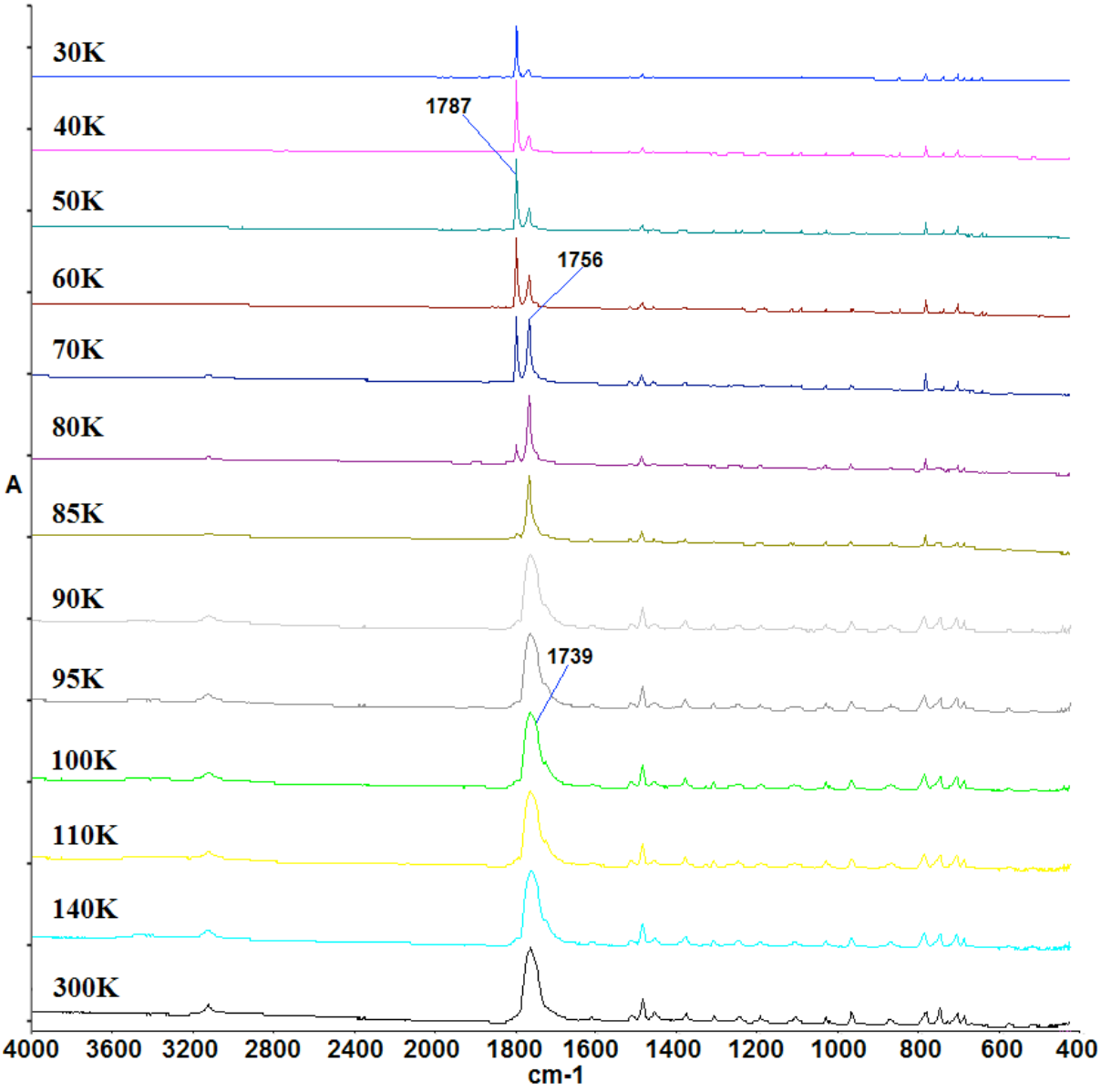


Figure S3. Warm-up of solid 3-phenylsydnone from 30 to 300 K [the more reactive site at 1787 cm^{-1} is decreasing, and the less reactive site originally at 1757 cm^{-1} is increasing due to aggregation]. .

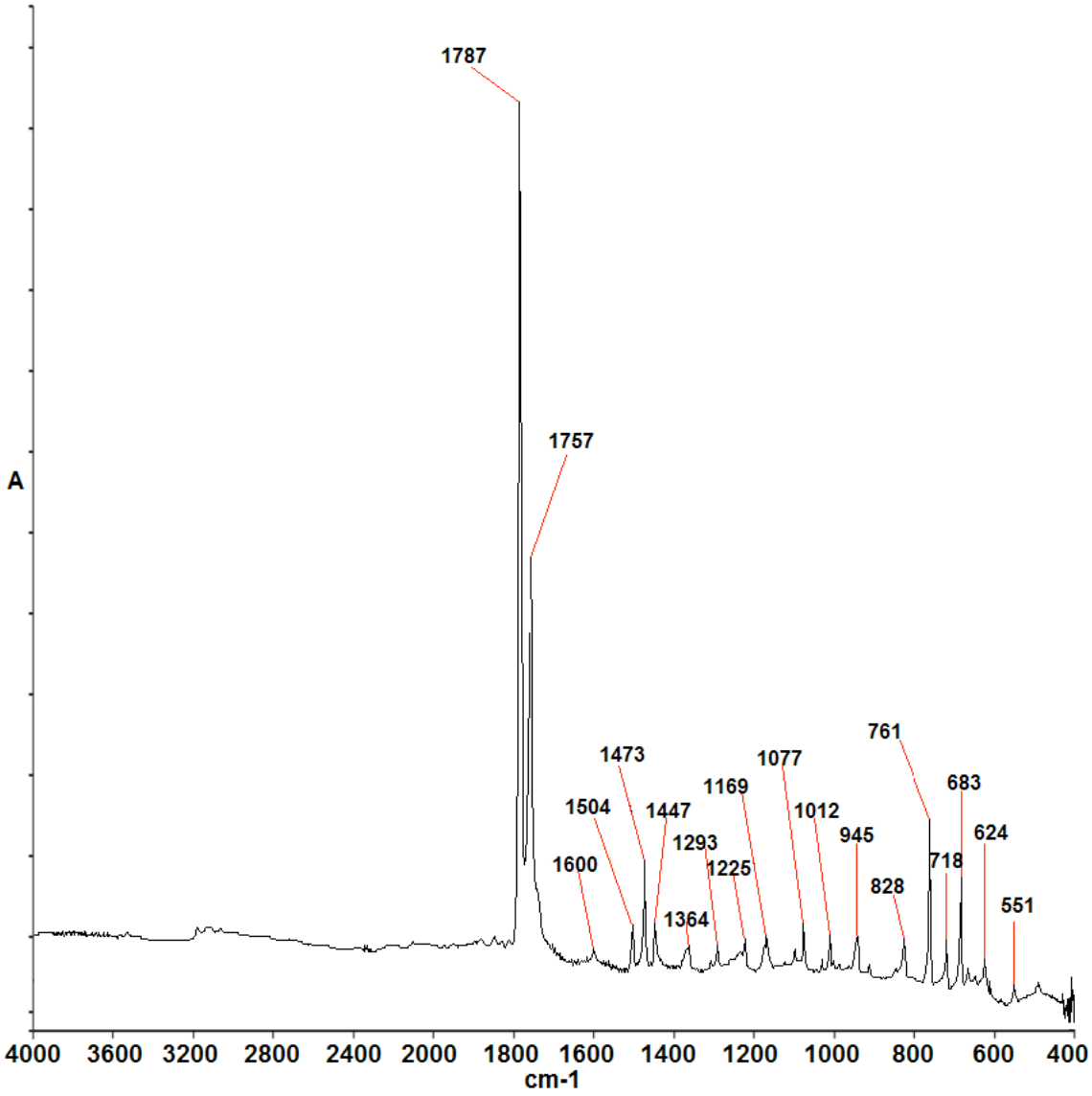


Figure S4. 3-Phenylsydnone in Xenon matrix at 20 K.

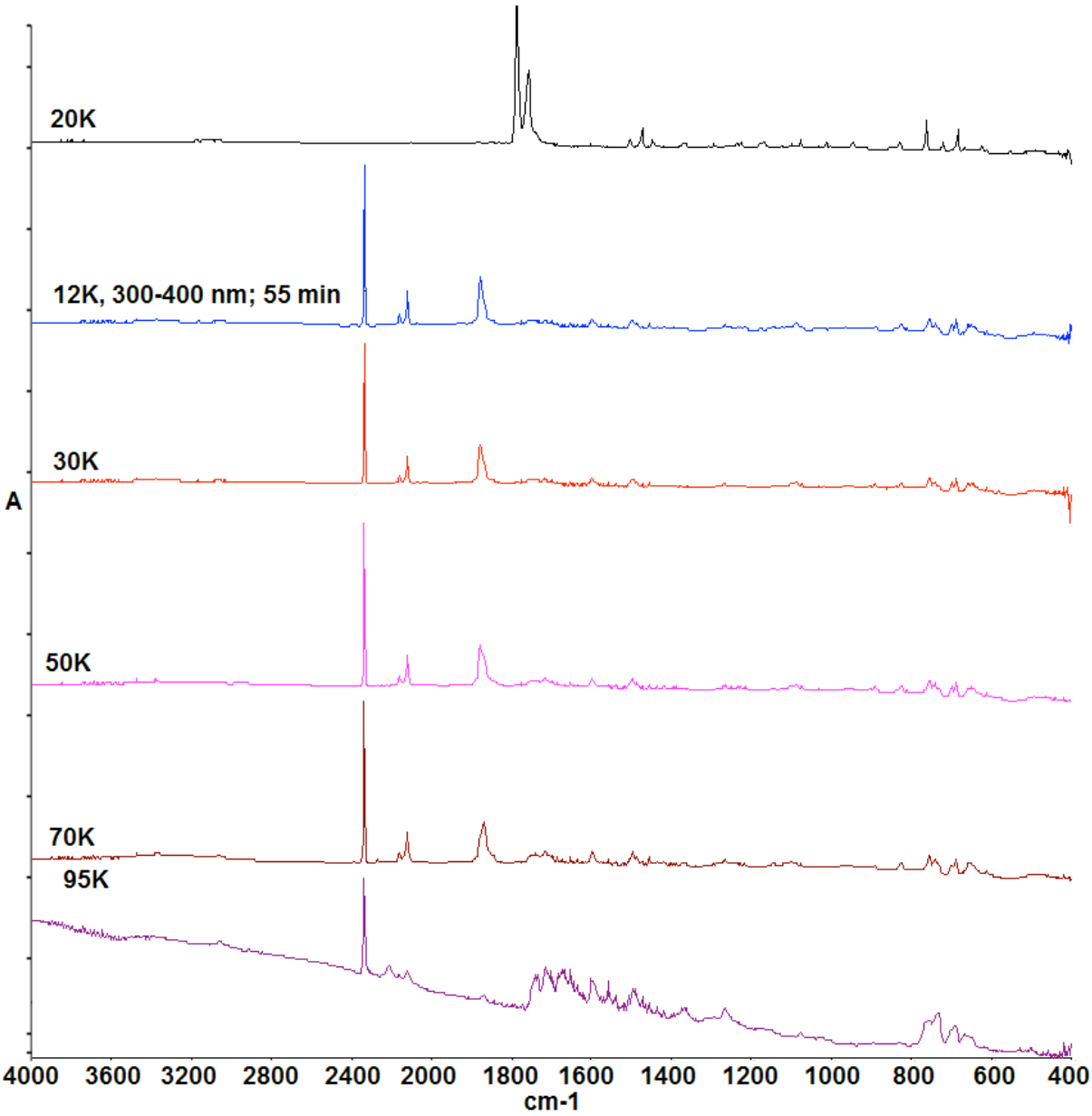


Figure S5. Warming of photoproducts of 3-phenylsydnone to 95 K in Xe matrix, indicating that the products are essentially stable till the softening of the xenon (ca. 80 K).

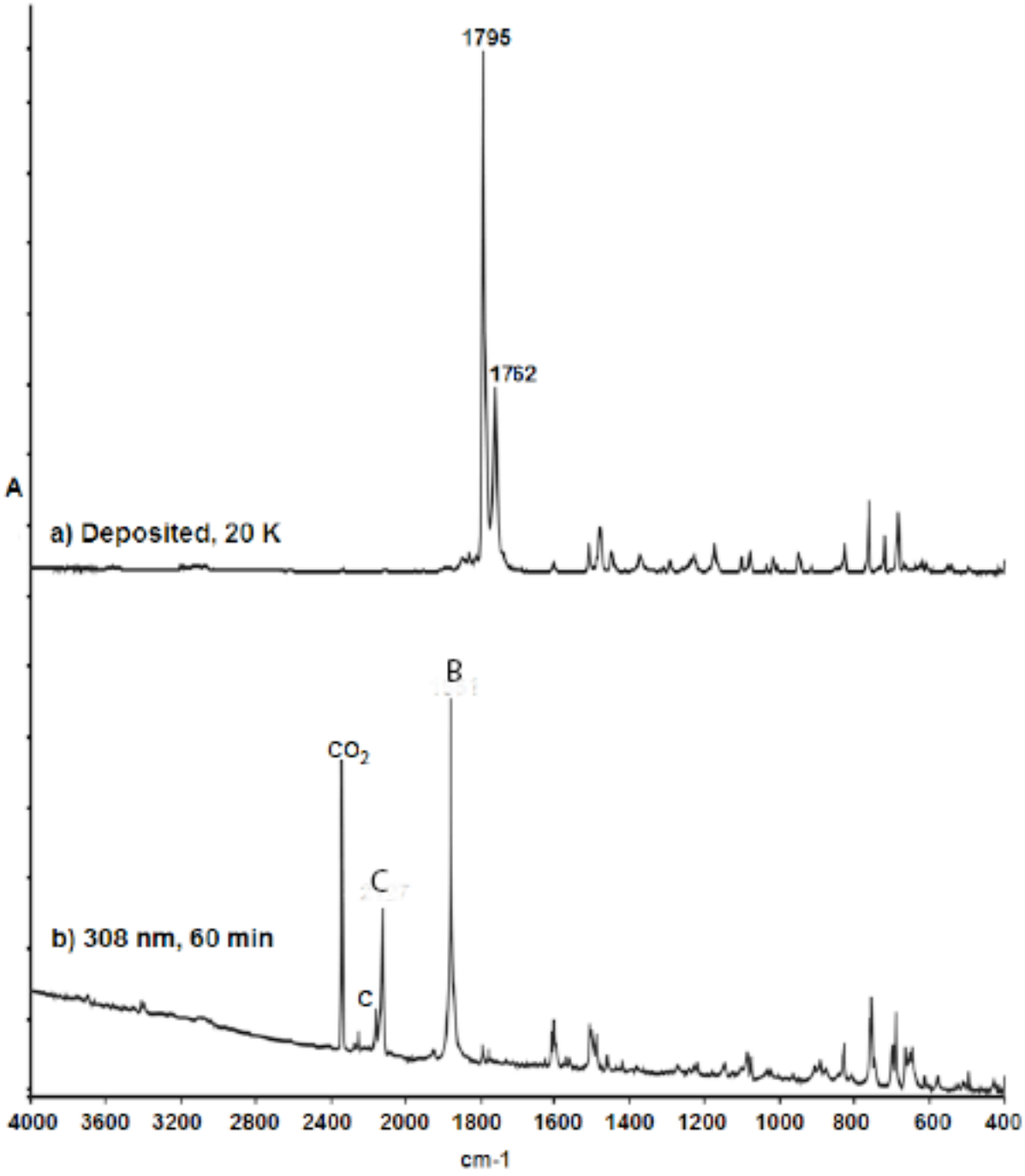


Figure S6. (a) IR spectrum of 3-phenylsydnone deposited in Ar matrix at 20 K. (b) Photolysis at 308 nm for 60 min at 12 K. Products: B = bicyclic lactone (1881 cm^{-1}). C = phenylcarbodiimide (2127 and 2163 cm^{-1}). CO_2 = 2340 cm^{-1}.

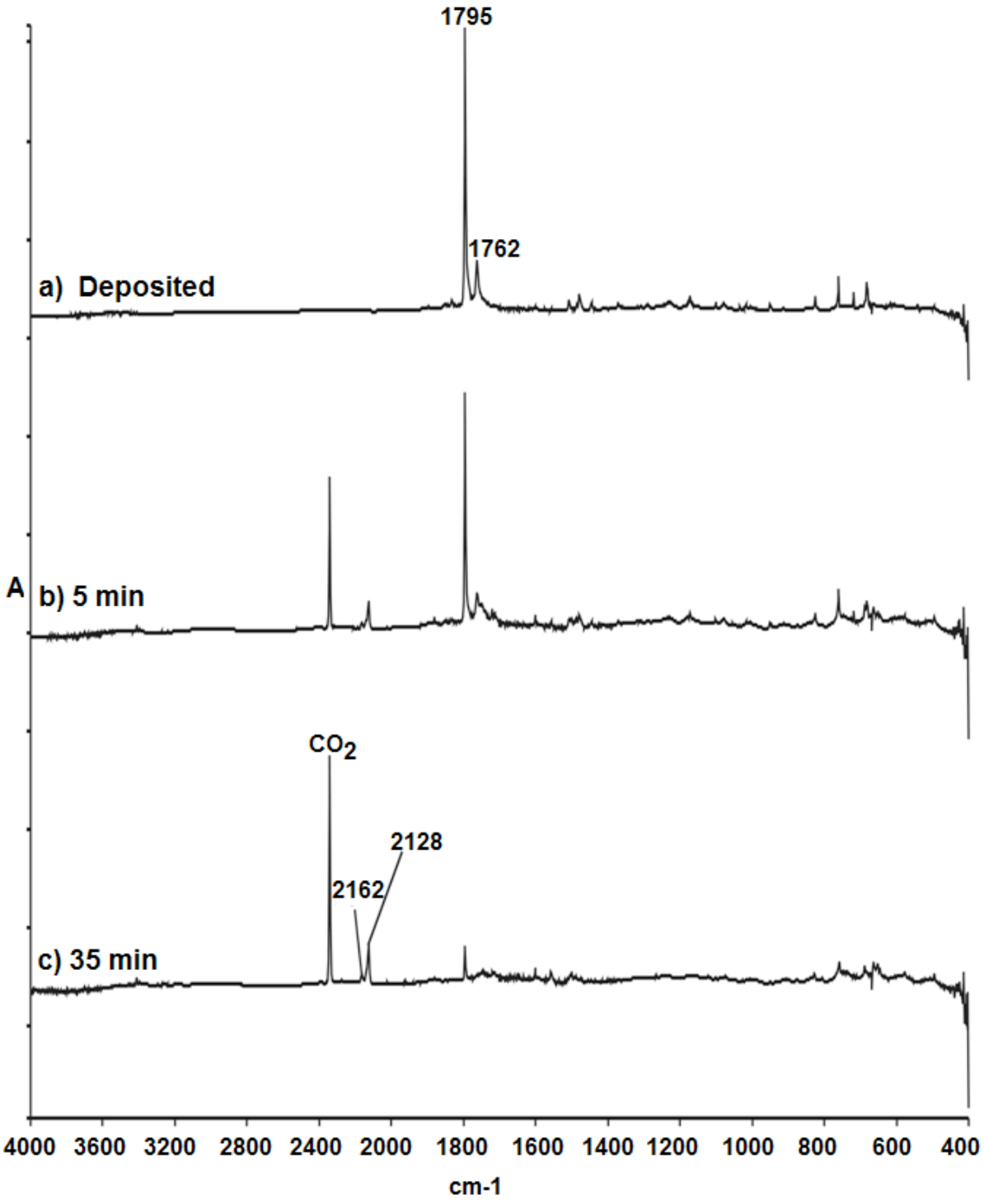


Figure S7. (a) Deposition of 3-phenylsydnone in Ar matrix at 20 K [a particularly large ratio of 'active' (1795 cm^{-1}) to 'inactive' (1762 cm^{-1}) site was obtained in this experiment]. (b) and (c) Photolysis at 222 nm for 5 and 35 min. Phenylcarbodiimide (2128, 2162 cm^{-1}) is the only detectable product (the bicyclic lactone is not stable at 222 nm).

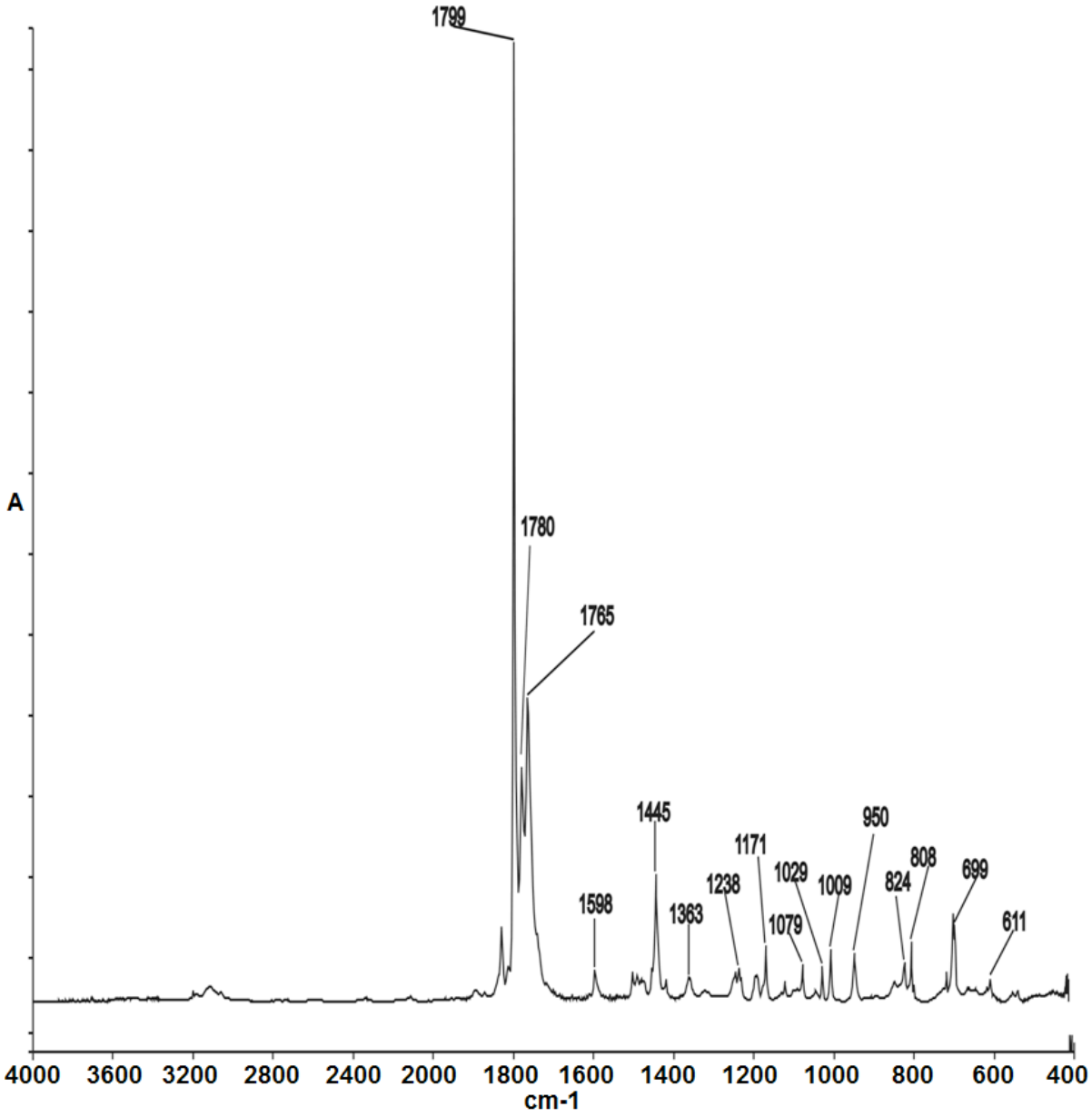


Figure S8. IR spectrum of 3-pyridylsydnone in Ar matrix at 20 K.

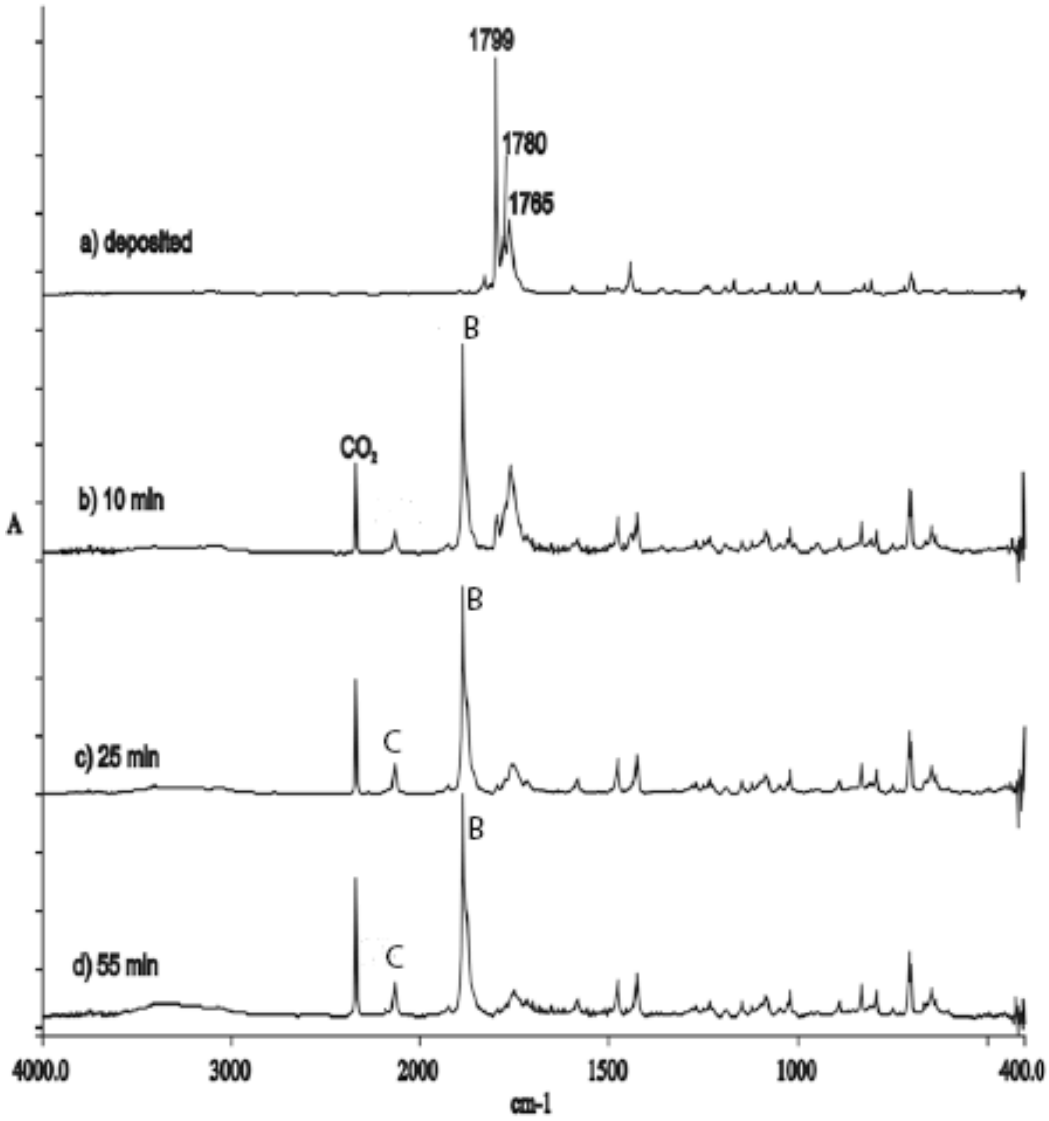


Figure S9. Photolysis of 3-pyridylsydnone at 310-390 nm for 10-55 min in Ar matrix at 12 K. The most reactive site absorbing at 1799 cm^{-1} disappears first. Products: B: bicyclic lactone (1886) cm^{-1}. C: 3-pyridylcarbodiimide (2135) cm^{-1}.

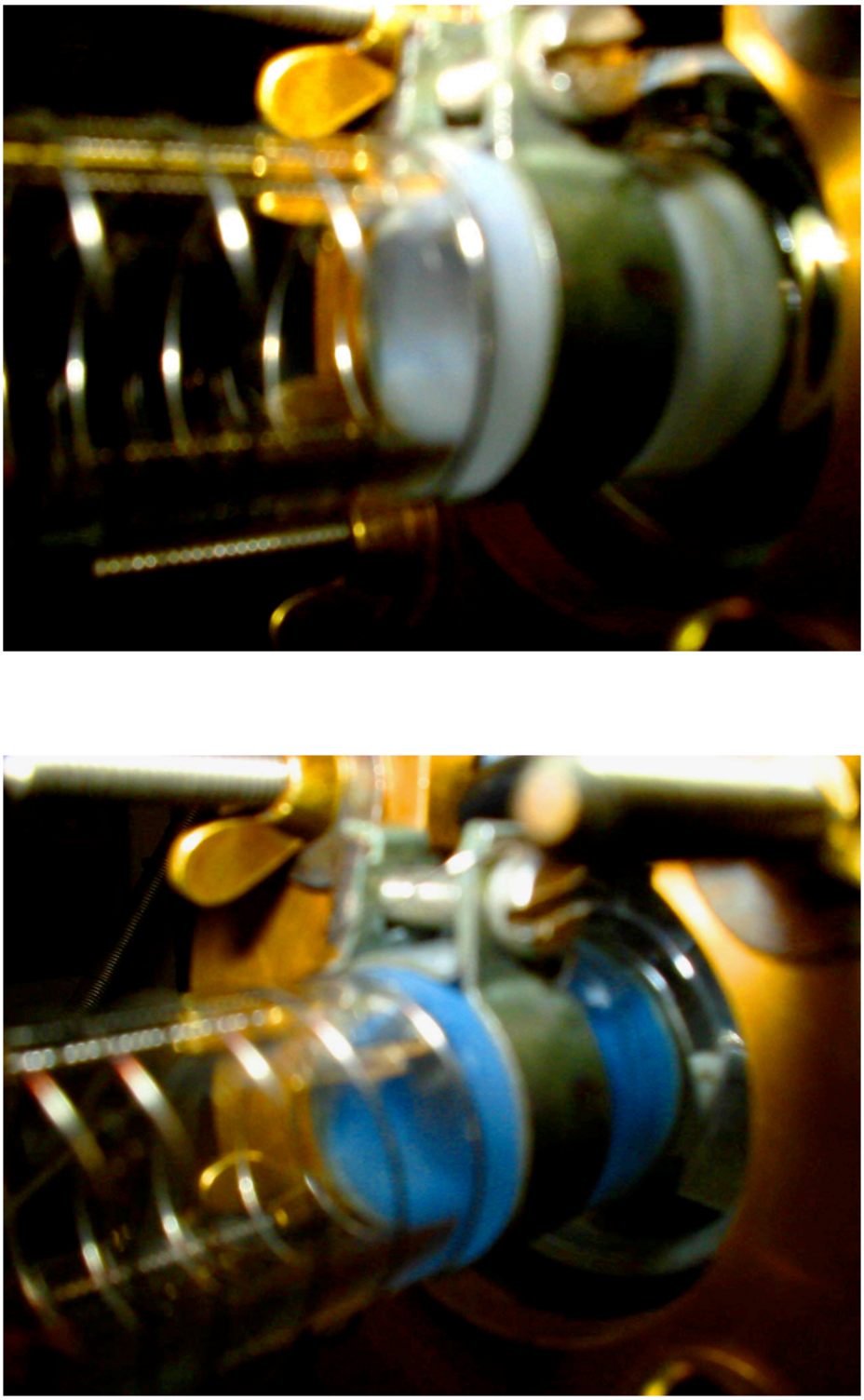


Figure S10. Blue color of solid, irradiated 3-pyridylsydnone at RT. Top: the colorless 3-pyridylsydnone deposited on inner surface of quartz tube at RT before irradiation. Bottom: blue color formed after irradiation at 308 nm at RT. This color disappeared after leaving the apparatus in the dark at RT overnight. The 20 K Ar matrix (not shown) remained colourless and did not develop a blue color at any stage of subsequent photolyses at 308 or 222 nm.

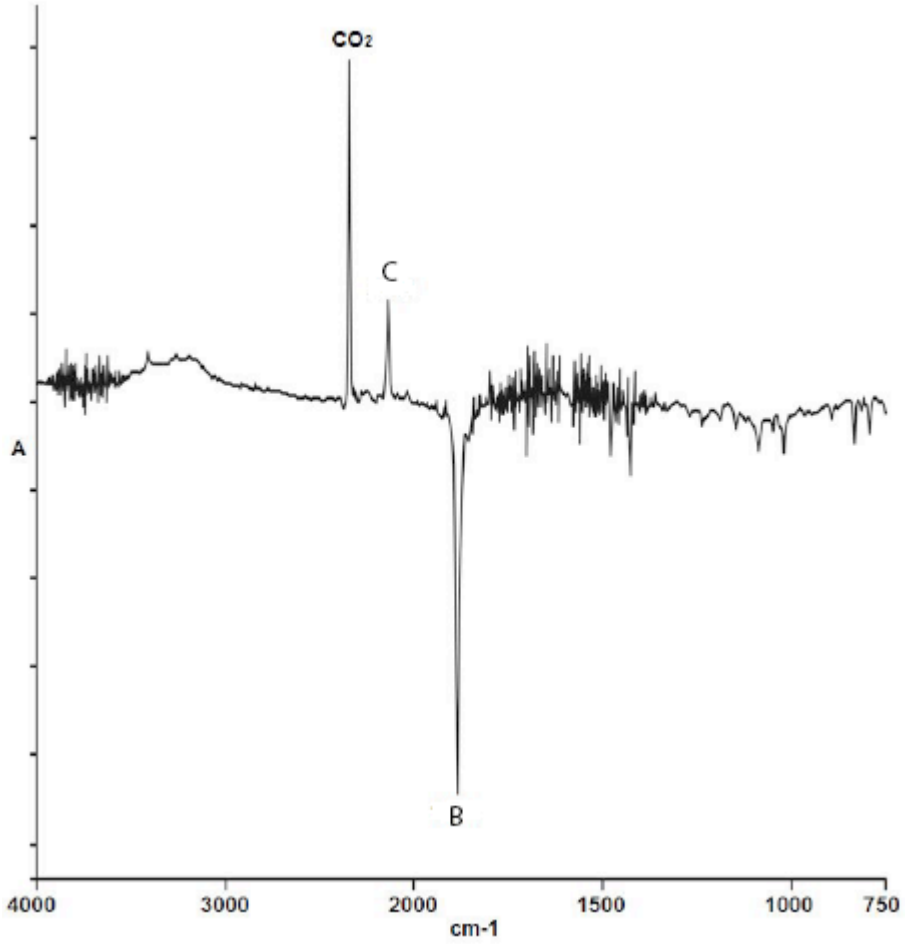


Figure S11. IR-difference spectrum showing initial product formed by irradiation of 3-pyridylsydnone at 308 nm as the negative peak B (bicyclic lactone, 1886 cm^{-1}) and the products formed on subsequent irradiation at 222 nm (20 min, Ar, 12 K): positive peak C = 3-pyridylcarbodiimide (2135 cm^{-1}) and CO_2 (2340 cm^{-1}).

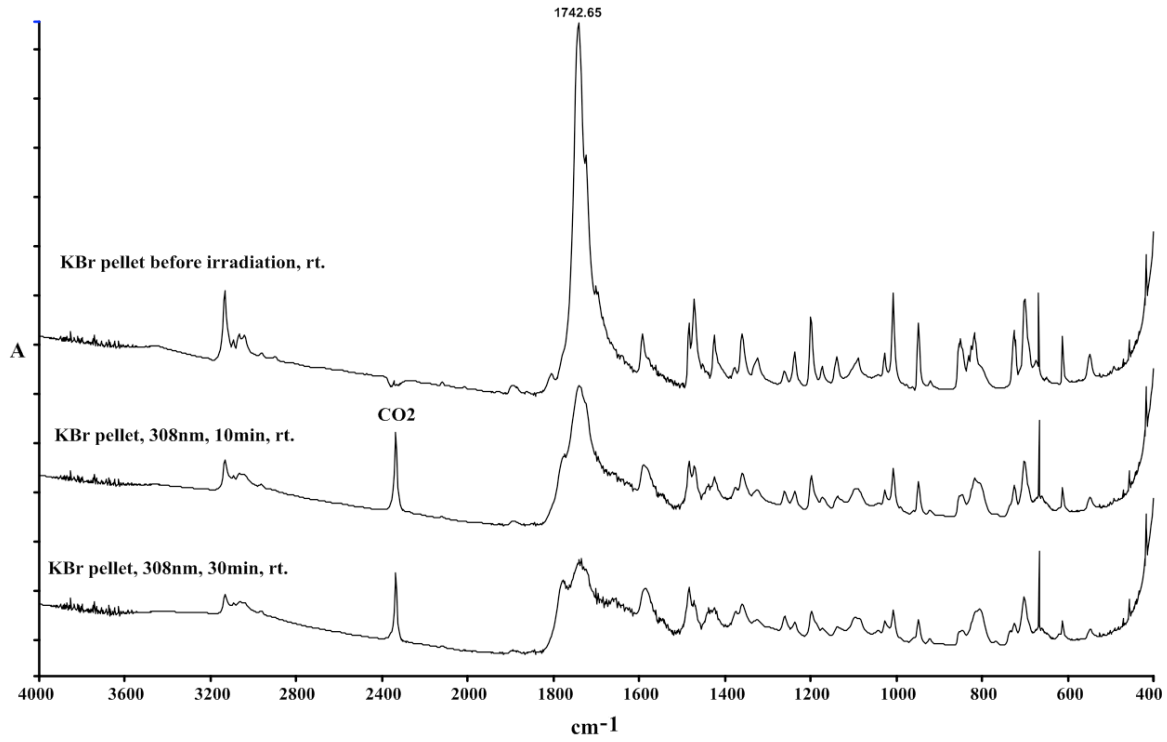


Figure S12. Photolysis of 3-pyridylsydnone in a KBr mull at 308 nm for 0-30 min. The mull turned blue, but no ketene was observable in the IR spectrum. 1742 cm^{-1} = neat 3-pyridylsydnone in KBr.

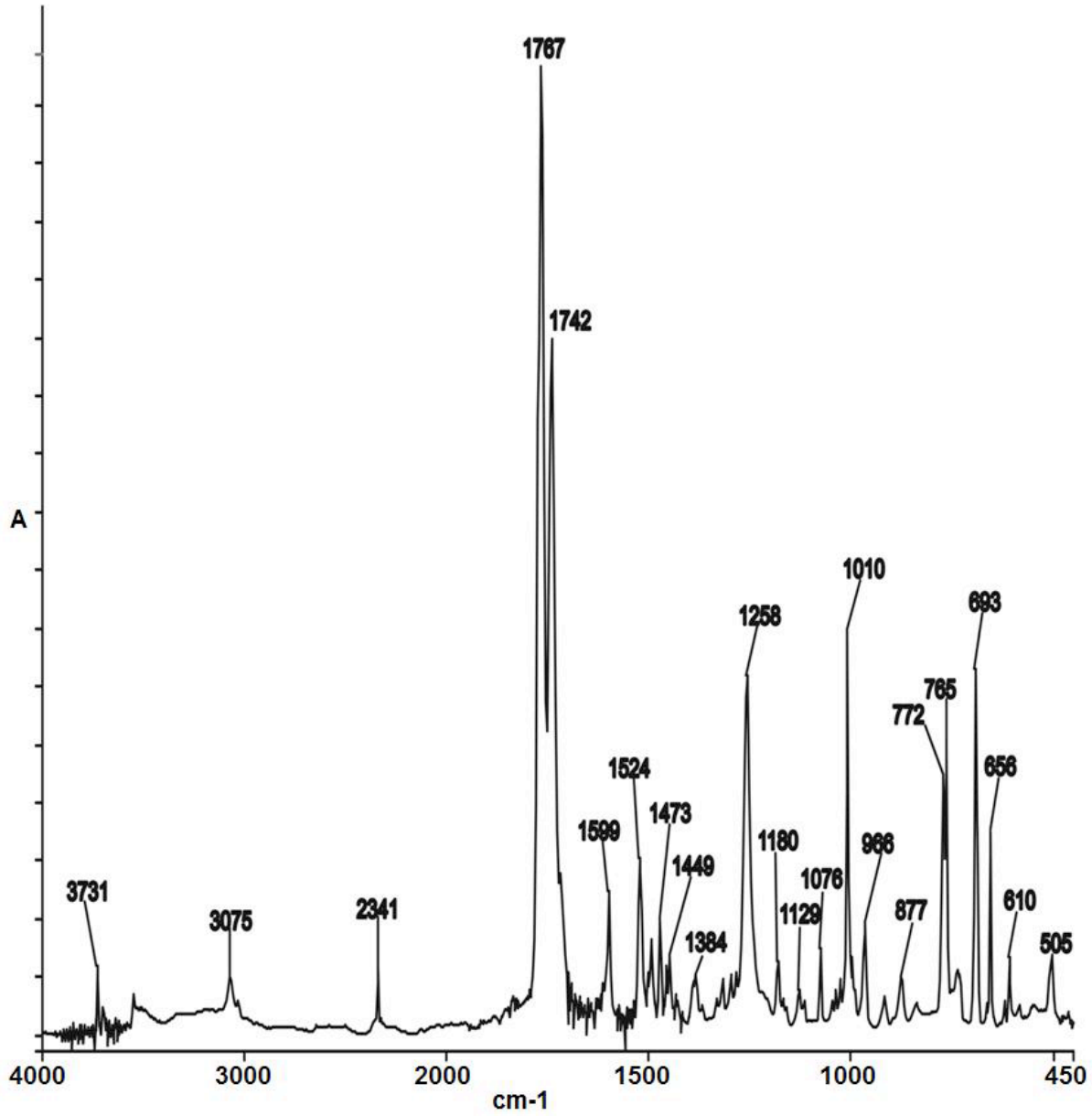


Figure S13. IR spectrum of 3,4-diphenylsydnone in Ar matrix at 20 K.

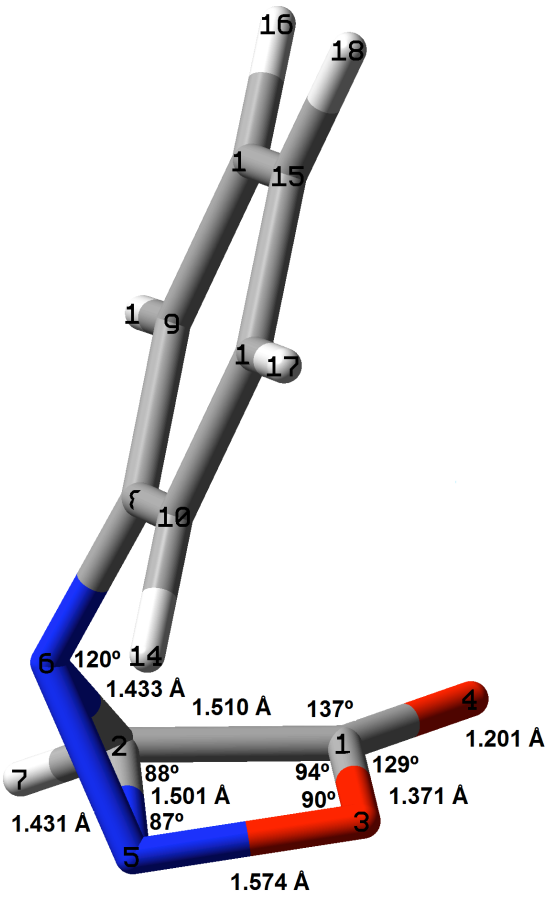
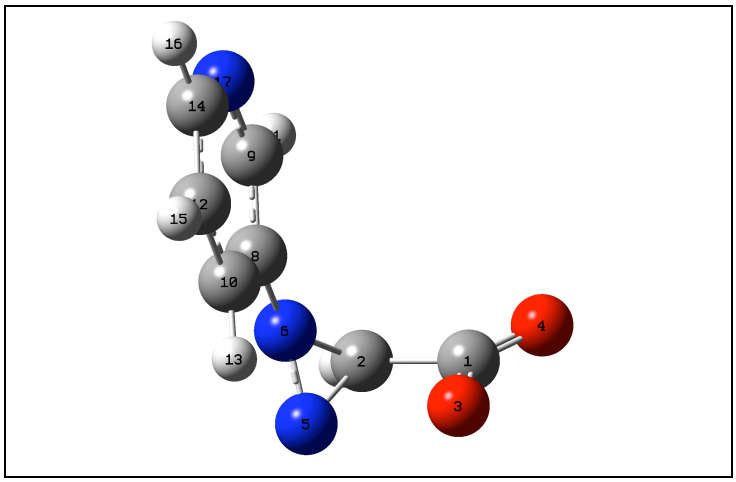


Figure S14. Calculated structure of ***endo*-17** at the QCISD level (*endo* isomer of Earl's bicyclic lactone derived from 3-phenylsydnone).



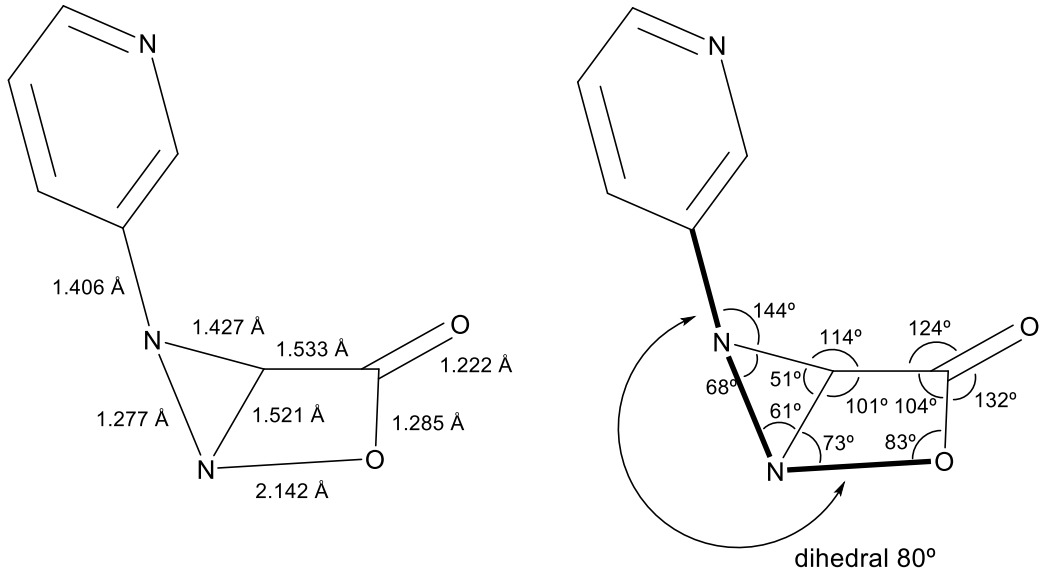


Figure S15. Calculated structure of ***endo*-20** at the B3LYP/6-31G* level.

Calculations

Calculations were performed using Gaussian 03 or 09.[1,2,3]

3-Phenylsydnone
Energies related to Scheme 12 at the B3LYP/6-31+G** level + ZPVE:

B3LYP/6-31+G** (R= phenyl)	HF +ZPVE (Hartree)	ΔE (cf. **19**) (kcal/mol)	$< S^2 >$
16	-568.228313	**0.0**	
exo-17	-568.165645	39.3	
TS (*exo-/endo-17*)	-568.157120	44.7	
endo-17	-568.175784	33.0	
18	-379.746422	-60.8	
CO_2 + 32	-379.669238	-12.4	
CO_2 + 31	-379.641378	5.1	
CO_2 + 34Z T0 Cs	-379.666306	-10.6	
CO_2 + 34Z S1 C1	-379.654020	-2.8	
CO_2 + 34E T0 C1	-379.665073	-9.8	
CO_2 + 34E S1 C1	-379.650603	-0.7	
CO_2 + 34E S2 C1	-379.649904	-0.3	
TS (**19**-**20** ***exo***)	-568.116445	70.2	
TS (*exo*-17-**31**)	-568.157121	44.7	
TS (*endo*-17-**32**)	-568.170699	36.2	
TS (**31**-**33**)	-568.128517	62.6	
TS (**31**-**32**)	-379.592071	36.0	
TS (**31**-**32**) 180º	-379.591191	36.6	
TS (**31**-**34 S1**)	-379.648655	0.5	0.213644
TS (**34Z S1**-18)	-379.627610	13.7	

TS (**34E S1**-18)	**-379.619691**	18.7
CO_2	-188.578829	

QCISD/6-31+G** (R= phenyl)	HF +ZPVE (Hartree)	ΔE (cf. **19**) (kcal/mol)	$< S^2 >$
exo-20	-566.719601	946.7	
endo-20	-566.722479	944.9	

3-(3-Pyridyl)sydnone
Energies calculated at the B3LYP/6-31+G** level

+ ZPVE:

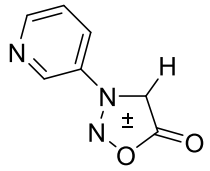
RB3LYP/6-31+G** (R= 3-pyridyl)	HF +ZPVE (Hartree)	ΔE (cf. **16**) (kcal/mol)
16	-584.270532	-37.9
exo-17	**-584.210076**	**0.0**
endo-17	-584.216774	-4.2
CO_2 + 31	-395.714712	-52.4
13E	-584.233592	-14.8
13Z	-584.233987	-15.0
14	-584.219825	-6.1
3	-584.231671	-13.6
TS (*exo-/endo*-**17**)	-584.200451	6.0
CO_2	-188.578829	

CO_2

```
RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: D*H
State=1-SGG
HF= -188.5903926\RMSD=1.161e-10\RMSF=5.958e-05
Zero-point correction= 0.011564
Sum of electronic and thermal Free Energies= -188.578829

 C                  0.00000000    0.00000000    0.00000000
 O                  0.00000000    0.00000000    1.16943400
 O                  0.00000000    0.00000000   -1.16943400
```

3-Pyridylsydnone, 19



RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: C1
State=1-A
HF=-584.3894347\RMSD=2.828e-09\RMSF=6.203e-05
Zero-point correction= 0.118903
Sum of electronic and thermal Free Energies= -584.270532

O	2.50098200	-0.97997400	0.43450500
O	3.94320500	0.67032000	-0.33100800
N	-2.89260800	-1.09679100	-0.38864500
N	0.62304900	-0.08523900	0.05356800
N	1.16313600	-1.17660600	0.54768600
C	-3.51196400	0.05159500	-0.08398500
C	-1.55854200	-1.12049500	-0.34261200
C	-0.80656400	0.00248900	0.01782200
C	-1.44572600	1.19855700	0.33837600
C	-2.83714200	1.22090100	0.27893800
C	2.80393300	0.31079000	-0.14984900
C	1.50654500	0.84374100	-0.37464300
H	-4.59789900	0.03517400	-0.13235900
H	-1.06273700	-2.05166300	-0.60049600
H	-0.87648300	2.07203300	0.63924900
H	-3.38927400	2.12268200	0.52120400
H	1.21461300	1.76399600	-0.84812200

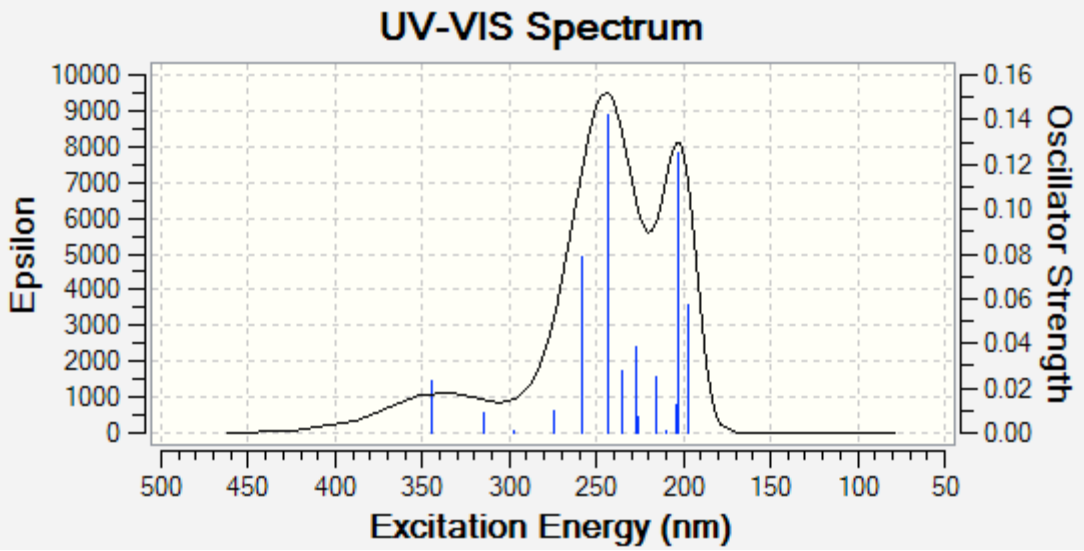
Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	46.9	0.4	0
2	A	88.4	4.3	0
3	A	115.2	2.7	0
4	A	225.4	1.3	0
5	A	296.8	0.3	0
6	A	325.1	4.6	1
7	A	396.5	2.2	0
8	A	400.2	2.1	0
9	A	470.3	2.3	0
10	A	541.3	10.4	1
11	A	595.5	3.0	0
12	A	604.4	29.8	3
13	A	625.5	15.1	2
14	A	642.0	10.4	1
15	A	683.8	36.0	4
16	A	689.1	11.4	1
17	A	690.5	11.8	1
18	A	789.1	24.1	3
19	A	798.4	39.5	4
20	A	909.5	2.4	0
21	A	935.0	14.7	2
22	A	939.9	5.3	1
23	A	968.6	0.2	0
24	A	986.6	26.2	3
25	A	1006.3	5.2	1
26	A	1026.1	1.6	0
27	A	1065.2	15.4	2
28	A	1099.6	11.0	1
29	A	1156.9	31.3	3
30	A	1178.8	23.2	3
31	A	1214.1	27.0	3
32	A	1252.3	2.7	0
33	A	1304.0	10.8	1
34	A	1343.1	55.8	6

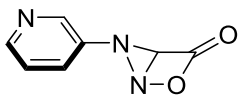
35	A	1396.6	22.2	2
36	A	1444.2	35.0	4
37	A	1461.6	27.1	3
38	A	1565.1	25.1	3
39	A	1573.5	1.5	0
40	A	1789.2	926.5	100
41	A	3063.8	9.4	1
42	A	3082.9	5.6	1
43	A	3085.3	1.9	0
44	A	3097.6	3.2	0
45	A	3202.6	10.9	1

Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	3.6005 eV	344.35 nm	f=0.0233
Excited State 2:	Singlet-A	3.9415 eV	314.56 nm	f=0.0085
Excited State 3:	Singlet-A	4.1752 eV	296.95 nm	f=0.0011
Excited State 4:	Singlet-A	4.5108 eV	274.86 nm	f=0.0100
Excited State 5:	Singlet-A	4.8066 eV	257.95 nm	f=0.0015
Excited State 6:	Singlet-A	4.8087 eV	257.83 nm	f=0.0785
Excited State 7:	Singlet-A	5.0852 eV	243.82 nm	f=0.1419
Excited State 8:	Singlet-A	5.2766 eV	234.97 nm	f=0.0273
Excited State 9:	Singlet-A	5.4584 eV	227.14 nm	f=0.0387
Excited State 10:	Singlet-A	5.4816 eV	226.18 nm	f=0.0075
Excited State 11:	Singlet-A	5.7559 eV	215.40 nm	f=0.0250
Excited State 12:	Singlet-A	5.9129 eV	209.69 nm	f=0.0013
Excited State 13:	Singlet-A	6.0717 eV	204.20 nm	f=0.0126
Excited State 14:	Singlet-A	6.0955 eV	203.40 nm	f=0.1252
Excited State 15:	Singlet-A	6.2818 eV	197.37 nm	f=0.0569



***exo*-20, R= 3-pyridyl**



RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: C1
State=1-A
HF= -584.3274708\RMSD=5.084e-09\RMSF=3.972e-05

Zero-point correction= 0.117394
Sum of electronic and thermal Free Energies= -584.210076

C	2.86526100	-0.27540400	-0.00140600
C	1.46639300	-0.50245100	0.52916200
O	2.63511800	1.08358300	-0.13821300
O	3.86319800	-0.89130700	-0.20851200
N	1.28417900	0.95397400	0.51926100
N	0.57992600	0.10224200	-0.45708200
H	1.12840800	-1.15484700	1.32693700
C	-0.82820700	0.02844400	-0.19424500
C	-1.46202700	-1.21738200	-0.11826300
C	-1.60465500	1.18833500	-0.13354800
H	-0.88018700	-2.13526800	-0.17909700
C	-2.98235800	1.04484400	0.00916100
H	-1.13497100	2.16445200	-0.19173800
C	-3.52598900	-0.24163000	0.07884500
H	-3.62694100	1.91608900	0.06605000
H	-4.59785400	-0.38471500	0.19038500
N	-2.78489000	-1.35513800	0.01539700

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.78646	1.99950	3.16509	0.04895	5.21354
C	2	-0.01480	1.99920	3.99527	0.02033	6.01480
O	3	-0.38587	1.99980	6.36368	0.02239	8.38587
O	4	-0.51460	1.99976	6.48852	0.02631	8.51460
N	5	-0.00502	1.99957	4.98219	0.02327	7.00502
N	6	-0.30673	1.99940	5.27075	0.03657	7.30673
H	7	0.27457	0.00000	0.72342	0.00200	0.72543
C	8	0.07372	1.99890	3.90517	0.02220	5.92628
C	9	-0.00545	1.99910	3.98143	0.02492	6.00545
C	10	-0.20788	1.99902	4.19405	0.01480	6.20788
H	11	0.23815	0.00000	0.76041	0.00144	0.76185
C	12	-0.26716	1.99912	4.25417	0.01387	6.26716
H	13	0.26742	0.00000	0.73056	0.00202	0.73258
C	14	0.00299	1.99923	3.97184	0.02594	5.99701
H	15	0.25905	0.00000	0.73952	0.00142	0.74095
H	16	0.24000	0.00000	0.75880	0.00120	0.76000
N	17	-0.43488	1.99947	5.40764	0.02777	7.43488

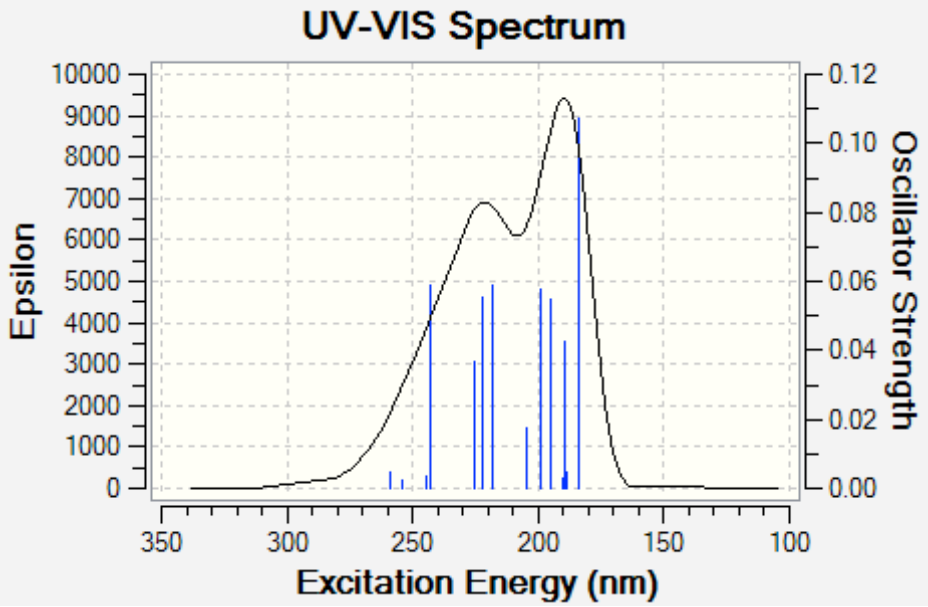
Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	31.1	3.6	1
2	A	91.2	3.9	1
3	A	103.2	3.4	1
4	A	185.2	8.1	1
5	A	267.0	0.3	0
6	A	317.9	0.2	0
7	A	386.1	6.0	1
8	A	396.2	3.6	1
9	A	500.4	2.3	0
10	A	505.9	2.3	0
11	A	588.9	4.1	1
12	A	621.5	8.3	1
13	A	637.0	26.7	4
14	A	687.1	27.0	4
15	A	693.8	50.6	8

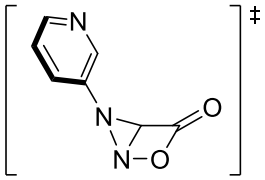
16	A	737.0	9.8	2
17	A	779.9	28.8	5
18	A	802.0	8.1	1
19	A	820.5	40.9	7
20	A	878.4	9.4	2
21	A	895.8	0.8	0
22	A	926.0	1.3	0
23	A	945.6	2.7	0
24	A	960.7	0.1	0
25	A	992.8	17.4	3
26	A	1011.8	16.7	3
27	A	1030.9	9.2	1
28	A	1068.9	68.2	11
29	A	1096.6	6.0	1
30	A	1131.5	22.5	4
31	A	1176.5	13.2	2
32	A	1207.4	34.9	6
33	A	1254.7	5.7	1
34	A	1261.9	33.2	5
35	A	1311.5	3.8	1
36	A	1405.9	40.7	7
37	A	1452.7	37.4	6
38	A	1557.0	8.1	1
39	A	1567.7	6.4	1
40	A	1867.9	625.9	100
41	A	3045.2	14.9	2
42	A	3060.3	7.7	1
43	A	3083.0	10.7	2
44	A	3095.7	0.2	0
45	A	3097.2	2.4	0

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	4.7827 eV	259.23 nm	f=0.0046
Excited State	2:	Singlet-A	4.8764 eV	254.25 nm	f=0.0026
Excited State	3:	Singlet-A	5.0703 eV	244.53 nm	f=0.0033
Excited State	4:	Singlet-A	5.1008 eV	243.07 nm	f=0.0590
Excited State	5:	Singlet-A	5.4946 eV	225.65 nm	f=0.0365
Excited State	6:	Singlet-A	5.5886 eV	221.85 nm	f=0.0556
Excited State	7:	Singlet-A	5.6755 eV	218.45 nm	f=0.0591
Excited State	8:	Singlet-A	6.0478 eV	205.01 nm	f=0.0174
Excited State	9:	Singlet-A	6.2351 eV	198.85 nm	f=0.0576
Excited State	10:	Singlet-A	6.3637 eV	194.83 nm	f=0.0547
Excited State	11:	Singlet-A	6.5077 eV	190.52 nm	f=0.0027
Excited State	12:	Singlet-A	6.5550 eV	189.14 nm	f=0.0425
Excited State	13:	Singlet-A	6.5809 eV	188.40 nm	f=0.0049
Excited State	14:	Singlet-A	6.7298 eV	184.23 nm	f=0.1070
Excited State	15:	Singlet-A	6.7502 eV	183.68 nm	f=0.0204



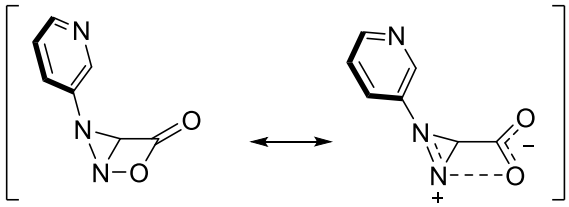
TS (*exo*-20 – *endo*-20), R= 3-pyridyl



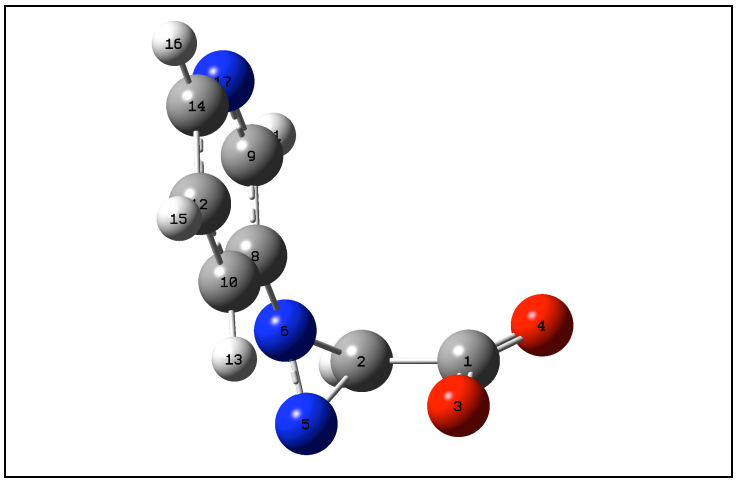

```
RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: C1
State=1-A
HF= -584.3167105\RMSD=3.426e-09\RMSF=1.044e-05
Zero-point correction= 0.116259
Sum of electronic and thermal Free Energies= -584.200451
Imaginary frequency= -307.8230 cm-1

 C                 -2.87410000    0.25955100   -0.12557600
 C                 -1.67218500    0.31107700    0.81664300
 O                 -2.67610700   -0.97498100   -0.59394000
 O                 -3.76177200    1.03848900   -0.36117800
 N                 -1.32836700   -1.11053400    0.54602800
 N                 -0.53535900   -0.13695000    0.08692300
 H                 -1.60455600    0.73615700    1.81397700
 C                  0.86532000   -0.03956900    0.03131300
 C                  1.46395600    1.22687900   -0.01045900
 C                  1.66338200   -1.18535700   -0.03087100
 H                  0.85276400    2.12601200    0.02510600
 C                  3.04013100   -1.00381500   -0.12703700
 H                  1.21496400   -2.17282000   -0.00358900
 C                  3.55561100    0.29621200   -0.15125900
 H                  3.70621800   -1.85892400   -0.17889300
 H                  4.62653000    0.46622600   -0.22391000
 N                  2.78578500    1.39111500   -0.09127400
```

endo-20, R= 3-pyridyl



RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: C1
State=1-A
HF= -584.3335776\RMSD=2.114e-09\RMSF=2.866e-05
Zero-point correction= 0.116804
Sum of electronic and thermal Free Energies= -584.216774



C	-2.47985200	0.28790600	-0.48154500
C	-1.88946400	0.18378300	0.92932300
O	-2.16964900	-0.83185800	-1.03117500
O	-3.10933000	1.25478600	-0.88528800
N	-1.38565400	-1.25182600	0.91754700
N	-0.54436100	-0.29249400	0.96156700
H	-2.28709100	0.62126300	1.83978300
C	0.74840200	-0.11120700	0.44001000
C	1.34267800	1.15459000	0.51145600
C	1.43549100	-1.18963100	-0.12556300
H	0.80334600	1.99558300	0.94124900
C	2.71753000	-0.93985700	-0.60051300
H	0.96566900	-2.16443300	-0.20244000
C	3.24148400	0.35427200	-0.48570500
H	3.30207100	-1.72833700	-1.06230000
H	4.24218200	0.57481600	-0.84810800
N	2.57402000	1.38411300	0.05499300

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.72124	1.99954	3.22466	0.05456	5.27876
C	2	0.00569	1.99927	3.96968	0.02537	5.99431
O	3	-0.56262	1.99981	6.54944	0.01337	8.56262
O	4	-0.61584	1.99979	6.59220	0.02386	8.61584
N	5	-0.00055	1.99969	4.97171	0.02916	7.00055
N	6	-0.11889	1.99926	5.08220	0.03742	7.11889

H	7	0.26703	0.00000	0.73149	0.00147	0.73297
C	8	0.06211	1.99892	3.92016	0.01882	5.93789
C	9	0.03892	1.99914	3.93716	0.02478	5.96108
C	10	-0.17970	1.99904	4.16603	0.01464	6.17970
H	11	0.25158	0.00000	0.74693	0.00149	0.74842
C	12	-0.26578	1.99913	4.25290	0.01375	6.26578
H	13	0.27963	0.00000	0.71852	0.00185	0.72037
C	14	0.03462	1.99924	3.94051	0.02564	5.96538
H	15	0.26721	0.00000	0.73146	0.00133	0.73279
H	16	0.24726	0.00000	0.75161	0.00113	0.75274
N	17	-0.43190	1.99948	5.40454	0.02787	7.43190

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	23.2	14.0	2
2	A	52.8	12.5	2
3	A	96.3	3.8	1
4	A	165.2	84.5	14
5	A	181.2	7.7	1
6	A	229.2	63.8	11
7	A	380.1	6.9	1
8	A	383.6	2.0	0
9	A	406.1	0.4	0
10	A	450.1	6.3	1
11	A	502.3	29.1	5
12	A	524.4	6.3	1
13	A	600.1	2.8	0
14	A	638.1	17.5	3
15	A	675.8	24.1	4
16	A	707.2	5.8	1
17	A	752.7	5.6	1
18	A	786.6	44.7	8
19	A	834.3	3.3	1
20	A	856.3	4.8	1
21	A	898.0	2.3	0
22	A	937.2	1.8	0
23	A	967.4	0.0	0
24	A	992.5	9.9	2
25	A	1005.6	14.2	2
26	A	1017.2	1.0	0
27	A	1083.1	10.1	2
28	A	1095.0	10.6	2
29	A	1165.4	14.2	2
30	A	1184.1	21.1	4
31	A	1222.5	31.1	5
32	A	1264.8	5.3	1
33	A	1274.2	49.5	8
34	A	1312.9	2.3	0
35	A	1408.2	27.1	5
36	A	1450.8	3.8	1
37	A	1521.3	236.2	40
38	A	1556.5	11.5	2
39	A	1564.7	58.6	10
40	A	1711.2	584.5	100
41	A	3062.2	6.2	1
42	A	3068.0	4.0	1
43	A	3085.3	3.1	1
44	A	3090.8	4.4	1
45	A	3102.5	2.3	0

Excitation energies and oscillator strengths:

```
Excited State   1:      Singlet-A      2.3152 eV  535.52 nm  f=0.0201
Excited State   2:      Singlet-A      2.6598 eV  466.14 nm  f=0.0004
Excited State   3:      Singlet-A      3.5138 eV  352.85 nm  f=0.0054
Excited State   4:      Singlet-A      3.6214 eV  342.36 nm  f=0.2297
Excited State   5:      Singlet-A      4.2609 eV  290.98 nm  f=0.0180
Excited State   6:      Singlet-A      4.4199 eV  280.51 nm  f=0.0170
Excited State   7:      Singlet-A      4.5370 eV  273.27 nm  f=0.0106
Excited State   8:      Singlet-A      4.6349 eV  267.50 nm  f=0.0082
Excited State   9:      Singlet-A      4.7851 eV  259.10 nm  f=0.0998
Excited State  10:      Singlet-A      4.8902 eV  253.54 nm  f=0.0049
Excited State  11:      Singlet-A      5.0704 eV  244.52 nm  f=0.0028
Excited State  12:      Singlet-A      5.1430 eV  241.07 nm  f=0.0187
Excited State  13:      Singlet-A      5.3848 eV  230.25 nm  f=0.0021
Excited State  14:      Singlet-A      5.4039 eV  229.44 nm  f=0.0346
Excited State  15:      Singlet-A      5.4906 eV  225.81 nm  f=0.0107
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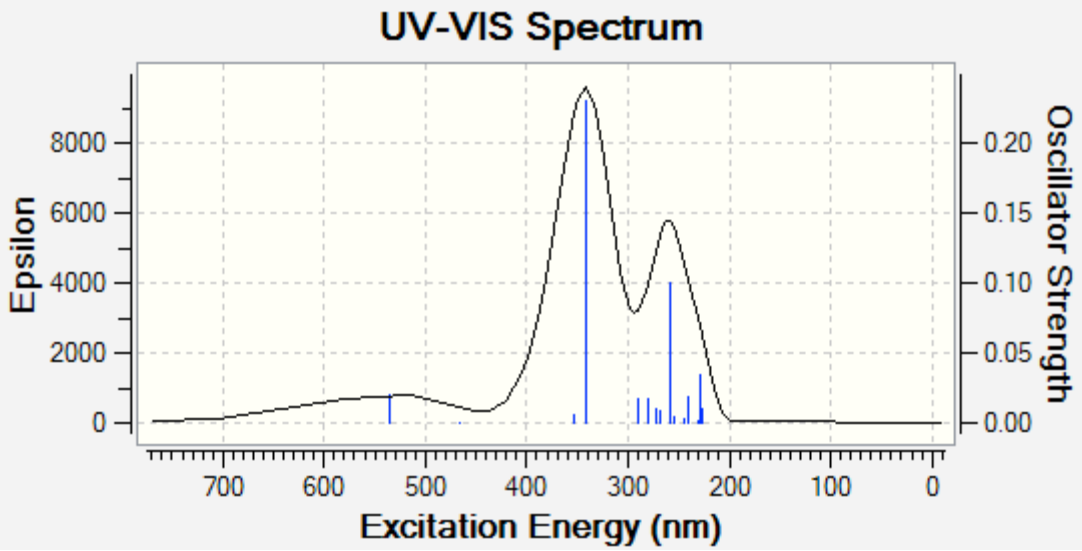
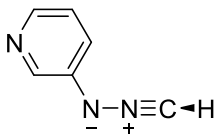


32, R= 3-pyridyl




```
RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: C1
State=1-A
HF= -395.8162365\RMSD=4.264e-09\RMSF=4.178e-05
Zero-point correction= 0.101525
Sum of electronic and thermal Free Energies= -395.714712

 C                -2.49709500    0.41315800   -0.00285700
 C                -0.94484700   -1.27117900    0.00537500
 C                 0.12670600   -0.36028800    0.00771400
 C                -0.16713200    1.01023200    0.00511200
 C                -1.50565300    1.39757100   -0.00297800
 N                 1.42116400   -0.92386300    0.00194500
 H                -3.54941700    0.68653300   -0.00571200
 H                -0.73079900   -2.33739500    0.00512500
 H                 0.62713100    1.75065500    0.00562000
 H                -1.77831300    2.44857000   -0.00750600
 N                 2.38431300   -0.13823800    0.02048600
```

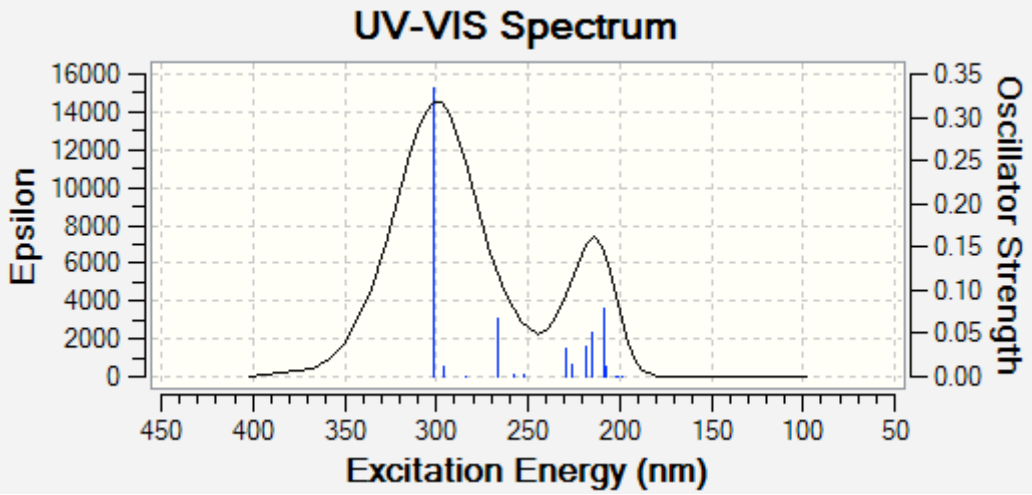
C	3.37307700	0.51787000	-0.13599000
H	4.06159100	0.95022900	0.57648200
N	-2.22555200	-0.90115300	0.00153000

Vibrational frequencies (scaled by 0.9613):

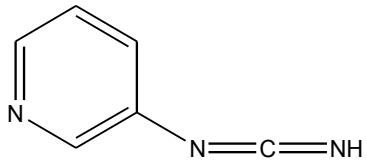
ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	69.6	1.6	0
2	A	136.8	0.2	0
3	A	217.7	4.6	1
4	A	352.9	2.5	0
5	A	399.5	3.4	0
6	A	444.3	3.6	0
7	A	447.3	36.8	5
8	A	468.9	19.8	3
9	A	600.6	1.6	0
10	A	621.7	770.1	100
11	A	652.6	15.0	2
12	A	670.5	13.1	2
13	A	692.3	40.0	5
14	A	784.4	31.3	4
15	A	806.8	2.8	0
16	A	895.3	0.6	0
17	A	917.8	2.8	0
18	A	952.5	0.0	0
19	A	989.3	10.5	1
20	A	1022.1	1.6	0
21	A	1094.0	15.2	2
22	A	1132.7	22.2	3
23	A	1175.4	5.0	1
24	A	1255.6	16.7	2
25	A	1297.9	41.3	5
26	A	1311.0	20.4	3
27	A	1406.8	56.9	7
28	A	1448.5	38.6	5
29	A	1548.6	5.4	1
30	A	1564.0	9.7	1
31	A	2041.5	713.9	93
32	A	3055.3	9.6	1
33	A	3061.3	10.0	1
34	A	3071.3	10.6	1
35	A	3084.6	10.8	1
36	A	3148.4	38.8	5

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	4.1159 eV	301.23 nm	f=0.3346
Excited State	2:	Singlet-A	4.1862 eV	296.17 nm	f=0.0127
Excited State	3:	Singlet-A	4.3628 eV	284.19 nm	f=0.0009
Excited State	4:	Singlet-A	4.6510 eV	266.58 nm	f=0.0682
Excited State	5:	Singlet-A	4.8045 eV	258.06 nm	f=0.0027
Excited State	6:	Singlet-A	4.9226 eV	251.87 nm	f=0.0031
Excited State	7:	Singlet-A	5.4004 eV	229.58 nm	f=0.0328
Excited State	8:	Singlet-A	5.4936 eV	225.69 nm	f=0.0135
Excited State	9:	Singlet-A	5.6855 eV	218.07 nm	f=0.0354
Excited State	10:	Singlet-A	5.7705 eV	214.86 nm	f=0.0512
Excited State	11:	Singlet-A	5.9421 eV	208.65 nm	f=0.0779
Excited State	12:	Singlet-A	5.9814 eV	207.28 nm	f=0.0118
Excited State	13:	Singlet-A	6.1511 eV	201.56 nm	f=0.0005
Excited State	14:	Singlet-A	6.1727 eV	200.86 nm	f=0.0004
Excited State	15:	Singlet-A	6.2491 eV	198.40 nm	f=0.0004



3-Pyridylcarbodiimide:



a) Method: B3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.574490	0.330115	0.031757
2	7	2.233906	-0.962337	0.037091
3	6	0.937198	-1.264472	0.005250
4	6	-0.079300	-0.301808	-0.028815
5	6	0.288108	1.046966	-0.036526
6	6	1.640279	1.364497	-0.005680
7	7	-1.408055	-0.748998	-0.067874
8	6	-2.457344	-0.136308	0.016530
9	7	-3.555394	0.392645	-0.060893
10	1	3.638002	0.547276	0.057033

```
   11          1                    0.668774   -2.316572
0.006480
   12          1                   -0.468891    1.823061   -
0.071117
   13          1                    1.967570    2.397572   -
0.012124
   14          1                   -4.119233    0.545557
0.766363
 -------------------------------------------------------------------
-
```

Energy = -395.978101
E+ZPVE = -395.875796

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	48.9	4.7	0
2	A	107.2	2.0	0
3	A	222.6	13.4	1
4	A	375.7	8.2	1
5	A	405.9	41.2	3
6	A	423.6	45.7	3
7	A	481.3	0.9	0
8	A	503.1	20.9	2
9	A	586.2	43.5	3
10	A	630.0	3.5	0
11	A	667.4	29.3	2
12	A	716.3	28.6	2
13	A	807.7	4.5	0
14	A	814.0	37.1	3
15	A	873.8	437.5	32
16	A	931.8	1.2	0
17	A	954.2	2.5	0
18	A	986.1	0.0	0
19	A	1036.0	13.2	1
20	A	1060.2	1.9	0
21	A	1134.2	26.8	2
22	A	1160.2	34.0	2
23	A	1219.1	7.1	1
24	A	1279.9	7.3	1
25	A	1354.1	0.6	0
26	A	1417.8	1.6	0
27	A	1466.9	38.8	3
28	A	1513.8	74.0	5
29	A	1602.6	2.0	0
30	A	1623.9	21.4	2
31	A	2231.5	1384.4	100
32	A	3157.0	12.5	1
33	A	3164.3	9.5	1
34	A	3172.2	8.2	1
35	A	3190.4	9.8	1

```
  36        A          3586.9       99.1          7
```

b) Method: B3LYP6-31G*

```
---------------------------------------------------------------------
-
 Center     Atomic                     Coordinates (Angstroms)
 Number     Number                    X           Y           Z
 ---------------------------------------------------------------------
-
    1             6                          2.577094     0.331785
0.025777
    2             7                          2.240093    -0.964057
0.030179
    3             6                          0.940465    -1.264935
0.004635
    4           6                         -0.079655    -0.302796    -
0.022894
    5           6                          0.287651     1.049046    -
0.029769
    6           6                          1.641439     1.368353    -
0.004736
    7           7                         -1.406768    -0.755190    -
0.054557
    8             6                           -2.459297    -0.132548
0.020575
    9           7                         -3.566922     0.388793    -
0.076177
   10             1                          3.642996     0.550696
0.046199
   11             1                          0.671071    -2.319252
0.005548
   12           1                         -0.474391     1.823692    -
0.058301
   13           1                          1.968442     2.404064    -
0.010082
   14             1                           -4.119112     0.560546
0.758989
 ---------------------------------------------------------------------------------------------------
---
```

Energy = -395.8683033
E+ZPVE = -395.765237

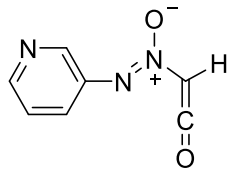
Vibrational Frequencies:

Scaled by a factor of 0.9613

```
ModeNr.  Symmetry  Wavenumber  Abs.Int.  Rel.Int.
   1        A           54.4       4.4         0
   2        A          101.9       1.7         0
```

3	A	220.4	13.7	1
4	A	361.3	6.5	1
5	A	394.0	44.6	4
6	A	410.4	38.4	3
7	A	460.5	0.7	0
8	A	478.5	17.5	2
9	A	565.8	43.5	4
10	A	604.3	4.0	0
11	A	634.1	27.7	2
12	A	694.1	18.9	2
13	A	779.0	5.2	0
14	A	793.3	26.1	2
15	A	874.1	468.1	41
16	A	902.8	0.3	0
17	A	928.2	3.1	0
18	A	951.0	0.1	0
19	A	997.7	15.3	1
20	A	1027.4	0.9	0
21	A	1100.0	22.5	2
22	A	1123.6	30.2	3
23	A	1183.7	4.1	0
24	A	1253.6	5.9	1
25	A	1316.2	0.4	0
26	A	1374.9	1.1	0
27	A	1424.3	41.0	4
28	A	1472.5	65.7	6
29	A	1558.5	1.9	0
30	A	1581.1	17.4	2
31	A	2160.1	1143.9	100
32	A	3056.5	16.4	1
33	A	3065.1	15.0	1
34	A	3071.3	11.9	1
35	A	3088.6	13.7	1
36	A	3427.0	57.4	5

14E, R= 3-pyridyl



RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: C1
State=1-A
HF= -584.3506824\RMSD=3.828e-09\RMSF=3.224e-05
Zero-point correction= 0.117091
Sum of electronic and thermal Free Energies= -584.233592

C	-3.50492300	-0.27588700	0.00002800
N	-2.93955600	0.93652300	0.00008500

C	-1.60355000	1.02600400	0.00006700
C	-0.76184200	-0.11507700	-0.00001000
C	-1.38308400	-1.38081900	-0.00006700
C	-2.76741100	-1.46482600	-0.00004900
N	0.63545700	-0.18323400	-0.00004100
C	2.76697700	0.63851900	0.00002000
C	3.21566200	-0.61552500	-0.00004400
O	3.66588200	-1.68667800	-0.00009800
N	1.35723200	0.88106100	-0.00000600
O	0.98907300	2.08185500	0.00010100
H	-4.59246600	-0.29805700	0.00004600
H	-1.18482200	2.02156500	0.00011300
H	-0.75764800	-2.26797800	-0.00012600
H	-3.27043600	-2.42667600	-0.00009300
H	3.42283600	1.49495000	0.00010600

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	34.8	0.9	0
2	A	77.1	0.0	0
3	A	86.6	0.2	0
4	A	125.6	5.1	1
5	A	203.1	2.3	0
6	A	270.0	3.3	0
7	A	342.1	1.8	0
8	A	351.8	19.4	2
9	A	397.1	2.7	0
10	A	491.2	6.2	1
11	A	498.7	15.1	1
12	A	507.3	0.7	0
13	A	516.3	31.4	3
14	A	545.7	7.2	1
15	A	599.4	3.1	0
16	A	672.2	16.9	2
17	A	682.3	26.2	3
18	A	725.4	0.0	0
19	A	790.8	31.5	3
20	A	860.3	1.4	0
21	A	906.3	1.1	0
22	A	934.7	2.3	0
23	A	960.5	0.1	0
24	A	978.6	21.2	2
25	A	984.7	8.2	1
26	A	1027.5	0.9	0
27	A	1083.2	1.7	0
28	A	1097.1	9.6	1
29	A	1178.1	8.5	1
30	A	1205.5	20.1	2
31	A	1243.2	15.6	2
32	A	1286.5	86.9	9
33	A	1311.9	1.0	0
34	A	1351.7	158.0	16
35	A	1399.2	32.7	3
36	A	1438.8	30.4	3
37	A	1478.1	304.0	30
38	A	1533.5	12.1	1
39	A	1568.2	28.4	3
40	A	2137.1	1011.0	100
41	A	3052.3	11.9	1
42	A	3076.4	11.4	1
43	A	3090.5	10.5	1

```
  44        A          3146.3        0.5          0
  45        A          3160.4       33.5          3

Excitation energies and oscillator strengths:
Excited State   1:      Singlet-A      2.9740 eV  416.89 nm  f=0.0001
Excited State   2:      Singlet-A      3.4984 eV  354.41 nm  f=0.0000
Excited State   3:      Singlet-A      3.7541 eV  330.26 nm  f=0.1972
Excited State   4:      Singlet-A      4.0633 eV  305.14 nm  f=0.3063
Excited State   5:      Singlet-A      4.0747 eV  304.28 nm  f=0.0000
Excited State   6:      Singlet-A      4.1574 eV  298.22 nm  f=0.0001
Excited State   7:      Singlet-A      4.5318 eV  273.59 nm  f=0.0051
Excited State   8:      Singlet-A      4.6493 eV  266.67 nm  f=0.0286
Excited State   9:      Singlet-A      4.7431 eV  261.40 nm  f=0.0000
Excited State  10:      Singlet-A      4.7704 eV  259.91 nm  f=0.0038
Excited State  11:      Singlet-A      5.1165 eV  242.32 nm  f=0.0591
Excited State  12:      Singlet-A      5.3306 eV  232.59 nm  f=0.1624
Excited State  13:      Singlet-A      5.4499 eV  227.50 nm  f=0.0007
Excited State  14:      Singlet-A      5.7105 eV  217.12 nm  f=0.0102
Excited State  15:      Singlet-A      5.7349 eV  216.19 nm  f=0.0082
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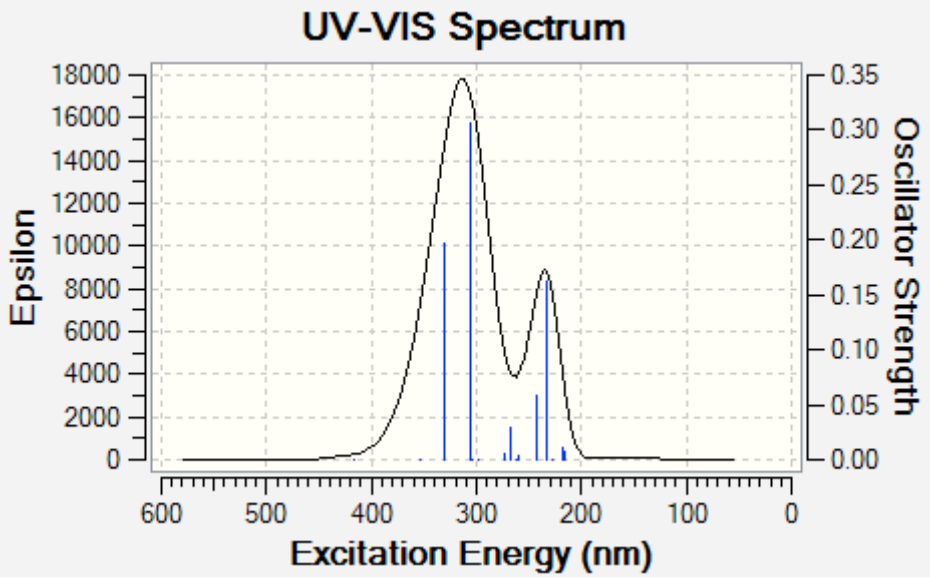
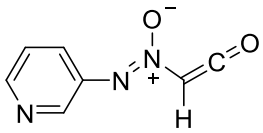


14Z, R= 3-pyridyl




```
RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: C1
State=1-A
HF= -584.351054\RMSD=3.485e-09\RMSF=6.774e-05
Zero-point correction= 0.117067
Sum of electronic and thermal Free Energies= -584.233987

 C                 -3.64490800   -0.48753700   -0.00005200
 N                 -2.68885200   -1.42352500   -0.00010300
 C                 -1.40671400   -1.03654900   -0.00007000
 C                 -1.02196900    0.32832600    0.00001900
 C                 -2.04940400    1.29372600    0.00007100
 C                 -3.37476600    0.88524500    0.00003600
```

N	0.26041400	0.89107800	0.00006500
C	2.53689300	0.85738200	0.00006800
C	3.65648000	0.13083200	0.00001800
O	4.67088000	-0.43271300	-0.00002100
N	1.30486100	0.15173800	0.00003000
O	1.38389000	-1.11501600	-0.00005800
H	-4.67048400	-0.85030500	-0.00008200
H	-0.66356800	-1.82003600	-0.00011300
H	-1.77512200	2.34392000	0.00013900
H	-4.18486400	1.60766400	0.00007500
H	2.54724100	1.93699900	0.00013000

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	48.5	0.0	0
2	A	62.2	2.2	0
3	A	90.4	0.0	0
4	A	123.7	1.5	0
5	A	222.9	2.7	0
6	A	279.1	2.8	0
7	A	306.6	1.4	0
8	A	347.3	17.9	1
9	A	397.6	2.4	0
10	A	428.9	13.2	1
11	A	484.3	7.0	1
12	A	493.5	9.3	1
13	A	551.9	34.9	3
14	A	593.4	5.7	0
15	A	615.3	8.0	1
16	A	671.9	11.3	1
17	A	682.1	32.9	3
18	A	781.7	2.2	0
19	A	793.1	28.6	2
20	A	825.0	0.7	0
21	A	910.6	0.9	0
22	A	939.0	2.5	0
23	A	963.0	0.0	0
24	A	972.0	37.1	3
25	A	985.8	8.3	1
26	A	1024.9	2.1	0
27	A	1072.8	0.5	0
28	A	1096.0	9.9	1
29	A	1173.6	7.5	1
30	A	1181.4	16.3	1
31	A	1242.1	11.6	1
32	A	1285.7	62.4	5
33	A	1315.8	12.7	1
34	A	1351.3	24.0	2
35	A	1396.7	7.7	1
36	A	1444.6	14.6	1
37	A	1474.0	371.1	29
38	A	1534.0	15.0	1
39	A	1569.9	44.9	4
40	A	2148.2	1276.6	100
41	A	3051.8	12.1	1
42	A	3076.8	11.8	1
43	A	3091.0	11.7	1
44	A	3148.4	22.1	2
45	A	3149.2	5.1	0

Excitation energies and oscillator strengths:

```
Excited State   1:      Singlet-A      3.0902 eV  401.21 nm  f=0.0001
Excited State   2:      Singlet-A      3.4913 eV  355.12 nm  f=0.0000
Excited State   3:      Singlet-A      3.9429 eV  314.45 nm  f=0.0005
Excited State   4:      Singlet-A      3.9888 eV  310.83 nm  f=0.0001
Excited State   5:      Singlet-A      4.0612 eV  305.29 nm  f=0.6842
Excited State   6:      Singlet-A      4.1537 eV  298.49 nm  f=0.0001
Excited State   7:      Singlet-A      4.5410 eV  273.03 nm  f=0.0013
Excited State   8:      Singlet-A      4.5948 eV  269.84 nm  f=0.0439
Excited State   9:      Singlet-A      4.7604 eV  260.45 nm  f=0.0038
Excited State  10:      Singlet-A      4.8359 eV  256.38 nm  f=0.0000
Excited State  11:      Singlet-A      4.9608 eV  249.93 nm  f=0.0241
Excited State  12:      Singlet-A      5.2394 eV  236.64 nm  f=0.0928
Excited State  13:      Singlet-A      5.3920 eV  229.94 nm  f=0.0008
Excited State  14:      Singlet-A      5.8059 eV  213.55 nm  f=0.0101
Excited State  15:      Singlet-A      5.8402 eV  212.30 nm  f=0.0039
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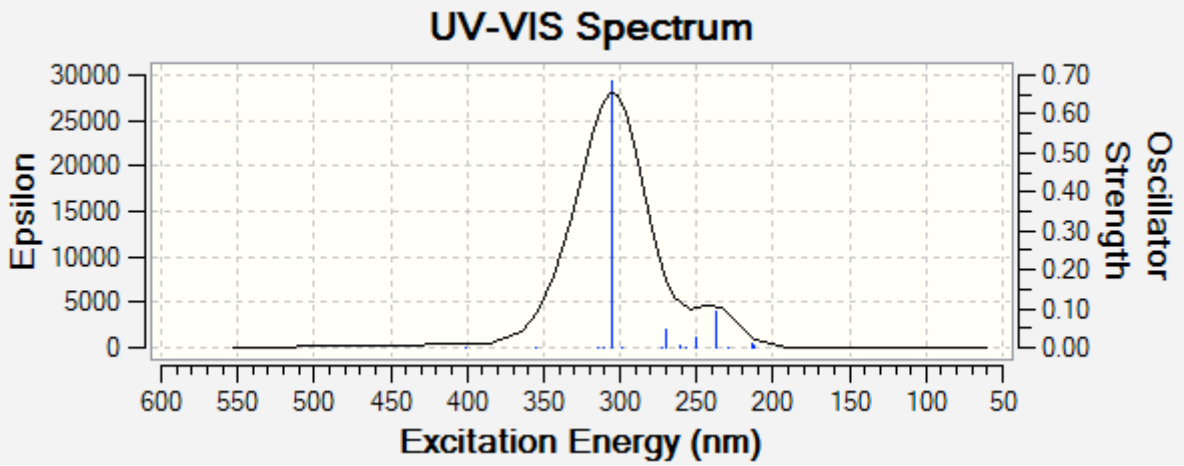
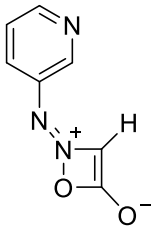


15, R= 3-pyridyl




```
RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: C1
State=1-A
HF= -584.3371182\RMSD=3.801e-09\RMSF=2.624e-05
Zero-point correction= 0.117294
Sum of electronic and thermal Free Energies= -584.219825

 C                 -3.53620200    0.65075500    0.08804900
 N                 -2.52104400    1.48526400   -0.16785400
 C                 -1.29001600    0.97251300   -0.25517600
 C                 -1.01373700   -0.39977900   -0.09402600
 C                 -2.09602600   -1.26566300    0.13869000
 C                 -3.37315100   -0.73092000    0.24131000
 N                  0.23973200   -1.02310600   -0.20745200
 C                  1.83140300    0.86074300    0.22605900
 C                  3.14588400    0.29874400    0.10909100
 O                  4.31130700    0.52453900    0.18171700
```

N	1.28437200	-0.34822300	-0.07179000
O	2.53506000	-1.02377400	-0.23361800
H	-4.52105200	1.10471700	0.16435500
H	-0.50585100	1.67997500	-0.50274300
H	-1.90662500	-2.32962100	0.23686200
H	-4.23132300	-1.36752200	0.43067600
H	1.36356300	1.79042800	0.49173800

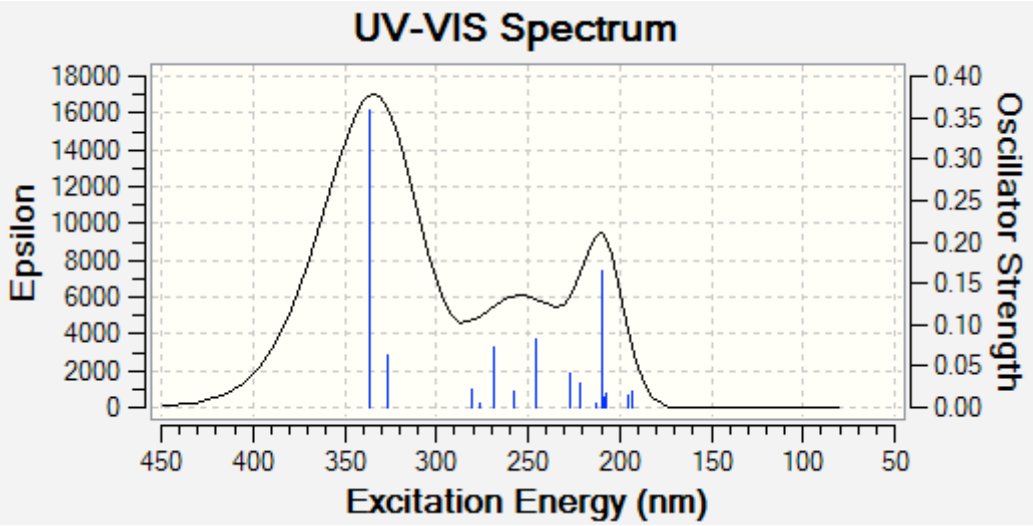
Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	34.6	2.5	0
2	A	79.8	6.6	1
3	A	114.3	1.6	0
4	A	168.6	0.3	0
5	A	260.1	1.2	0
6	A	300.9	0.2	0
7	A	335.7	3.5	0
8	A	395.3	5.4	1
9	A	467.4	8.8	1
10	A	491.1	26.4	3
11	A	511.3	28.6	3
12	A	556.2	27.4	3
13	A	577.0	4.7	1
14	A	599.9	0.8	0
15	A	640.6	14.0	2
16	A	683.8	19.0	2
17	A	694.1	14.8	2
18	A	747.5	9.6	1
19	A	794.5	27.5	3
20	A	815.4	2.7	0
21	A	888.3	0.9	0
22	A	931.5	9.4	1
23	A	936.8	78.3	9
24	A	964.6	0.9	0
25	A	988.5	3.5	0
26	A	1023.3	0.8	0
27	A	1025.7	31.1	4
28	A	1094.1	9.0	1
29	A	1155.2	13.4	2
30	A	1185.3	12.4	1
31	A	1231.1	45.0	5
32	A	1246.0	20.7	2
33	A	1261.3	10.0	1
34	A	1316.4	6.9	1
35	A	1402.6	13.2	2
36	A	1454.4	16.1	2
37	A	1542.4	47.9	6
38	A	1552.5	475.0	55
39	A	1588.1	801.3	93
40	A	1894.3	864.9	100
41	A	3061.2	8.5	1
42	A	3083.0	13.8	2
43	A	3086.6	1.3	0
44	A	3096.7	5.0	1
45	A	3215.5	9.9	1

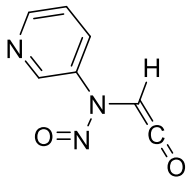
Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	3.6908 eV	335.93 nm	f=0.3582
Excited State	2:	Singlet-A	3.7946 eV	326.74 nm	f=0.0642
Excited State	3:	Singlet-A	4.4270 eV	280.06 nm	f=0.0214
Excited State	4:	Singlet-A	4.4937 eV	275.91 nm	f=0.0043

```
Excited State   5:      Singlet-A      4.6249 eV  268.08 nm  f=0.0736
Excited State   6:      Singlet-A      4.8130 eV  257.60 nm  f=0.0193
Excited State   7:      Singlet-A      5.0526 eV  245.39 nm  f=0.0830
Excited State   8:      Singlet-A      5.4602 eV  227.07 nm  f=0.0401
Excited State   9:      Singlet-A      5.5885 eV  221.85 nm  f=0.0293
Excited State  10:      Singlet-A      5.8289 eV  212.71 nm  f=0.0050
Excited State  11:      Singlet-A      5.9283 eV  209.14 nm  f=0.1641
Excited State  12:      Singlet-A      5.9532 eV  208.26 nm  f=0.0117
Excited State  13:      Singlet-A      5.9723 eV  207.60 nm  f=0.0167
Excited State  14:      Singlet-A      6.3294 eV  195.89 nm  f=0.0153
Excited State  15:      Singlet-A      6.4253 eV  192.96 nm  f=0.0202
```



3, R= 3-pyridyl




```
RB3LYP/6-31+G**; Gaussian 09, Revision C.01
Point group: C1
State=1-A
HF= -584.3473426\RMSD=4.732e-09\RMSF=1.190e-05
Zero-point correction= 0.115671
Sum of electronic and thermal Free Energies= -584.231671

 C                 -3.20872300   -0.62139200   -0.10762900
 N                 -2.89503300    0.58748600    0.37880100
 C                 -1.60251700    0.90045600    0.50056900
 C                 -0.56978400    0.01916800    0.14186500
 C                 -0.90503100   -1.24084600   -0.35971400
 C                 -2.25368200   -1.56752000   -0.48536800
 N                  0.80233100    0.39201800    0.30840600
 C                  1.73955100   -0.53630100    0.83092900
 C                  2.86503700   -0.81640700    0.18246800
 O                  3.86971500   -1.07995900   -0.35025000
 N                  1.34688400    1.56556100   -0.16966800
 O                  0.57659200    2.29905000   -0.75767000
 H                 -4.27004900   -0.84280000   -0.19081400
 H                 -1.37436600    1.88310100    0.89962900
```

H	-0.12652100	-1.94369800	-0.63843800
H	-2.55860700	-2.53553100	-0.86985600
H	1.59071200	-0.95219400	1.82134200

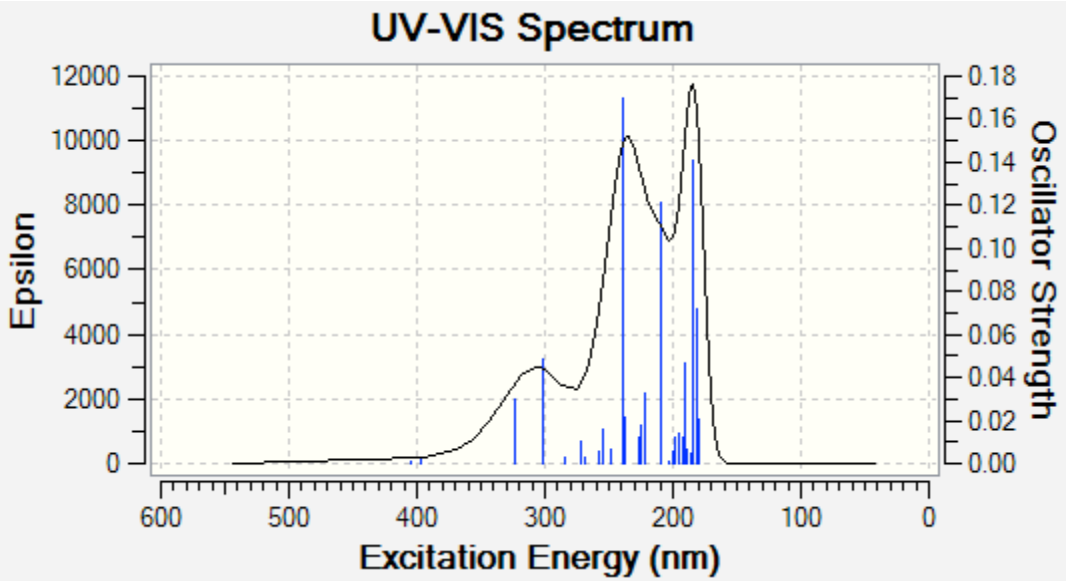
Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	36.7	1.0	0
2	A	43.2	1.9	0
3	A	81.9	1.4	0
4	A	135.1	2.2	0
5	A	184.9	1.8	0
6	A	250.8	3.1	0
7	A	271.1	1.8	0
8	A	299.5	5.6	1
9	A	394.7	4.2	1
10	A	403.9	4.6	1
11	A	452.5	9.3	1
12	A	483.7	4.4	1
13	A	502.2	0.4	0
14	A	570.8	82.1	10
15	A	589.6	7.8	1
16	A	620.5	3.6	0
17	A	687.3	28.4	4
18	A	745.7	9.2	1
19	A	763.1	8.9	1
20	A	791.8	19.9	3
21	A	901.3	3.4	0
22	A	931.0	1.5	0
23	A	961.0	0.1	0
24	A	977.5	182.5	23
25	A	995.3	27.0	3
26	A	1026.8	25.5	3
27	A	1055.6	8.6	1
28	A	1096.9	2.2	0
29	A	1143.6	76.8	10
30	A	1181.2	10.7	1
31	A	1235.4	7.1	1
32	A	1256.9	0.2	0
33	A	1314.7	2.3	0
34	A	1379.4	7.2	1
35	A	1407.7	49.0	6
36	A	1452.0	25.5	3
37	A	1529.6	244.9	31
38	A	1556.6	7.5	1
39	A	1566.7	5.1	1
40	A	2129.0	786.5	100
41	A	3057.7	10.2	1
42	A	3078.7	11.3	1
43	A	3084.9	17.9	2
44	A	3088.6	4.3	1
45	A	3091.9	5.4	1

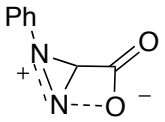
Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	3.0612 eV	405.02 nm	f=0.0007
Excited State	2:	Singlet-A	3.1261 eV	396.60 nm	f=0.0019
Excited State	3:	Singlet-A	3.8364 eV	323.18 nm	f=0.0295
Excited State	4:	Singlet-A	4.1011 eV	302.32 nm	f=0.0481
Excited State	5:	Singlet-A	4.3660 eV	283.97 nm	f=0.0026
Excited State	6:	Singlet-A	4.5673 eV	271.46 nm	f=0.0098
Excited State	7:	Singlet-A	4.6003 eV	269.51 nm	f=0.0032
Excited State	8:	Singlet-A	4.8031 eV	258.13 nm	f=0.0034

```
Excited State   9:      Singlet-A      4.8062 eV  257.97 nm  f=0.0053
Excited State  10:      Singlet-A      4.8641 eV  254.90 nm  f=0.0161
Excited State  11:      Singlet-A      4.9923 eV  248.35 nm  f=0.0066
Excited State  12:      Singlet-A      5.2000 eV  238.43 nm  f=0.1702
Excited State  13:      Singlet-A      5.2347 eV  236.85 nm  f=0.0217
Excited State  14:      Singlet-A      5.4666 eV  226.80 nm  f=0.0119
Excited State  15:      Singlet-A      5.5046 eV  225.24 nm  f=0.0036
```



***endo*-17 (R= Phenyl)**

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TD-B3LYP/6-31+G** excitation energies and oscillator strengths:
Excited State   1:      Singlet-A      1.9084 eV  649.67
nm  f=0.0108  <S**2>=0.000
Excited State   2:      Singlet-A      2.2304 eV  555.88
nm  f=0.0003  <S**2>=0.000
Excited State   3:      Singlet-A      3.0621 eV  404.89
nm  f=0.1808  <S**2>=0.000
Excited State   4:      Singlet-A      3.8341 eV  323.38
nm  f=0.0112  <S**2>=0.000
Excited State   5:      Singlet-A      4.2605 eV  291.01
nm  f=0.0859  <S**2>=0.000
Excited State   6:      Singlet-A      4.3640 eV  284.10
nm  f=0.0489  <S**2>=0.000
Excited State   7:      Singlet-A      4.4297 eV  279.89
nm  f=0.0524  <S**2>=0.000
Excited State   8:      Singlet-A      4.6345 eV  267.52
nm  f=0.0457  <S**2>=0.000
Excited State   9:      Singlet-A      4.8553 eV  255.36
nm  f=0.0035  <S**2>=0.000
Excited State  10:      Singlet-A      4.9079 eV  252.62
nm  f=0.0040  <S**2>=0.000
Excited State  11:      Singlet-A      5.1426 eV  241.09
nm  f=0.0165  <S**2>=0.000
Excited State  12:      Singlet-A      5.2234 eV  237.36
nm  f=0.0106  <S**2>=0.000
```
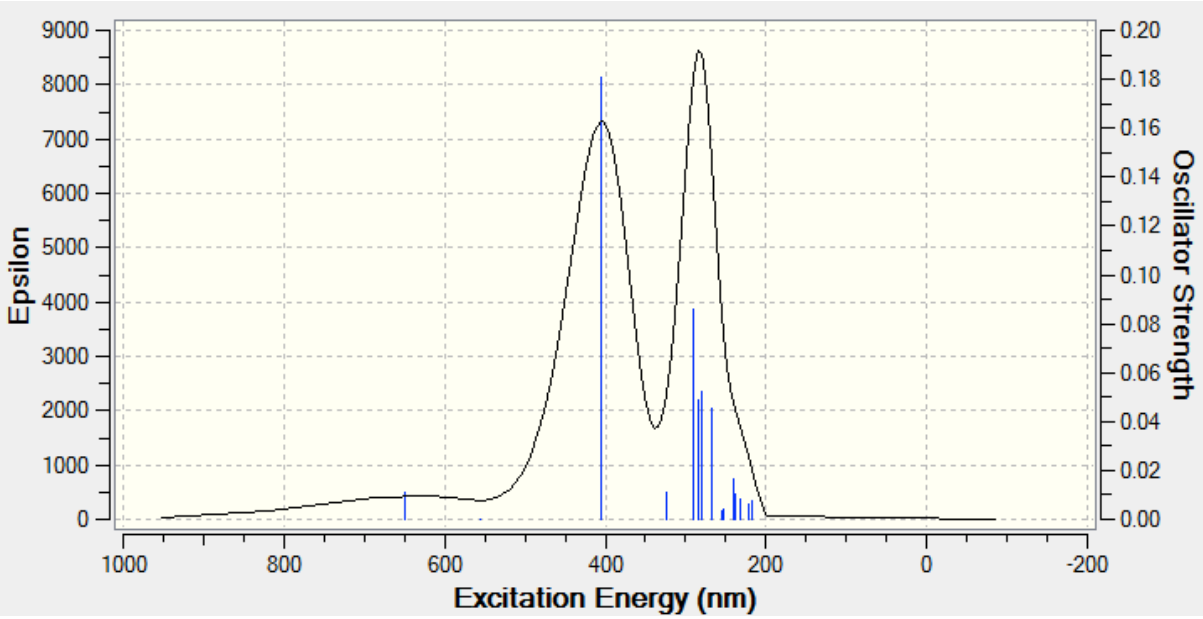
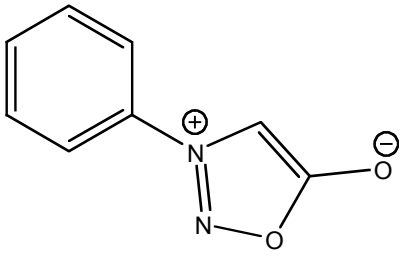

```
Excited State  13:      Singlet-A      5.3467 eV  231.89
nm  f=0.0082  <S**2>=0.000
Excited State  14:      Singlet-A      5.6029 eV  221.29
nm  f=0.0063  <S**2>=0.000
Excited State  15:      Singlet-A      5.7027 eV  217.41
nm  f=0.0079  <S**2>=0.000
```



Calculated UV-vis spectrum of ***endo*-17** (TD-B3LYP/6-31+G**).

3-Phenylsydnone:



a) Method: B3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.560194	0.145983	-0.059802
2	6	-2.924836	-1.061913	-0.345161

```
    3          6                    -1.536344   -1.151023   -
0.314036
    4          6                    -0.799407   -0.015891
0.013789
    5          6                    -1.416566    1.196468
0.310390
    6          6                    -2.805986    1.271889
0.266722
    7          7                     0.635551   -0.100261
0.049835
    8          7                     1.182991   -1.186978
0.532353
    9          8                     2.515760   -0.984406
0.423166
   10          6                     2.811995    0.316379   -
0.149958
   11          6                     1.512053    0.836697   -
0.370396
   12          8                     3.942932    0.679341   -
0.324329
   13          1                    -4.641514    0.209477   -
0.090213
   14          1                    -3.509211   -1.937690   -
0.600637
   15          1                    -1.025154   -2.077301   -
0.540228
   16          1                    -0.823957    2.058452
0.590062
   17          1                    -3.297131    2.209254
0.498640
   18          1                     1.213353    1.757458   -
0.832925
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-
```

Energy = -568.4812811
E+ZPVE = -568.350926

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	51.1	0.3	0
2	A	92.4	2.9	0
3	A	123.9	1.8	0
4	A	235.6	2.0	0
5	A	316.7	1.0	0
6	A	339.4	3.3	0
7	A	414.7	1.3	0
8	A	417.6	0.0	0
9	A	495.9	4.9	0
10	A	559.2	15.0	2
11	A	624.7	3.3	0
12	A	632.5	19.2	2
13	A	638.3	25.3	3

14	A	667.3	9.3	1
15	A	687.1	26.5	3
16	A	702.5	32.8	3
17	A	722.5	16.9	2
18	A	779.2	47.8	5
19	A	820.8	26.7	3
20	A	850.0	0.3	0
21	A	939.7	3.5	0
22	A	971.3	23.6	2
23	A	991.5	0.2	0
24	A	1012.6	0.1	0
25	A	1018.1	1.5	0
26	A	1034.5	9.7	1
27	A	1052.3	7.5	1
28	A	1103.1	8.8	1
29	A	1105.3	20.3	2
30	A	1186.8	0.4	0
31	A	1196.0	22.3	2
32	A	1199.5	17.4	2
33	A	1247.8	27.6	3
34	A	1326.6	16.3	2
35	A	1350.7	1.4	0
36	A	1396.3	46.1	5
37	A	1463.6	28.7	3
38	A	1499.5	38.7	4
39	A	1528.8	20.0	2
40	A	1637.9	2.3	0
41	A	1638.8	2.3	0
42	A	1857.7	987.0	100
43	A	3176.5	0.0	0
44	A	3186.6	5.4	1
45	A	3194.5	8.5	1
46	A	3202.6	3.0	0
47	A	3214.2	0.6	0
48	A	3314.9	10.3	1

b) Method: B3LYP/6-31G*

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.564698	0.147736	-0.055654
2	6	-2.929368	-1.068194	-0.318000
3	6	-1.538987	-1.157608	-0.290028

```
    4          6                    -0.798465   -0.014225
0.013594
    5          6                    -1.416075    1.206560
0.287164
    6          6                    -2.807667    1.281495
0.245762
    7          7                     0.634313   -0.099061
0.044227
    8          7                     1.179942   -1.209968
0.487677
    9          8                     2.517247   -1.001348
0.386142
   10          6                     2.815674    0.318119   -
0.135741
   11          6                     1.513867    0.851822   -
0.334588
   12          8                     3.951378    0.689744   -
0.298529
   13          1                    -4.648474    0.211310   -
0.084735
   14          1                    -3.515684   -1.950986   -
0.554428
   15          1                    -1.026756   -2.089100   -
0.501264
   16          1                    -0.821111    2.074937
0.549993
   17          1                    -3.298192    2.226260
0.459592
   18          1                     1.215748    1.789384   -
0.768439
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-
```

Energy = -568.3270141
E+ZPVE = -568.195670

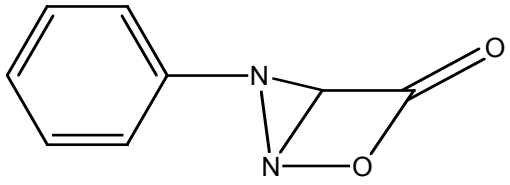
Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	54.2	0.3	0
2	A	90.2	2.9	0
3	A	123.1	1.8	0
4	A	227.5	1.9	0
5	A	308.6	1.0	0
6	A	328.3	3.1	0
7	A	397.8	1.6	0
8	A	403.1	0.0	0
9	A	478.8	3.0	0
10	A	535.8	9.8	1
11	A	597.1	20.9	3

12	A	605.3	12.9	2
13	A	627.6	8.9	1
14	A	643.9	5.5	1
15	A	664.5	29.4	4
16	A	675.7	20.9	3
17	A	692.3	17.2	2
18	A	751.1	38.8	5
19	A	798.7	24.5	3
20	A	821.0	0.4	0
21	A	902.9	3.7	0
22	A	938.2	15.6	2
23	A	940.2	4.2	1
24	A	967.9	0.3	0
25	A	980.6	2.4	0
26	A	1000.4	9.9	1
27	A	1018.4	5.2	1
28	A	1066.6	17.4	2
29	A	1072.3	11.6	1
30	A	1150.7	0.4	0
31	A	1159.5	31.4	4
32	A	1163.2	7.2	1
33	A	1211.0	26.7	3
34	A	1289.9	10.2	1
35	A	1314.6	3.0	0
36	A	1353.3	28.3	4
37	A	1424.9	28.1	4
38	A	1460.1	41.2	5
39	A	1488.6	19.1	2
40	A	1593.1	1.0	0
41	A	1593.8	2.7	0
42	A	1823.6	781.6	100
43	A	3075.0	0.0	0
44	A	3085.0	8.0	1
45	A	3093.1	15.6	2
46	A	3101.0	4.7	1
47	A	3116.1	0.3	0
48	A	3213.7	7.0	1

5-Phenyl-2-oxa-1, 5-diaza-bicyclo [2.1.0] pentan-3-one (*exo* conformer):



a) Method: B3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.592637	-0.070315	-0.455119
2	7	1.298176	-0.981422	0.452148
3	8	2.647813	-1.060132	-0.214436
4	6	2.875329	0.281365	0.019471
5	6	1.478465	0.467963	0.566728
6	8	3.865950	0.907882	-0.145242
7	1	1.138036	1.059450	1.406820
8	6	-0.819560	-0.007012	-0.192278
9	6	-1.570362	-1.179422	-0.101410
10	6	-1.441785	1.241151	-0.148251
11	6	-2.953022	-1.093662	0.038547
12	1	-1.072074	-2.139772	-0.136571
13	6	-2.825852	1.312915	-0.010605
14	1	-0.850460	2.145694	-0.237149
15	6	-3.585464	0.148102	0.084257
16	1	-3.536853	-2.003885	0.113039
17	1	-3.309017	2.282650	0.020554
18	1	-4.661924	0.207609	0.192777

Energy = -568.4165154
E+ZPVE = -568.287722

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	33.9	1.3	0
2	A	95.1	2.3	0
3	A	108.2	1.0	0
4	A	194.6	8.2	1
5	A	279.9	0.4	0
6	A	331.1	0.4	0
7	A	408.2	4.6	1
8	A	415.9	2.5	0
9	A	517.9	10.3	2
10	A	530.1	5.1	1
11	A	617.1	2.5	0
12	A	627.7	5.6	1
13	A	666.3	32.7	5
14	A	701.7	25.4	4
15	A	715.0	47.8	7
16	A	764.1	24.7	4
17	A	766.9	40.9	6
18	A	832.7	17.9	3
19	A	845.2	1.6	0
20	A	850.3	34.9	5
21	A	912.1	14.8	2
22	A	921.0	4.9	1
23	A	980.2	3.6	1
24	A	982.1	0.6	0
25	A	999.6	0.0	0
26	A	1015.5	0.4	0
27	A	1043.4	10.1	2
28	A	1060.1	25.7	4
29	A	1099.2	64.5	10
30	A	1106.8	9.8	1
31	A	1171.3	24.8	4
32	A	1183.3	0.5	0
33	A	1196.6	1.4	0
34	A	1241.3	39.0	6
35	A	1300.5	34.8	5
36	A	1331.9	0.3	0
37	A	1353.1	0.3	0
38	A	1484.5	4.8	1
39	A	1519.4	51.6	8
40	A	1627.7	3.4	1
41	A	1636.5	38.0	6
42	A	1937.1	663.0	100
43	A	3168.5	1.8	0
44	A	3175.4	2.2	0
45	A	3184.1	13.0	2

46	A	3194.6	11.5	2
47	A	3202.2	0.3	0
48	A	3204.2	1.5	0

b) **Method: B3LYP/6-31G***

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.592973	-0.075867	-0.469582
2	7	1.293065	-0.976846	0.461136
3	8	2.649480	-1.065445	-0.202041
4	6	2.877629	0.280477	0.020908
5	6	1.474454	0.475758	0.551796
6	8	3.877898	0.905938	-0.138720
7	1	1.122991	1.077116	1.383715
8	6	-0.819543	-0.008670	-0.201801
9	6	-1.572925	-1.182187	-0.108558
10	6	-1.440928	1.242310	-0.151946
11	6	-2.956272	-1.094667	0.041242
12	1	-1.073319	-2.144214	-0.147215
13	6	-2.826227	1.315676	-0.006050
14	1	-0.845599	2.146979	-0.240993
15	6	-3.587760	0.150008	0.092826
16	1	-3.541753	-2.006479	0.119140
17	1	-3.308350	2.288527	0.030663
18	1	-4.665829	0.210878	0.209394

Energy = -568.263726

E+ZPVE = -568.134078

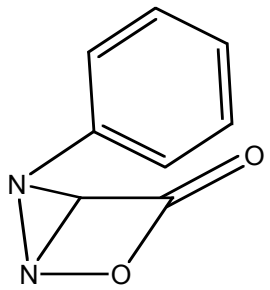
Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	32.6	1.2	0
2	A	92.2	2.4	0
3	A	104.2	0.9	0
4	A	187.7	7.3	1
5	A	271.6	0.3	0
6	A	318.6	0.3	0
7	A	391.1	5.2	1
8	A	401.1	1.0	0
9	A	499.0	5.6	1
10	A	509.2	5.3	1
11	A	592.1	2.0	0
12	A	603.5	5.1	1
13	A	638.5	27.0	5
14	A	677.3	13.5	2
15	A	688.6	44.0	8
16	A	735.6	11.5	2
17	A	739.5	45.0	8
18	A	802.7	18.6	3
19	A	816.3	0.9	0
20	A	820.6	30.6	6
21	A	879.4	11.8	2
22	A	884.6	4.9	1
23	A	928.8	0.0	0
24	A	946.9	2.7	0
25	A	956.1	0.2	0
26	A	978.5	1.1	0
27	A	1009.4	8.3	2
28	A	1024.3	13.5	2
29	A	1069.0	25.9	5
30	A	1078.4	48.0	9
31	A	1133.8	21.3	4
32	A	1147.6	0.4	0
33	A	1160.4	1.1	0
34	A	1206.9	41.4	8
35	A	1263.6	29.7	5
36	A	1297.5	1.0	0
37	A	1312.9	0.3	0
38	A	1444.2	5.0	1
39	A	1479.6	48.0	9
40	A	1583.8	3.3	1
41	A	1593.4	32.6	6
42	A	1887.5	547.2	100
43	A	3065.9	2.2	0
44	A	3072.8	2.9	1

45	A	3081.1	19.6	4
46	A	3091.4	18.7	3
47	A	3102.7	2.7	0
48	A	3104.1	0.4	0

5-Phenyl-2-oxa-1, 5-diaza-bicyclo [2.1.0] pentan-3-one (*endo* conformer):



a) Method: B3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.347379	0.460269	0.391608
2	6	2.912387	-0.864256	0.496725
3	6	1.620290	-1.207683	0.125745
4	6	0.780373	-0.197360	-0.351205
5	6	1.192928	1.131470	-0.462507
6	6	2.490441	1.453891	-0.082835
7	7	-0.527734	-0.521189	-0.741703
8	7	-1.309824	-1.493786	-0.625126
9	8	-2.390560	-0.570915	1.234922
10	6	-2.590944	0.338392	0.382141
11	6	-1.873047	-0.096269	-0.908880
12	8	-3.204470	1.397461	0.407615
13	1	4.357098	0.718202	0.688396

```
   14          1                    3.581294   -1.627043
0.876089
   15          1                    1.253817   -2.223140
0.210887
   16          1                    0.504052    1.886661   -
0.821248
   17          1                    2.830076    2.479886   -
0.151754
   18          1                   -2.182042    0.147169   -
1.919615
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-
```

Energy = -568.4277994
E+ZPVE = -568.299645

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	38.1	5.7	1
2	A	58.1	11.7	2
3	A	85.7	1.6	0
4	A	175.6	41.4	7
5	A	191.0	50.3	8
6	A	204.1	22.1	4
7	A	376.5	10.4	2
8	A	407.5	1.3	0
9	A	418.0	2.6	0
10	A	465.6	10.0	2
11	A	502.4	12.8	2
12	A	530.7	2.5	0
13	A	625.5	0.3	0
14	A	648.6	20.5	3
15	A	686.5	23.7	4
16	A	712.8	9.5	2
17	A	770.2	51.6	8
18	A	791.3	27.6	4
19	A	840.9	5.2	1
20	A	843.8	1.3	0
21	A	876.0	6.2	1
22	A	941.5	4.2	1
23	A	992.2	0.0	0
24	A	1013.5	0.3	0
25	A	1016.6	1.3	0
26	A	1040.2	2.3	0
27	A	1051.7	14.1	2
28	A	1100.2	8.4	1
29	A	1121.4	10.1	2
30	A	1189.0	0.2	0
31	A	1197.1	5.5	1
32	A	1232.6	14.6	2
33	A	1276.5	29.4	5

34	A	1333.4	41.2	7
35	A	1349.6	5.3	1
36	A	1357.9	4.2	1
37	A	1492.9	8.9	1
38	A	1513.3	4.7	1
39	A	1605.5	86.9	14
40	A	1629.0	0.8	0
41	A	1647.2	156.8	25
42	A	1747.4	625.7	100
43	A	3177.0	5.4	1
44	A	3180.8	0.1	0
45	A	3190.8	3.8	1
46	A	3195.6	2.3	0
47	A	3204.2	0.5	0
48	A	3207.4	4.5	1

b) Method: B3LYP/6-31G*

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.230700	0.087117	-0.584408
2	6	-2.534868	-1.123232	-0.519801
3	6	-1.255892	-1.172925	0.029386
4	6	-0.691880	0.011138	0.511772
5	6	-1.371649	1.230490	0.458149
6	6	-2.647311	1.261061	-0.099509
7	7	0.591643	-0.025418	1.107329
8	7	1.484719	-0.970673	1.133622
9	8	1.999168	-1.016050	-0.766149
10	6	2.375726	0.217161	-0.580077
11	6	1.912875	0.454375	0.856839
12	8	2.966366	0.990392	-1.304329
13	1	-4.225642	0.117017	-1.018619
14	1	-2.983816	-2.031768	-0.909745

```
   15             1                            -0.685973    -2.094789
0.063867
   16             1                            -0.903648     2.131513
0.842486
   17           1                            -3.185829     2.202243    -
0.154645
   18             1                             2.388294     1.062572
1.619721
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```

Energy = -568.2694997
E+ZPVE = -568.140198

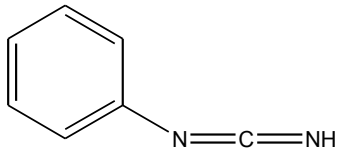
Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	28.6	4.4	1
2	A	49.8	22.7	5
3	A	113.8	6.5	1
4	A	160.9	109.5	23
5	A	184.0	2.5	1
6	A	265.1	62.4	13
7	A	384.9	5.0	1
8	A	398.5	0.0	0
9	A	423.9	2.9	1
10	A	455.4	6.5	1
11	A	524.9	33.1	7
12	A	555.7	21.2	4
13	A	605.1	1.0	0
14	A	664.8	15.8	3
15	A	669.1	7.1	1
16	A	690.5	9.3	2
17	A	736.1	31.0	6
18	A	758.9	45.1	9
19	A	811.8	0.3	0
20	A	847.7	2.1	0
21	A	870.1	5.8	1
22	A	891.9	6.3	1
23	A	933.6	0.1	0
24	A	964.6	0.1	0
25	A	979.7	2.0	0
26	A	998.6	15.6	3
27	A	1010.5	2.4	1
28	A	1058.6	9.6	2
29	A	1084.1	13.2	3
30	A	1135.1	32.0	7
31	A	1150.3	0.9	0
32	A	1163.0	2.4	1

33	A	1208.9	45.3	9
34	A	1263.0	26.1	5
35	A	1304.3	2.4	0
36	A	1316.2	2.5	1
37	A	1448.3	8.3	2
38	A	1458.3	93.6	20
39	A	1485.7	133.8	28
40	A	1583.4	3.6	1
41	A	1589.3	0.4	0
42	A	1775.5	477.9	100
43	A	3075.0	0.1	0
44	A	3083.7	5.2	1
45	A	3091.0	13.1	3
46	A	3098.7	12.4	3
47	A	3099.1	4.0	1
48	A	3110.6	1.1	0

10. Phenyl-carbodiimide:



a) Method: B3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.603390	0.431269	0.023751
2	6	2.253086	-0.918090	0.028166
3	6	0.914052	-1.297392	0.004027
4	6	-0.088087	-0.323401	-0.021753
5	6	0.261612	1.033321	-0.027948
6	6	1.602605	1.402939	-0.005445
7	7	-1.425395	-0.760183	-0.052877
8	6	-2.471528	-0.142905	0.016327

```
    9          7                    -3.571150    0.385605   -
0.073626
   10          1                     3.646548    0.724616
0.041349
   11          1                     3.024258   -1.679749
0.048701
   12          1                     0.627080   -2.341808
0.003866
   13          1                    -0.515238    1.789594   -
0.055908
   14          1                     1.866432    2.454595   -
0.012183
   15          1                    -4.124060    0.560351
0.756938
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Energy = -379.9393949
E+ZPVE = -379.825247

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	48.4	5.6	0
2	A	107.5	1.8	0
3	A	224.6	14.6	1
4	A	383.2	6.5	0
5	A	415.8	72.4	5
6	A	420.7	12.6	1
7	A	470.1	1.0	0
8	A	505.3	24.4	2
9	A	581.8	44.4	3
10	A	631.7	0.6	0
11	A	655.7	34.9	3
12	A	702.3	32.7	2
13	A	773.2	59.1	4
14	A	791.9	6.3	0
15	A	843.4	0.1	0
16	A	887.6	428.4	31
17	A	921.7	6.4	0
18	A	980.3	0.1	0
19	A	997.0	0.1	0
20	A	1016.3	0.3	0
21	A	1044.9	6.9	1
22	A	1099.4	11.6	1
23	A	1143.7	33.5	2
24	A	1181.3	0.0	0
25	A	1196.8	0.1	0
26	A	1319.4	6.2	0
27	A	1351.7	0.6	0
28	A	1426.9	4.2	0

29	A	1481.7	1.2	0
30	A	1530.7	67.9	5
31	A	1618.9	8.8	1
32	A	1637.4	60.6	4
33	A	2228.8	1379.0	100
34	A	3163.9	2.3	0
35	A	3171.8	2.5	0
36	A	3180.2	14.0	1
37	A	3189.5	16.0	1
38	A	3197.6	5.2	0
39	A	3582.3	85.2	6

b) Method: B3LYP/6-31G*

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.603390	0.431269	0.023751
2	6	2.253086	-0.918090	0.028166
3	6	0.914052	-1.297392	0.004027
4	6	-0.088087	-0.323401	-0.021753
5	6	0.261612	1.033321	-0.027948
6	6	1.602605	1.402939	-0.005445
7	7	-1.425395	-0.760183	-0.052877
8	6	-2.471528	-0.142905	0.016327
9	7	-3.571150	0.385605	-0.073626
10	1	3.646548	0.724616	0.041349
11	1	3.024258	-1.679749	0.048701
12	1	0.627080	-2.341808	0.003866
13	1	-0.515238	1.789594	-0.055908
14	1	1.866432	2.454595	-0.012183
15	1	-4.124060	0.560351	0.756938

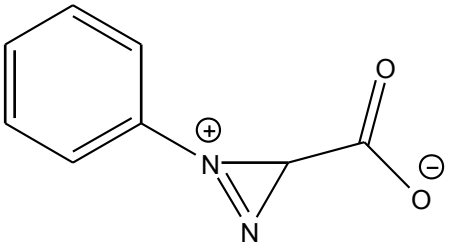
Energy = -379.939395
E+ZPVE = -379.825247

Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	53.9	5.3	0
2	A	102.3	1.5	0
3	A	220.8	14.6	1
4	A	368.5	6.5	1
5	A	400.9	61.4	5
6	A	407.0	15.7	1
7	A	449.9	0.5	0
8	A	479.3	20.2	2
9	A	560.1	44.3	4
10	A	607.3	1.0	0
11	A	622.5	31.6	3
12	A	677.6	17.2	2
13	A	748.1	46.4	4
14	A	763.1	6.2	1
15	A	817.7	0.0	0
16	A	886.3	231.0	20
17	A	889.3	233.8	21
18	A	929.5	0.1	0
19	A	955.4	0.3	0
20	A	979.7	0.2	0
21	A	1013.1	4.8	0
22	A	1066.2	8.7	1
23	A	1108.0	30.0	3
24	A	1145.9	0.1	0
25	A	1160.8	0.1	0
26	A	1285.5	4.0	0
27	A	1313.0	1.3	0
28	A	1381.5	5.3	0
29	A	1442.1	1.2	0
30	A	1490.5	61.4	5
31	A	1575.8	8.9	1
32	A	1595.0	48.2	4
33	A	2157.6	1136.1	100
34	A	3061.0	2.5	0
35	A	3068.9	3.8	0
36	A	3077.0	21.4	2
37	A	3086.3	23.9	2
38	A	3095.4	7.6	1
39	A	3420.4	46.0	4

Phenyldiazirinium-3-carboxylate



a) Method: B3LYP/6-31G*

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.790486	1.213472	-0.219894
2	6	-0.793713	0.280228	0.097602
3	6	-1.075178	-1.069674	0.343827
4	6	-2.400840	-1.484081	0.289643
5	6	-3.413344	-0.567556	-0.016056
6	6	-3.108314	0.774022	-0.274056
7	1	-1.526427	2.250020	-0.402852
8	1	-0.254035	-1.756883	0.512872
9	1	-2.644477	-2.526396	0.469042
10	1	-4.445828	-0.901331	-0.060810
11	1	-3.899834	1.477697	-0.512169
12	6	1.919393	0.652595	0.641840
13	1	2.117922	0.877387	1.689645
14	7	0.533094	0.700468	0.180136
15	7	1.207915	1.720523	-0.094666
16	6	2.703807	-0.432405	-0.155320
17	8	1.877365	-1.017039	-0.909892
18	8	3.899843	-0.553840	0.092450

Energy = -568.266546
E+ZPVE = -568.137830

Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	42.6	2.5	0
2	A	64.1	0.5	0
3	A	83.7	7.1	1
4	A	149.0	0.9	0
5	A	174.0	19.5	3
6	A	282.1	5.5	1
7	A	301.6	9.9	1
8	A	343.6	8.9	1
9	A	395.8	0.9	0
10	A	437.7	4.6	1
11	A	484.7	43.9	6
12	A	493.4	40.7	5
13	A	599.9	3.1	0
14	A	635.8	16.4	2
15	A	657.4	22.9	3
16	A	685.3	2.6	0
17	A	722.8	21.0	3
18	A	745.4	43.9	6
19	A	806.9	39.8	5
20	A	816.2	0.1	0
21	A	837.1	5.8	1
22	A	910.0	2.9	0
23	A	944.1	0.0	0
24	A	972.3	0.1	0
25	A	979.6	1.8	0
26	A	1007.3	2.8	0
27	A	1021.2	10.5	1
28	A	1048.5	15.0	2

29	A	1077.4	3.9	1
30	A	1151.8	0.1	0
31	A	1155.1	11.9	2
32	A	1189.6	5.9	1
33	A	1226.9	6.0	1
34	A	1276.1	82.0	11
35	A	1306.5	4.8	1
36	A	1321.6	7.8	1
37	A	1449.3	9.0	1
38	A	1468.0	4.9	1
39	A	1566.5	22.9	3
40	A	1577.3	1.1	0
41	A	1616.7	61.5	8
42	A	1745.9	746.8	100
43	A	3048.6	15.8	2
44	A	3079.8	0.4	0
45	A	3090.7	6.3	1
46	A	3098.0	6.9	1
47	A	3104.4	5.7	1
48	A	3120.8	3.3	0

b) Method: B3LYP/6-311++G**

scrf, dielectric constant = 36.64

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.829684	1.195734	0.204151
2	6	0.892662	0.180264	-0.079249
3	6	1.272484	-1.161474	-0.262574
4	6	2.617346	-1.482285	-0.174672
5	6	3.561520	-0.482637	0.093267
6	6	3.165948	0.850823	0.287159

7	1	1.504845	2.221920	0.325205
8	1	0.522135	-1.912590	-0.476869
9	1	2.946229	-2.502687	-0.326219
10	1	4.614780	-0.737387	0.142067
11	1	3.913854	1.609865	0.482819
12	6	-1.806711	0.270910	-0.714745
13	1	-1.915380	0.154395	-1.789355
14	7	-0.436815	0.524263	-0.269282
15	7	-1.131188	1.552334	-0.300927
16	6	-2.897672	-0.314839	0.223432
17	8	-2.592987	-0.414800	1.419917
18	8	-3.959765	-0.548783	-0.398267

Energy = -568.4563583

E+ZPVE = -568.328236

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	38.6	0.2	0
2	A	63.3	7.5	1
3	A	71.2	22.3	3
4	A	146.4	1.1	0
5	A	177.1	21.6	2
6	A	275.7	5.3	1
7	A	303.5	7.8	1
8	A	371.9	2.3	0
9	A	405.4	0.3	0
10	A	468.0	0.9	0
11	A	507.1	80.8	9
12	A	522.6	67.8	8
13	A	617.6	4.2	0
14	A	661.3	37.6	4
15	A	692.9	21.5	2

16	A	708.7	60.4	7
17	A	782.7	78.7	9
18	A	792.3	30.1	3
19	A	832.9	2.3	0
20	A	853.0	86.7	10
21	A	878.8	109.3	12
22	A	962.9	0.6	0
23	A	1008.3	61.5	7
24	A	1011.4	1.9	0
25	A	1030.8	0.4	0
26	A	1044.4	0.6	0
27	A	1068.2	258.6	29
28	A	1080.9	80.8	9
29	A	1114.7	40.7	5
30	A	1193.3	16.0	2
31	A	1204.6	5.4	1
32	A	1253.7	37.3	4
33	A	1287.0	534.3	61
34	A	1349.9	8.9	1
35	A	1356.5	183.0	21
36	A	1377.5	23.1	3
37	A	1490.2	42.9	5
38	A	1499.4	4.1	0
39	A	1581.8	512.2	58
40	A	1601.3	97.4	11
41	A	1683.2	123.8	14
42	A	1715.3	883.4	100
43	A	3152.8	14.2	2
44	A	3188.7	7.7	1
45	A	3195.6	0.9	0
46	A	3197.7	16.9	2
47	A	3207.4	7.5	1
48	A	3210.6	8.2	1

c) Method: B3LYP/6-31G*

scrf, dielectric constant = 36.64

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.817685	1.193937	0.256895
2	6	0.865556	0.210725	-0.085777
3	6	1.223460	-1.125680	-0.342095
4	6	2.565032	-1.474456	-0.267207
5	6	3.525907	-0.505894	0.058376
6	6	3.151230	0.822282	0.324277
7	1	1.505482	2.218228	0.432962
8	1	0.454463	-1.850789	-0.586934
9	1	2.875033	-2.494143	-0.469937
10	1	4.575783	-0.781767	0.098168
11	1	3.910287	1.559708	0.564870
12	6	-1.840663	0.394906	-0.704833
13	1	-1.969870	0.409968	-1.786787
14	7	-0.460423	0.577542	-0.241535
15	7	-1.152786	1.612624	-0.161535
16	6	-2.848877	-0.359955	0.206955
17	8	-2.373046	-0.706526	1.304062
18	8	-3.978791	-0.459418	-0.317861

Energy = -568.2878093

E+ZPVE = -568.158952

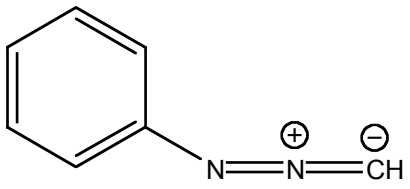
Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	34.1	8.5	1
2	A	56.7	17.5	2
3	A	62.4	7.4	1
4	A	137.3	4.0	0
5	A	161.5	27.7	3
6	A	267.5	5.2	1
7	A	289.9	12.6	2
8	A	344.1	13.2	2
9	A	391.3	0.5	0
10	A	445.6	8.3	1
11	A	483.5	166.0	20
12	A	487.7	14.2	2
13	A	594.8	3.5	0
14	A	642.3	25.7	3
15	A	662.5	10.2	1
16	A	680.4	22.7	3
17	A	739.7	33.4	4
18	A	751.2	64.0	8
19	A	805.5	0.8	0
20	A	822.0	41.0	5
21	A	840.3	124.3	15
22	A	923.8	0.8	0
23	A	958.9	0.1	0
24	A	974.2	31.5	4
25	A	999.5	1.0	0
26	A	1001.0	0.4	0
27	A	1027.9	81.8	10
28	A	1041.5	108.6	13
29	A	1078.9	26.4	3
30	A	1155.3	16.5	2
31	A	1163.4	4.4	1
32	A	1213.8	17.6	2

33	A	1247.9	235.6	28
34	A	1307.2	2.2	0
35	A	1314.1	242.2	29
36	A	1338.3	18.3	2
37	A	1447.3	31.2	4
38	A	1459.9	2.3	0
39	A	1544.0	336.3	41
40	A	1560.5	76.0	9
41	A	1628.1	29.6	4
42	A	1724.1	827.3	100
43	A	3044.2	29.7	4
44	A	3094.2	2.2	0
45	A	3099.1	1.0	0
46	A	3101.8	6.1	1
47	A	3110.2	0.8	0
48	A	3113.5	3.4	0

***N*-Phenylformonitrile imine (cf. ref. 41,** D. Bégué, G. Qiao, C. Wentrup, *J. Am. Chem. Soc.* **2012**, *134*, 5539.)



a) Method: B3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.515565	0.512363	-0.003353
2	6	-0.919733	-1.302935	0.005574

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    3             6                           0.134646    -0.380971
0.008064
    4             6                          -0.143390     0.992716
0.005002
    5            6                          -1.465016     1.429441    -
0.002260
    6             7                           1.438491    -0.931372
0.001690
    7            1                          -3.542130     0.859561    -
0.006608
    8             1                          -0.685077    -2.360551
0.005642
    9             1                           0.666073     1.713310
0.005725
   10            1                          -1.674035     2.493467    -
0.006375
   11             7                           2.394883    -0.146948
0.021271
   12            6                           3.374899     0.514545    -
0.135422
   13             1                           4.062729     0.957140
0.568153
   14             6                          -2.235136    -0.855047
0.001241
   15            1                          -3.045411    -1.575353    -
0.000345
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Energy = -379.8583205
E+ZPVE = -379.745424

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	74.1	3.6	0
2	A	144.8	0.8	0
3	A	227.3	4.4	1
4	A	372.8	1.7	0
5	A	420.5	0.2	0
6	A	457.4	4.4	1
7	A	472.3	44.6	6
8	A	495.2	20.0	3
9	A	624.0	775.7	100
10	A	630.2	0.3	0
11	A	667.1	3.8	0
12	A	682.7	20.9	3
13	A	708.4	64.9	8
14	A	779.9	38.9	5
15	A	828.9	0.8	0
16	A	839.6	0.1	0
17	A	914.5	5.4	1
18	A	978.3	0.1	0

19	A	994.5	0.0	0
20	A	1012.7	0.7	0
21	A	1043.1	5.3	1
22	A	1103.2	8.7	1
23	A	1154.6	17.1	2
24	A	1181.0	0.0	0
25	A	1199.1	0.7	0
26	A	1328.9	1.3	0
27	A	1340.9	70.5	9
28	A	1356.6	10.8	1
29	A	1483.3	1.3	0
30	A	1516.9	62.2	8
31	A	1617.4	4.5	1
32	A	1633.8	46.6	6
33	A	2107.4	733.8	95
34	A	3164.7	2.0	0
35	A	3173.0	7.1	1
36	A	3183.8	10.2	1
37	A	3190.5	14.4	2
38	A	3196.5	7.8	1
39	A	3256.0	36.6	5

b) Method: B3LYP/6-31G*

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.517948	0.513357	0.004307
2	6	-0.920366	-1.304337	0.006104
3	6	0.135376	-0.381364	-0.000371
4	6	-0.142482	0.994346	-0.006195
5	6	-1.465303	1.431933	-0.004998
6	7	1.438762	-0.936790	-0.014512
7	1	-3.546785	0.861874	0.007515
8	1	-0.683178	-2.363642	0.006969
9	1	0.672073	1.712634	-0.017007
10	1	-1.674253	2.498554	-0.011376
11	7	2.396048	-0.146593	0.025908

```
   12            6                          3.381019     0.521754    -
0.125942
   13             1                           4.045374     0.933881
0.622580
   14             6                          -2.238092    -0.855954
0.009770
   15             1                          -3.050121    -1.578031
0.015493
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-
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Energy = -379.7569649
E+ZPVE = -379.643140

Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	70.0	3.4	1
2	A	138.7	0.5	0
3	A	222.1	4.4	1
4	A	358.1	0.5	0
5	A	404.8	0.1	0
6	A	440.0	2.3	0
7	A	454.4	27.4	4
8	A	479.2	13.6	2
9	A	606.2	0.0	0
10	A	636.5	101.4	16
11	A	656.4	110.8	18
12	A	676.5	537.5	87
13	A	686.6	70.9	12
14	A	755.0	33.6	5
15	A	800.3	1.0	0
16	A	816.6	0.0	0
17	A	883.2	5.1	1
18	A	929.3	0.1	0
19	A	954.5	0.3	0
20	A	976.7	0.3	0
21	A	1012.0	3.5	1
22	A	1069.4	6.6	1
23	A	1119.7	15.4	3
24	A	1145.3	0.1	0
25	A	1162.6	0.7	0
26	A	1292.4	5.3	1
27	A	1299.4	51.2	8
28	A	1317.2	0.8	0
29	A	1444.1	1.5	0
30	A	1478.4	53.7	9
31	A	1575.3	4.5	1
32	A	1591.8	37.3	6
33	A	2044.1	615.7	100

34	A	3061.4	2.3	0
35	A	3069.8	10.0	2
36	A	3080.6	16.9	3
37	A	3087.2	21.5	3
38	A	3094.0	10.1	2
39	A	3139.8	13.0	2

c) Method: B3LYP/6-311+G**

scrf, dielectric constant = 36.64

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.514681	0.514457	-0.002859
2	6	-0.920932	-1.303017	0.004336
3	6	0.135084	-0.382832	0.005327
4	6	-0.141781	0.991115	0.002699
5	6	-1.462693	1.429869	-0.003046
6	7	1.438586	-0.934899	0.002977
7	1	-3.540433	0.863875	-0.000288
8	1	-0.687503	-2.361041	0.009017
9	1	0.667663	1.711604	0.007249
10	1	-1.669740	2.494093	-0.002235
11	7	2.394629	-0.148258	0.021421
12	6	3.371983	0.515722	-0.132963
13	1	4.058314	0.973213	0.562173
14	6	-2.235852	-0.853220	0.001200
15	1	-3.047565	-1.572203	0.005140

Energy = -379.8588586

E+ZPVE = -379.746150

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	74.0	5.4	0
2	A	145.2	1.6	0
3	A	227.7	6.7	0
4	A	372.1	12.0	1
5	A	419.8	1.4	0
6	A	457.1	22.0	1
7	A	467.9	375.2	21
8	A	492.9	113.4	6
9	A	560.4	1764.2	98
10	A	630.3	0.0	0
11	A	669.0	4.7	0
12	A	681.9	31.7	2
13	A	705.5	89.3	5
14	A	778.4	52.5	3
15	A	829.0	1.6	0
16	A	841.0	0.0	0
17	A	916.1	6.1	0
18	A	981.3	0.1	0
19	A	998.7	0.1	0
20	A	1012.5	1.0	0
21	A	1043.0	11.3	1
22	A	1102.8	16.5	1
23	A	1153.8	34.9	2
24	A	1180.9	0.0	0
25	A	1199.6	1.8	0
26	A	1328.7	3.8	0
27	A	1336.7	203.1	11
28	A	1355.9	17.2	1
29	A	1483.3	2.2	0
30	A	1515.1	153.9	9
31	A	1617.3	8.3	0
32	A	1632.5	115.6	6

33	A	2095.6	1791.7	100
34	A	3165.3	9.6	1
35	A	3172.9	11.5	1
36	A	3184.4	23.6	1
37	A	3190.4	23.3	1
38	A	3195.5	22.6	1
39	A	3260.1	109.8	6

d) Method: B3LYP/6-31G*

scrf, dielectric constant = 36.64

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.517367	0.514443	0.004504
2	6	-0.921027	-1.304374	0.004949
3	6	0.135482	-0.382375	-0.002039
4	6	-0.141580	0.993478	-0.007840
5	6	-1.463955	1.432231	-0.005400
6	7	1.439070	-0.938978	-0.012861
7	1	-3.545656	0.864290	0.011709
8	1	-0.684412	-2.363947	0.008935
9	1	0.672890	1.711782	-0.015718
10	1	-1.671908	2.498851	-0.008334
11	7	2.395588	-0.146933	0.026173
12	6	3.380011	0.521979	-0.125563
13	1	4.039640	0.944107	0.621749
14	6	-2.238511	-0.854969	0.009644
15	1	-3.051474	-1.576181	0.018946

Energy = -379.7574646

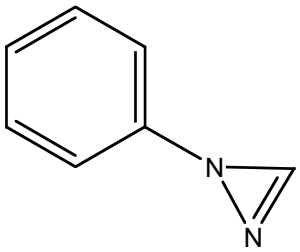
E+ZPVE = -379.643779

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	72.6	4.4	0
2	A	144.7	0.7	0
3	A	231.5	6.1	0
4	A	372.4	1.3	0
5	A	421.1	0.3	0
6	A	457.4	5.3	0
7	A	472.1	86.3	7
8	A	497.7	40.8	3
9	A	630.6	0.5	0
10	A	643.4	1206.8	96
11	A	674.9	302.8	24
12	A	688.9	147.5	12
13	A	713.0	50.7	4
14	A	784.7	38.9	3
15	A	832.5	1.8	0
16	A	849.5	0.0	0
17	A	919.0	5.4	0
18	A	967.0	0.1	0
19	A	993.4	0.3	0
20	A	1016.0	0.3	0
21	A	1052.6	6.2	0
22	A	1112.3	10.8	1
23	A	1164.1	26.7	2
24	A	1191.6	0.1	0
25	A	1209.7	1.1	0
26	A	1343.5	31.1	2
27	A	1349.3	87.1	7
28	A	1370.0	1.0	0
29	A	1502.2	2.1	0
30	A	1536.6	108.0	9

31	A	1638.8	7.5	1
32	A	1655.0	74.5	6
33	A	2114.9	1254.6	100
34	A	3185.9	7.3	1
35	A	3193.3	14.8	1
36	A	3205.2	32.0	3
37	A	3212.0	29.8	2
38	A	3216.9	23.7	2
39	A	3266.1	25.2	2

1-Phenyl-1*H*-diazirine



Method: B3LYP/6-31G*

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.531968	1.362276	0.018268
2	1	1.849419	2.401285	0.044091
3	6	2.481908	0.339225	0.075975
4	1	3.538629	0.581639	0.146092
5	6	2.068044	-0.995188	0.051703
6	1	2.802010	-1.794660	0.103461
7	6	0.713122	-1.305296	-0.029649
8	1	0.366179	-2.333652	-0.047307
9	6	-0.243389	-0.281392	-0.104212

10	6	0.174976	1.059356	-0.071424
11	7	-1.585400	-0.718341	-0.267228
12	7	-2.717864	0.093965	0.816137
13	6	-2.551376	0.279919	-0.404171
14	1	-2.927083	0.901979	-1.216643
15	1	-0.557836	1.860635	-0.090997

Energy = -379.7379557

E+ZPVE = -379.624478

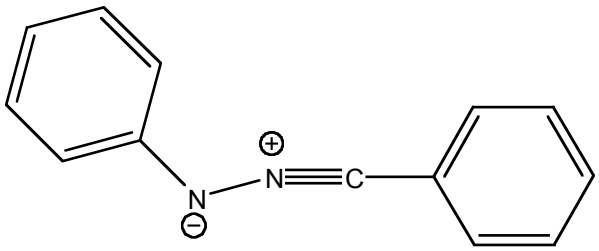
Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	58.7	6.8	19
2	A	145.8	7.6	21
3	A	219.0	5.5	15
4	A	286.0	35.6	99
5	A	374.1	7.4	21
6	A	404.6	0.7	2
7	A	448.3	34.2	95
8	A	514.8	5.4	15
9	A	575.5	2.6	7
10	A	606.3	0.3	1
11	A	676.3	21.0	58
12	A	748.9	25.1	70
13	A	767.5	16.0	44
14	A	817.1	0.4	1
15	A	850.9	9.5	26
16	A	893.3	3.2	9
17	A	933.0	0.4	1
18	A	959.9	0.1	0
19	A	977.2	1.1	3
20	A	991.9	15.5	43

21	A	1015.4	5.6	16
22	A	1070.3	5.3	15
23	A	1144.6	0.5	1
24	A	1150.0	0.9	2
25	A	1166.5	2.4	7
26	A	1228.7	20.8	58
27	A	1292.7	0.2	0
28	A	1313.4	1.5	4
29	A	1441.1	5.2	14
30	A	1475.2	17.1	48
31	A	1574.7	1.5	4
32	A	1589.1	1.9	5
33	A	1718.3	10.9	30
34	A	3054.9	26.3	73
35	A	3062.7	1.4	4
36	A	3071.5	7.7	21
37	A	3080.6	21.4	59
38	A	3088.0	18.8	52
39	A	3096.8	7.3	20

Diphenylnitrilimine (propargylic structure), cf. ref. 41, D. Bégué, G. Qiao, C. Wentrup, *J. Am. Chem. Soc.* **2012**, *134*, 5539.



a) Method: B3LYP/6-31G*

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-0.959445	-0.550113	0.002239
2	7	0.163384	-0.892889	0.001153
3	7	1.314364	-1.413721	0.000722
4	6	2.413421	-0.539133	0.000165
5	6	2.328606	0.864820	0.000079
6	6	3.682572	-1.145560	-0.000316
7	6	3.490226	1.635108	-0.000457
8	1	1.356587	1.350307	0.000410
9	6	4.834037	-0.366164	-0.000848
10	1	3.736043	-2.229979	-0.000234
11	6	4.748516	1.029922	-0.000918
12	1	3.408646	2.719414	-0.000534
13	1	5.806789	-0.851436	-0.001198
14	1	5.649633	1.636445	-0.001357
15	6	-2.326677	-0.181359	0.000946
16	6	-3.327783	-1.177750	-0.000601
17	6	-2.703591	1.179121	0.001381
18	6	-4.669274	-0.811364	-0.001699
19	1	-3.041345	-2.224578	-0.000946
20	6	-4.050615	1.524911	0.000163
21	1	-1.937279	1.947777	0.002614
22	6	-5.038764	0.536595	-0.001339
23	1	-5.431737	-1.585268	-0.002891
24	1	-4.330397	2.574686	0.000443
25	1	-6.088546	0.814697	-0.002202

Energy = -610.8234847

E+ZPVE = -610.627838

Vibrational Frequencies:

Scaled by 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	18.4	0.2	0
2	A	29.8	0.1	0
3	A	37.5	0.1	0
4	A	79.5	0.5	0
5	A	117.3	0.2	0
6	A	218.6	0.1	0
7	A	245.1	0.3	0
8	A	272.5	0.6	0
9	A	357.4	1.2	0
10	A	391.0	0.5	0
11	A	403.3	0.8	0
12	A	411.0	3.4	0
13	A	473.4	4.7	0
14	A	478.2	5.7	0
15	A	490.3	2.4	0
16	A	490.6	2.4	0
17	A	606.6	0.4	0
18	A	609.4	0.6	0
19	A	630.1	18.3	1
20	A	671.4	11.7	1
21	A	674.1	14.6	1
22	A	722.6	56.7	4
23	A	729.6	46.4	3
24	A	736.1	53.8	4
25	A	801.0	4.8	0
26	A	804.7	0.0	0
27	A	813.7	0.0	0
28	A	861.6	5.3	0
29	A	877.4	3.5	0
30	A	919.7	0.1	0
31	A	928.7	0.0	0
32	A	945.4	0.3	0

33	A	957.5	0.1	0
34	A	971.6	1.8	0
35	A	973.0	2.1	0
36	A	1010.1	7.5	1
37	A	1013.1	6.4	0
38	A	1063.5	50.9	3
39	A	1070.0	5.6	0
40	A	1071.2	43.1	3
41	A	1142.8	4.2	0
42	A	1149.1	0.1	0
43	A	1156.4	39.4	3
44	A	1167.6	1.7	0
45	A	1206.4	196.7	13
46	A	1276.3	0.8	0
47	A	1289.5	17.5	1
48	A	1315.2	12.7	1
49	A	1316.1	0.8	0
50	A	1368.6	426.3	28
51	A	1431.3	4.0	0
52	A	1443.1	1.0	0
53	A	1477.3	160.7	11
54	A	1480.3	14.6	1
55	A	1556.7	3.2	0
56	A	1568.8	7.0	0
57	A	1588.2	44.0	3
58	A	1592.5	137.4	9
59	A	2272.8	1502.4	100
60	A	3054.9	9.7	1
61	A	3063.3	9.5	1
62	A	3067.4	4.6	0
63	A	3073.4	22.7	2
64	A	3074.6	5.5	0
65	A	3082.8	31.4	2
66	A	3085.6	15.4	1

67	A	3090.2	19.2	1
68	A	3091.9	17.7	1
69	A	3096.1	11.7	1

b) Method: B3LYP/6-311+G**

scrf, dielectric constant = 36.64

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.731212	1.033758	0.188676
2	6	-3.683637	-1.121646	-0.162139
3	6	-2.405209	-0.538673	-0.069388
4	6	-2.314508	0.847525	0.156123
5	6	-3.468118	1.616645	0.282078
6	7	-1.318572	-1.404119	-0.210629
7	1	-5.624563	1.639557	0.288695
8	1	-3.748889	-2.189519	-0.335802
9	1	-1.343380	1.321526	0.238216
10	1	-3.374703	2.683290	0.457167
11	7	-0.161444	-0.882942	-0.149940
12	6	0.954602	-0.545975	-0.137555
13	6	-4.825375	-0.343284	-0.034090
14	1	-5.800495	-0.814468	-0.108957
15	6	2.322243	-0.181499	-0.061971
16	6	2.725680	1.137423	-0.345364
17	6	3.286870	-1.144288	0.294621
18	6	4.068635	1.481369	-0.260426
19	1	1.986799	1.876813	-0.629000
20	6	4.627029	-0.785451	0.360342

21	1	2.977959	-2.158713	0.514941
22	6	5.022548	0.524697	0.088366
23	1	4.374464	2.498597	-0.474349
24	1	5.366555	-1.529759	0.630872
25	1	6.069081	0.798484	0.146558

Energy = -610.9815137

E+ZPVE = -610.787312

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	8.5	1.6	0
2	A	35.6	0.1	0
3	A	42.2	0.6	0
4	A	88.3	3.8	0
5	A	126.8	0.9	0
6	A	221.7	3.4	0
7	A	267.9	11.5	0
8	A	284.8	1.5	0
9	A	370.0	4.0	0
10	A	403.3	0.5	0
11	A	418.1	0.5	0
12	A	436.8	10.3	0
13	A	481.1	11.6	0
14	A	502.1	19.9	1
15	A	505.2	22.9	1
16	A	528.6	7.8	0
17	A	630.3	3.1	0
18	A	633.2	1.1	0
19	A	657.3	53.5	2
20	A	688.3	35.0	1
21	A	695.7	37.8	1
22	A	745.8	187.5	6

23	A	749.8	96.8	3
24	A	762.4	68.5	2
25	A	827.6	0.0	0
26	A	831.6	8.2	0
27	A	847.3	2.2	0
28	A	883.8	9.1	0
29	A	930.9	2.9	0
30	A	966.6	0.1	0
31	A	975.2	0.1	0
32	A	989.3	0.0	0
33	A	1004.7	54.6	2
34	A	1010.2	0.3	0
35	A	1015.7	0.0	0
36	A	1040.1	5.8	0
37	A	1043.8	69.5	2
38	A	1089.0	277.5	9
39	A	1101.3	62.4	2
40	A	1104.7	8.9	0
41	A	1172.9	25.3	1
42	A	1189.8	2.5	0
43	A	1190.5	228.5	7
44	A	1203.5	3.3	0
45	A	1244.1	626.2	20
46	A	1312.2	11.1	0
47	A	1320.1	197.4	6
48	A	1352.7	210.6	7
49	A	1355.3	2.2	0
50	A	1371.7	2145.1	70
51	A	1472.5	10.5	0
52	A	1479.9	0.2	0
53	A	1510.8	571.6	19
54	A	1517.8	10.2	0
55	A	1603.0	7.1	0
56	A	1604.5	24.2	1

57	A	1629.0	529.7	17
58	A	1630.0	29.8	1
59	A	2330.3	3085.3	100
60	A	3148.8	60.0	2
61	A	3160.5	17.8	1
62	A	3176.5	90.7	3
63	A	3177.4	6.6	0
64	A	3182.8	0.3	0
65	A	3183.5	45.4	1
66	A	3187.4	30.4	1
67	A	3191.6	3.0	0
68	A	3196.8	14.2	0
69	A	3203.5	8.8	0

c) Method: B3LYP/6-31G*

scrf, dielectric constant = 36.64

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.961439	-0.552996	-0.004384
2	7	-0.160885	-0.887614	-0.004660
3	7	-1.320036	-1.418261	-0.006576
4	6	-2.408868	-0.543954	-0.002089
5	6	-2.329646	0.863149	0.004829
6	6	-3.684714	-1.144443	-0.004873
7	6	-3.490569	1.633743	0.008682
8	1	-1.358748	1.350037	0.007272
9	6	-4.834715	-0.364215	-0.000959
10	1	-3.738934	-2.229240	-0.010174
11	6	-4.751290	1.032703	0.005838

12	1	-3.404882	2.717920	0.014002
13	1	-5.808193	-0.851039	-0.003235
14	1	-5.651643	1.641472	0.008882
15	6	2.331936	-0.181274	-0.001972
16	6	3.329693	-1.179052	0.008876
17	6	2.702456	1.179584	-0.010503
18	6	4.671155	-0.811335	0.010909
19	1	3.044181	-2.226158	0.015531
20	6	4.049318	1.527024	-0.007786
21	1	1.935250	1.947420	-0.019137
22	6	5.036505	0.537718	0.002769
23	1	5.436424	-1.581675	0.019089
24	1	4.331168	2.575677	-0.014194
25	1	6.085630	0.816803	0.004598

Energy = -610.826281

E+ZPVE = -610.630824

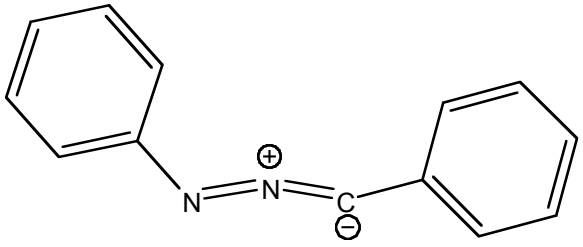
Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	4.2	0.3	0
2	A	38.9	0.1	0
3	A	40.2	0.3	0
4	A	94.5	0.4	0
5	A	124.2	1.4	0
6	A	225.6	0.2	0
7	A	270.9	1.6	0
8	A	283.2	3.5	0
9	A	368.2	5.7	0
10	A	403.9	0.5	0
11	A	419.3	1.6	0
12	A	427.1	2.4	0

13	A	491.2	5.0	0
14	A	498.8	36.2	1
15	A	511.2	3.2	0
16	A	516.7	1.3	0
17	A	630.9	4.4	0
18	A	633.5	1.7	0
19	A	655.1	52.7	1
20	A	697.3	19.3	1
21	A	700.6	12.5	0
22	A	747.5	231.8	7
23	A	756.3	70.5	2
24	A	762.0	40.4	1
25	A	835.1	8.7	0
26	A	835.3	0.2	0
27	A	847.4	0.0	0
28	A	881.9	9.5	0
29	A	925.9	1.8	0
30	A	950.6	0.3	0
31	A	971.0	0.5	0
32	A	973.2	0.0	0
33	A	1008.5	49.2	1
34	A	1011.2	0.0	0
35	A	1012.3	4.5	0
36	A	1049.2	28.1	1
37	A	1052.9	42.5	1
38	A	1096.0	314.9	9
39	A	1110.8	50.0	1
40	A	1114.6	7.0	0
41	A	1184.0	16.7	0
42	A	1200.5	0.7	0
43	A	1201.8	249.1	7
44	A	1214.9	3.4	0
45	A	1258.3	742.7	21
46	A	1331.3	10.0	0

47	A	1336.5	263.9	7
48	A	1366.0	576.3	16
49	A	1369.1	3.4	0
50	A	1384.2	2072.3	58
51	A	1489.3	11.9	0
52	A	1500.6	0.8	0
53	A	1532.4	661.8	19
54	A	1536.3	35.2	1
55	A	1622.4	5.9	0
56	A	1625.9	21.5	1
57	A	1649.6	52.0	1
58	A	1652.8	598.4	17
59	A	2353.5	3559.6	100
60	A	3163.3	95.7	3
61	A	3177.6	32.8	1
62	A	3192.9	178.4	5
63	A	3200.3	17.8	1
64	A	3203.5	59.5	2
65	A	3205.1	0.0	0
66	A	3206.4	32.0	1
67	A	3213.9	3.1	0
68	A	3219.0	24.0	1
69	A	3226.9	23.4	1

Diphenylnitrilimine (allenic structure); not observed, cf. ref. 41, D. Bégué, G. Qiao, C. Wentrup, *J. Am. Chem. Soc.* **2012**, *134*, 5539.



a) Method: B3LYP/6-31G*

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.960874	-0.284032	-0.890254
2	7	-0.127198	-0.710498	-0.653882
3	7	-1.251497	-1.260412	-0.604005
4	6	-2.345329	-0.458775	-0.209262
5	6	-2.264197	0.909737	0.097931
6	6	-3.588882	-1.106942	-0.140014
7	6	-3.412288	1.608606	0.466440
8	1	-1.306966	1.420676	0.046549
9	6	-4.728195	-0.399487	0.231092
10	1	-3.635147	-2.163988	-0.383621
11	6	-4.648593	0.962473	0.536521
12	1	-3.338314	2.667518	0.701668
13	1	-5.684565	-0.913650	0.280960
14	1	-5.538989	1.513109	0.826474
15	6	2.286299	-0.095375	-0.355737
16	6	3.173413	0.789331	-0.993106
17	6	2.714674	-0.801094	0.787038
18	6	4.458578	0.976320	-0.489938
19	1	2.840492	1.320647	-1.879138
20	6	4.005105	-0.618404	1.274458
21	1	2.030664	-1.486523	1.278247
22	6	4.877559	0.271921	0.640977
23	1	5.136191	1.666369	-0.984560
24	1	4.330525	-1.167218	2.153876
25	1	5.882869	0.413754	1.027865

Energy = -610.8232938

E+ZPVE = -610.627243

Vibrational Frequencies:

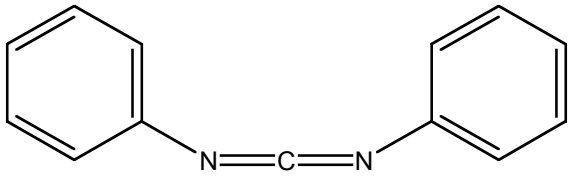
Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	18.6	0.4	0
2	A	34.8	1.6	0
3	A	39.0	0.5	0
4	A	93.7	12.6	1
5	A	120.9	0.1	0
6	A	230.9	6.9	1
7	A	265.8	6.5	1
8	A	292.9	0.9	0
9	A	363.4	16.1	2
10	A	399.9	2.0	0
11	A	405.5	0.0	0
12	A	425.8	21.0	2
13	A	475.0	15.7	2
14	A	483.0	2.0	0
15	A	511.9	167.9	19
16	A	526.8	8.8	1
17	A	606.2	0.4	0
18	A	608.0	0.5	0
19	A	626.4	54.2	6
20	A	674.6	9.0	1
21	A	676.4	23.2	3
22	A	737.5	26.4	3
23	A	739.4	28.1	3
24	A	746.2	48.7	6
25	A	798.4	6.0	1
26	A	812.6	0.0	0
27	A	826.7	0.6	0
28	A	872.0	6.1	1
29	A	902.9	4.1	0

30	A	924.2	0.1	0
31	A	937.7	0.0	0
32	A	948.7	0.3	0
33	A	965.5	0.1	0
34	A	974.8	0.9	0
35	A	977.8	3.0	0
36	A	1011.3	1.4	0
37	A	1013.6	7.5	1
38	A	1065.9	13.0	1
39	A	1067.6	8.9	1
40	A	1079.2	12.7	1
41	A	1143.3	2.1	0
42	A	1149.0	0.3	0
43	A	1153.5	15.6	2
44	A	1164.8	3.9	0
45	A	1192.0	56.2	6
46	A	1279.6	47.7	5
47	A	1291.8	9.1	1
48	A	1313.0	3.1	0
49	A	1315.0	7.1	1
50	A	1374.8	379.7	43
51	A	1432.3	6.1	1
52	A	1443.4	1.2	0
53	A	1477.6	103.4	12
54	A	1483.6	29.1	3
55	A	1565.2	9.4	1
56	A	1572.6	5.3	1
57	A	1589.6	16.9	2
58	A	1592.7	76.9	9
59	A	2122.6	882.4	100
60	A	3057.0	5.4	1
61	A	3065.2	11.7	1
62	A	3066.2	0.6	0
63	A	3075.3	5.9	1

64	A	3077.1	20.8	2
65	A	3083.9	26.9	3
66	A	3084.4	18.1	2
67	A	3090.6	17.0	2
68	A	3091.7	16.5	2
69	A	3096.2	11.8	1

Diphenylcarbodiimide:



a) Method: B3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.771333	0.846124	0.333816
2	6	-4.653970	-0.064966	-0.714848
3	6	-3.436020	-0.686732	-0.974473
4	6	-2.320595	-0.397650	-0.182907
5	6	-2.436507	0.517059	0.872441
6	6	-3.658290	1.132459	1.124937
7	7	-1.114925	-1.056820	-0.483382
8	6	-0.000001	-0.964155	-0.000114
9	7	1.114944	-1.057002	0.483070
10	6	2.320604	-0.397725	0.182789
11	6	3.436039	-0.687031	0.974259

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   12              6                            4.653977    -0.065164
0.714816
   13            6                           4.771318     0.846249    -
0.333570
   14            6                           3.658266     1.132801    -
1.124601
   15            6                           2.436495     0.517304    -
0.872284
   16             1                             -5.720822     1.328445
0.534642
   17            1                          -5.513851    -0.294729    -
1.333852
   18            1                          -3.331417    -1.398086    -
1.784594
   19             1                             -1.572780     0.738437
1.489880
   20             1                             -3.740623     1.838440
1.943780
   21             1                              3.331452    -1.398633
1.784163
   22             1                              5.513866    -0.295102
1.333744
   23            1                           5.720796     1.328652    -
0.534253
   24            1                           3.740582     1.839031    -
1.943231
   25            1                           1.572760     0.738859    -
1.489647
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Energy = -611.0449497
E+ZPVE = -610.849734

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	22.8	0.1	0
2	A	29.1	0.5	0
3	A	36.8	0.3	0
4	A	101.4	8.7	0
5	A	111.2	0.2	0
6	A	239.7	2.3	0
7	A	274.6	0.0	0
8	A	293.2	0.3	0
9	A	410.3	25.2	1
10	A	419.6	0.0	0
11	A	420.3	3.9	0
12	A	455.2	0.4	0
13	A	502.3	5.0	0
14	A	513.1	0.5	0
15	A	530.2	11.5	0

16	A	617.0	178.6	6
17	A	630.3	0.5	0
18	A	634.4	26.2	1
19	A	636.6	4.2	0
20	A	700.3	23.7	1
21	A	701.4	34.0	1
22	A	761.4	13.2	0
23	A	767.0	58.7	2
24	A	772.1	60.1	2
25	A	820.6	3.3	0
26	A	841.3	0.2	0
27	A	842.1	0.2	0
28	A	917.8	5.4	0
29	A	919.3	5.3	0
30	A	978.9	0.1	0
31	A	979.2	0.1	0
32	A	994.6	0.1	0
33	A	994.6	0.0	0
34	A	1015.5	0.5	0
35	A	1016.4	0.3	0
36	A	1043.6	2.1	0
37	A	1045.4	11.6	0
38	A	1098.6	3.0	0
39	A	1099.3	23.1	1
40	A	1118.4	9.8	0
41	A	1180.8	1.6	0
42	A	1180.9	0.0	0
43	A	1192.1	16.2	1
44	A	1196.2	0.1	0
45	A	1232.3	161.6	6
46	A	1318.7	41.5	1
47	A	1319.4	0.1	0
48	A	1351.0	0.3	0
49	A	1351.3	0.1	0
50	A	1477.8	0.8	0
51	A	1481.3	8.2	0
52	A	1485.5	0.3	0
53	A	1519.0	163.0	6
54	A	1559.0	19.4	1
55	A	1617.7	2.9	0
56	A	1618.2	29.3	1
57	A	1632.3	200.2	7
58	A	1639.8	5.8	0
59	A	2226.6	2773.9	100
60	A	3163.8	6.3	0
61	A	3163.9	0.8	0
62	A	3171.1	2.7	0
63	A	3171.1	2.1	0
64	A	3179.7	27.1	1
65	A	3179.8	0.7	0
66	A	3189.9	22.9	1

67	A	3189.9	12.2	0
68	A	3197.4	12.6	0
69	A	3197.5	0.4	0

b) Method: B3LYP/6-31G*

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.789635	0.378738	0.818388
2	6	4.663693	-0.727489	-0.024088
3	6	3.440569	-1.020118	-0.625015
4	6	2.328695	-0.203713	-0.383915
5	6	2.453826	0.909824	0.461746
6	6	3.680247	1.194383	1.057136
7	7	1.120807	-0.541901	-1.019396
8	6	-0.000028	-0.053344	-0.943720
9	7	-1.120834	0.423519	-1.074541
10	6	-2.328806	0.159039	-0.405166
11	6	-3.440153	0.944614	-0.734772
12	6	-4.663115	0.721669	-0.104304
13	6	-4.789492	-0.283962	0.856005
14	6	-3.680673	-1.069175	1.183001
15	6	-2.454418	-0.853586	0.558989
16	1	5.744004	0.605214	1.285199
17	1	5.521234	-1.366523	-0.216451
18	1	3.327416	-1.875336	-1.283684
19	1	1.590630	1.544754	0.643439
20	1	3.769466	2.058423	1.710287

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   21           1                       -3.326813     1.721284    -
1.484441
   22           1                       -5.520209     1.336179    -
0.366072
   23            1                           -5.743706    -0.456189
1.345729
   24            1                           -3.770088    -1.855278
1.928113
   25            1                           -1.591628    -1.465137
0.809722
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Energy = -610.8883691
E+ZPVE = -610.691841

Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	22.5	0.0	0
2	A	30.4	0.6	0
3	A	36.1	0.3	0
4	A	97.9	8.4	0
5	A	107.1	0.2	0
6	A	235.6	2.7	0
7	A	266.0	0.0	0
8	A	282.3	0.2	0
9	A	391.0	23.8	1
10	A	405.5	0.0	0
11	A	406.2	1.7	0
12	A	434.1	0.3	0
13	A	486.3	2.0	0
14	A	493.0	0.8	0
15	A	512.6	5.6	0
16	A	579.6	189.0	7
17	A	599.2	6.8	0
18	A	606.7	0.0	0
19	A	609.6	10.4	0
20	A	675.5	10.6	0
21	A	677.0	17.4	1
22	A	732.0	13.7	1
23	A	742.2	47.2	2
24	A	747.1	48.4	2
25	A	791.9	3.3	0
26	A	816.1	0.1	0
27	A	816.7	0.1	0
28	A	884.4	4.5	0
29	A	885.9	5.0	0
30	A	928.4	0.1	0
31	A	928.6	0.1	0

32	A	954.4	0.2	0
33	A	954.5	0.2	0
34	A	979.2	0.1	0
35	A	979.4	1.4	0
36	A	1011.9	1.6	0
37	A	1014.3	7.3	0
38	A	1066.0	2.6	0
39	A	1066.4	17.9	1
40	A	1082.8	8.7	0
41	A	1145.6	0.9	0
42	A	1145.7	0.1	0
43	A	1157.7	8.9	0
44	A	1160.8	0.1	0
45	A	1199.8	155.4	6
46	A	1285.1	35.1	1
47	A	1285.5	0.1	0
48	A	1312.7	2.7	0
49	A	1312.8	0.3	0
50	A	1438.5	0.6	0
51	A	1442.0	7.4	0
52	A	1443.8	0.0	0
53	A	1480.5	156.0	6
54	A	1515.4	18.7	1
55	A	1574.8	4.1	0
56	A	1575.1	31.3	1
57	A	1590.6	175.6	7
58	A	1597.5	4.4	0
59	A	2155.1	2532.0	100
60	A	3060.5	4.6	0
61	A	3060.8	3.0	0
62	A	3068.0	3.9	0
63	A	3068.3	3.8	0
64	A	3076.2	26.9	1
65	A	3076.6	15.8	1
66	A	3085.9	29.2	1
67	A	3086.2	24.1	1
68	A	3094.5	10.2	0
69	A	3095.1	8.3	0

Transition state connecting *exo*-3-pyridyl-bicyclic lactone and *N*-nitroso-*N*-(3-pyridyl)aminoketene (*s-Z*):

a) Method: B3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

```
    1             7                           -0.584411    -0.079029
0.542931
    2             7                          -1.335547    -1.048225    -
0.273697
    3             8                           -2.426792    -1.272996
0.371699
    4             6                          -2.818307     0.539632    -
0.042023
    5             6                          -1.447707     0.755058    -
0.259768
    6             8                          -3.919483     0.774052    -
0.299004
    7             1                          -1.090582     1.615719    -
0.811786
    8             6                           0.801157     0.010795
0.218228
    9             6                           1.474376     1.230461
0.282673
   10             6                           1.540681    -1.147738    -
0.054062
   11             6                           2.847519     1.240644
0.066214
   12             1                           0.943537     2.146898
0.515746
   13             1                           1.042848    -2.110699    -
0.098906
   14             6                           3.494613     0.037127    -
0.205400
   15             1                           3.407423     2.167111
0.110427
   16             1                           4.565257     0.011052    -
0.382188
   17             7                           2.855347    -1.134804    -
0.262093
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```

Energy = -584.3936663

E+ZPVE = -584.280504

Imaginary Frequency: -719.0345

b) Method: B3LYP/6-31G*

```
---------------------------------------------------------------------
 Center     Atomic                     Coordinates (Angstroms)
 Number     Number                  X           Y           Z
 ---------------------------------------------------------------------
-
    1             7                           -0.583720    -0.079078
0.553855
    2             7                          -1.343557    -1.056126    -
0.268789
```

```
    3              8                          -2.431924    -1.265948
0.386592
    4              6                          -2.816454     0.536206    -
0.046119
    5              6                          -1.444656     0.775248    -
0.226565
    6              8                          -3.920523     0.766751    -
0.340841
    7              1                          -1.084124     1.661658    -
0.739030
    8              6                           0.800469     0.010337
0.224927
    9              6                           1.479098     1.230563
0.289885
   10              6                           1.539743    -1.149199    -
0.056724
   11              6                           2.852918     1.239121
0.063018
   12              1                           0.949224     2.148375
0.530506
   13              1                           1.037990    -2.112811    -
0.103265
   14              6                           3.495773     0.033337    -
0.218984
   15              1                           3.415235     2.166977
0.106562
   16              1                           4.567423     0.005960    -
0.404714
   17              7                           2.854774    -1.140548    -
0.275450
 ---------------------------------------------------------------------
-
```

Energy = -584.2332865

E+ZPVE = -584.119325

Imaginary Frequency: -701.6843

Transition state connecting *exo*-phenyl-bicyclic lactone and *s-Z-N*-nitroso-*N*-phenylaminoketene:

a) Method: B3LYP/6-311++G**

```
---------------------------------------------------------------------
 Center     Atomic                     Coordinates (Angstroms)
 Number     Number                     X           Y           Z
 ---------------------------------------------------------------------
-
    1              7                           0.598958     0.087169
0.547761
    2              7                           1.353719     1.061146    -
0.247069
```

```
    3             8                           2.450977     1.264984
0.398648
    4             6                           2.824411    -0.546201    -
0.059949
    5             6                           1.451775    -0.740337    -
0.275278
    6             8                           3.923309    -0.782097    -
0.327990
    7             1                           1.079677    -1.581402    -
0.846923
    8             6                          -0.793009     0.009456
0.221509
    9             6                          -1.449214    -1.222462
0.294061
   10             6                         -1.514525     1.173188    -
0.056318
   11             6                          -2.823827    -1.286810
0.082493
   12             1                          -0.894713    -2.121955
0.537189
   13             6                         -2.888735     1.094870    -
0.265187
   14             1                         -1.001968     2.125173    -
0.105034
   15             6                         -3.549432    -0.130785    -
0.200205
   16             1                          -3.327546    -2.244722
0.143627
   17             1                         -3.444043     2.000421    -
0.481413
   18             1                         -4.619104    -0.184329    -
0.364300
 ---------------------------------------------------------------------
-
```

Energy = -568.3560423

E+ZPVE = -568.231035

Imaginary Frequency: -719.2275

b) Method: B3LYP/6-31G*

```
---------------------------------------------------------------------
 Center     Atomic                     Coordinates (Angstroms)
 Number     Number                    X           Y           Z
 ---------------------------------------------------------------------
-
    1             7                           0.598500     0.086933
0.561020
    2             7                           1.361401     1.069550    -
0.237905
    3             8                           2.456947     1.255585
0.415759
```

```
     4           6                        2.821440    -0.543608    -
0.066361
     5           6                        1.447269    -0.760515    -
0.243777
     6           8                        3.922641    -0.774545    -
0.373792
     7           1                        1.069688    -1.626388    -
0.778120
     8           6                       -0.792285     0.010756
0.228659
     9           6                       -1.453819    -1.221166
0.304273
    10           6                      -1.512138     1.176061    -
0.059954
    11           6                       -2.828766    -1.284237
0.081378
    12           1                       -0.900481    -2.121382
0.557713
    13           6                      -2.886352     1.098775    -
0.281194
    14           1                      -0.995110     2.128063    -
0.111736
    15           6                      -3.551113    -0.127230    -
0.215120
    16           1                       -3.334919    -2.243643
0.143759
    17           1                      -3.438733     2.006536    -
0.507859
    18           1                      -4.621870    -0.179910    -
0.388722
 -------------------------------------------------------------------
-
```

Energy = -568.19919

E+ZPVE = -568.073359

Imaginary Frequency: -702.7995

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