

**Supporting Information for**  
**Theoretical study on photochemistry of furoylazides:**  
**Curtius rearrangement and subsequent reactions**

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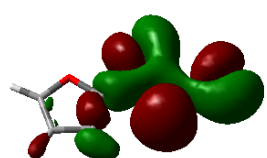
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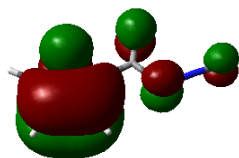
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Table S1. Relative TD-CAM-B3LYP vertical excitation energy ( $\Delta E$ ) and wavelength ( $\lambda$ ) at  $\mathbf{1-S}_0$  together with the electronic configuration (weight in the parenthesis, orbitals below the table) and oscillator strength ( $f$ )

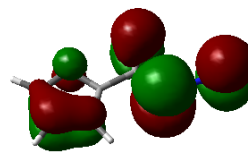
State	Configuration and weight	$\Delta E/eV$	$\lambda/nm$	Oscillator strength
S <sub>0</sub>	-	0.00	-	-
S <sub>1</sub>	HOMO-1→LUMO(0.68)	4.49	276	0.0001
S <sub>2</sub>	HOMO-2→LUMO+1(0.63)	4.79	259	0.0004
S <sub>3</sub>	HOMO→LUMO(0.65)	5.00	248	0.4295
S <sub>4</sub>	HOMO-2→LUMO(0.44)	5.45	228	0.0582
S <sub>5</sub>	HOMO→LUMO+1(0.65)	6.21	200	0.0001
S <sub>6</sub>	HOMO-3→LUMO(0.59)	6.26	198	0.0396
S <sub>7</sub>	HOMO-4→LUMO(0.57)	6.49	191	0.0004
S <sub>8</sub>	HOMO-1→LUMO+1(0.46)	6.60	188	0.1462
S <sub>9</sub>	HOMO→LUMO+2(0.60)	7.08	175	0.0110
S <sub>10</sub>	HOMO-2→LUMO+2(0.42)	7.34	169	0.0023



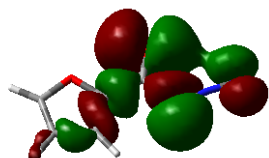
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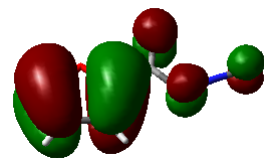
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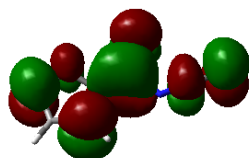
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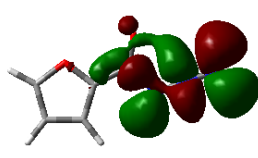
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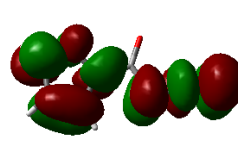
HOMO



LUMO



LUMO+1



LUMO+2

Table S2. Relative TD-M06-2X vertical excitation energy ( $\Delta E$ ) and wavelength ( $\lambda$ ) at  $1-S_0$  together with the electronic configuration (weight in the parenthesis, orbitals below the table) and oscillator strength ( $f$ )

State	Configuration and weight	$\Delta E/eV$	$\lambda/nm$	Oscillator strength
S <sub>0</sub>	-	0.00	-	-
S <sub>1</sub>	HOMO-2 $\rightarrow$ LUMO(0.62)	4.35	285	0.0000
S <sub>2</sub>	HOMO-1 $\rightarrow$ LUMO+1(0.57)	4.60	269	0.0003
S <sub>3</sub>	HOMO $\rightarrow$ LUMO(0.66)	5.08	244	0.4585
S <sub>4</sub>	HOMO-1 $\rightarrow$ LUMO(0.50)	5.57	222	0.0351
S <sub>5</sub>	HOMO $\rightarrow$ LUMO+1(0.65)	6.38	194	0.0000
S <sub>6</sub>	HOMO-3 $\rightarrow$ LUMO(0.61)	6.41	193	0.0498
S <sub>7</sub>	HOMO-4 $\rightarrow$ LUMO(0.53)	6.51	190	0.0006
S <sub>8</sub>	HOMO-2 $\rightarrow$ LUMO+1(0.43)	6.84	181	0.1663
S <sub>9</sub>	HOMO $\rightarrow$ LUMO+2(0.62)	7.33	169	0.0158
S <sub>10</sub>	HOMO-4 $\rightarrow$ LUMO+1(0.43)	7.62	163	0.0254

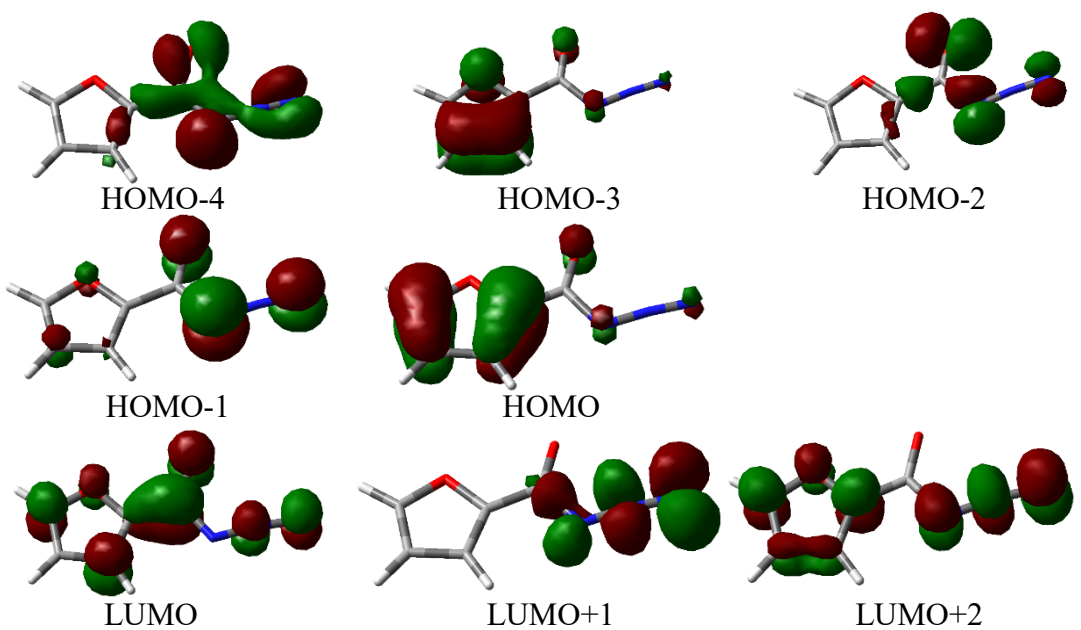
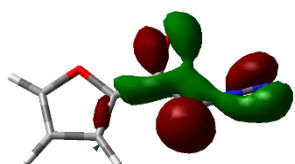
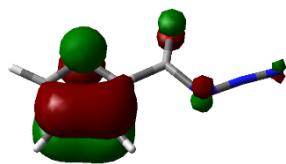


Table S3. Relative TD- $\omega$ B97XD vertical excitation energy ( $\Delta E$ ) and wavelength ( $\lambda$ ) at  $1-S_0$  together with the electronic configuration (weight in the parenthesis, orbitals below the table) and oscillator strength ( $f$ )

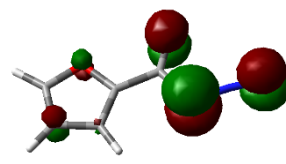
State	Configuration and weight	$\Delta E/eV$	$\lambda/nm$	Oscillator strength
S <sub>0</sub>	-	0.00	-	-
S <sub>1</sub>	HOMO-1 $\rightarrow$ LUMO(0.69)	4.48	276	0.0001
S <sub>2</sub>	HOMO-2 $\rightarrow$ LUMO+1(0.63)	4.86	255	0.0004
S <sub>3</sub>	HOMO $\rightarrow$ LUMO(0.65)	5.01	247	0.4348
S <sub>4</sub>	HOMO-1 $\rightarrow$ LUMO+1(0.44)	5.46	227	0.0617
S <sub>5</sub>	HOMO-3 $\rightarrow$ LUMO(0.58)	6.26	198	0.0369
S <sub>6</sub>	HOMO $\rightarrow$ LUMO+1(0.64)	6.32	196	0.0001
S <sub>7</sub>	HOMO-4 $\rightarrow$ LUMO(0.57)	6.50	190	0.0003
S <sub>8</sub>	HOMO-1 $\rightarrow$ LUMO+1(0.46)	6.59	188	0.1426
S <sub>9</sub>	HOMO $\rightarrow$ LUMO+2(0.58)	7.14	173	0.0179
S <sub>10</sub>	HOMO-2 $\rightarrow$ LUMO+2(0.40)	7.36	168	0.0052



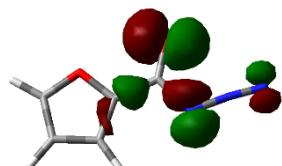
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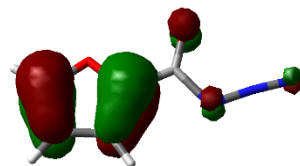
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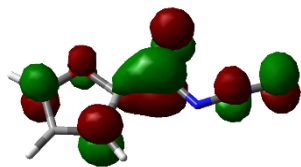
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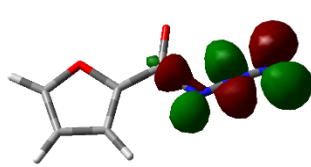
HOMO-1



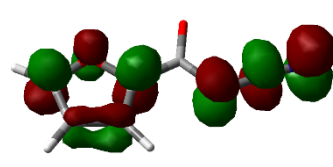
HOMO



LUMO



LUMO+1



LUMO+2

Table S4. Relative CASPT2 vertical excitation energy ( $\Delta E$ ) and wavelength ( $\lambda$ ) at  $5-S_0$  together with the electronic configuration (weight in the parenthesis, orbitals below the table) and oscillator strength ( $f$ )

State	Configuration and weight	$\Delta E/eV$	$\lambda/nm$	Oscillator strength
$S_0$	-	0.00	-	-
$S_1$	2u22222d0000(0.72)	3.97	312	0.0010
$S_2$	22u2222d0000(0.37) 2u222220d000(0.31)	4.93	251	0.1065
$S_3$	22222u2d0000(0.55)	5.04	246	0.0535
$S_4$	22u22220d000(0.83)	5.11	243	0.0011

The figure displays 12 molecular orbital diagrams, numbered 1 through 12, arranged in a 4x3 grid. Each diagram shows a chemical structure with electron density lobes represented in green and red. The orbitals are labeled 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, and 12.

"u" and "d" stand for singly occupied orbitals with electrons of spin up (u) or spin down (d).

Table S5. Relative TD-CAM-B3LYP vertical excitation energy ( $\Delta E$ ) and wavelength ( $\lambda$ ) at **5**-S<sub>0</sub> together with the electronic configuration (weight in the parenthesis, orbitals below the table) and oscillator strength ( $f$ )

State	Configuration and weight	$\Delta E/eV$	$\lambda/nm$	Oscillator strength
S <sub>0</sub>	-	0.00	-	-
S <sub>1</sub>	HOMO-1→LUMO(0.68)	4.53	274	0.0001
S <sub>2</sub>	HOMO-2→LUMO+1(0.66)	4.85	256	0.0005
S <sub>3</sub>	HOMO→LUMO(0.67)	5.21	238	0.1293
S <sub>4</sub>	HOMO-2→LUMO(0.47)	5.37	231	0.0101
S <sub>5</sub>	HOMO-3→LUMO(0.56)	6.27	198	0.2572
S <sub>6</sub>	HOMO→LUMO+1(0.69)	6.33	196	0.0000
S <sub>7</sub>	HOMO-4→LUMO(0.59)	6.50	191	0.0004
S <sub>8</sub>	HOMO-1→LUMO+1(0.48)	6.66	186	0.1754
S <sub>9</sub>	HOMO→LUMO+2(0.62)	6.93	179	0.2280
S <sub>10</sub>	HOMO-4→LUMO+1(0.46)	7.45	166	0.0685

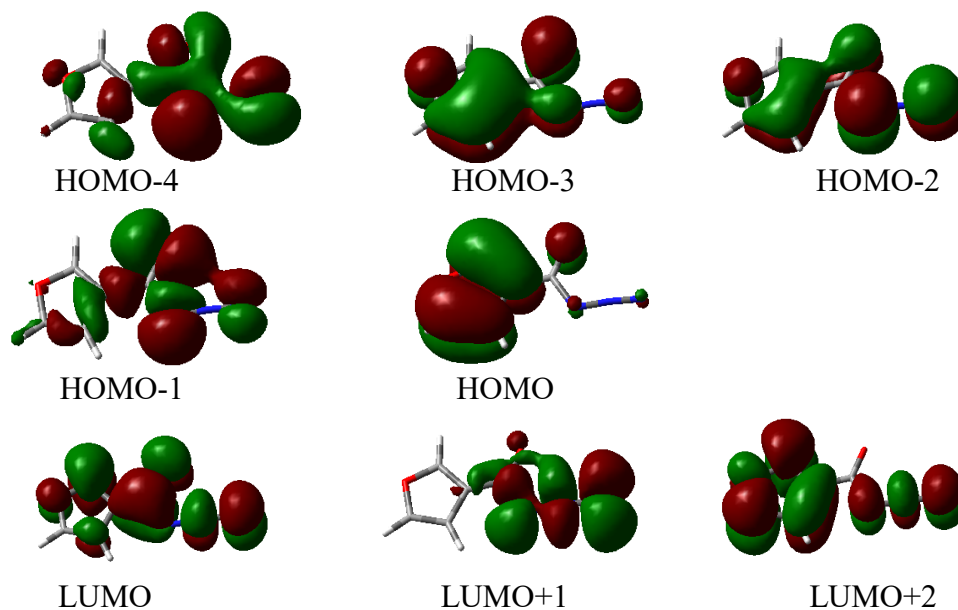


Table S6. Relative TD-M06-2X vertical excitation energy ( $\Delta E$ ) and wavelength ( $\lambda$ ) at  $\mathbf{5-S_0}$  together with the electronic configuration (weight in the parenthesis, orbitals below the table) and oscillator strength ( $f$ )

State	Configuration and weight	$\Delta E/eV$	$\lambda/nm$	Oscillator strength
S <sub>0</sub>	-	0.00	-	-
S <sub>1</sub>	HOMO-2→LUMO(0.62)	4.49	276	0.0000
S <sub>2</sub>	HOMO-1→LUMO+1(0.58)	4.75	261	0.0004
S <sub>3</sub>	HOMO→LUMO(0.68)	5.46	227	0.1298
S <sub>4</sub>	HOMO-3→LUMO(0.58)	5.62	220	0.0293
S <sub>5</sub>	HOMO-1→LUMO(0.49)	6.49	191	0.2382
S <sub>6</sub>	HOMO→LUMO+1(0.69)	6.57	189	0.0000
S <sub>7</sub>	HOMO-4→LUMO(0.57)	6.61	188	0.0006
S <sub>8</sub>	HOMO-2→LUMO+1(0.54)	6.96	178	0.2270
S <sub>9</sub>	HOMO→LUMO+2(0.64)	7.76	160	0.0001
S <sub>10</sub>	HOMO-3→LUMO+1(0.64)	7.81	159	0.0475

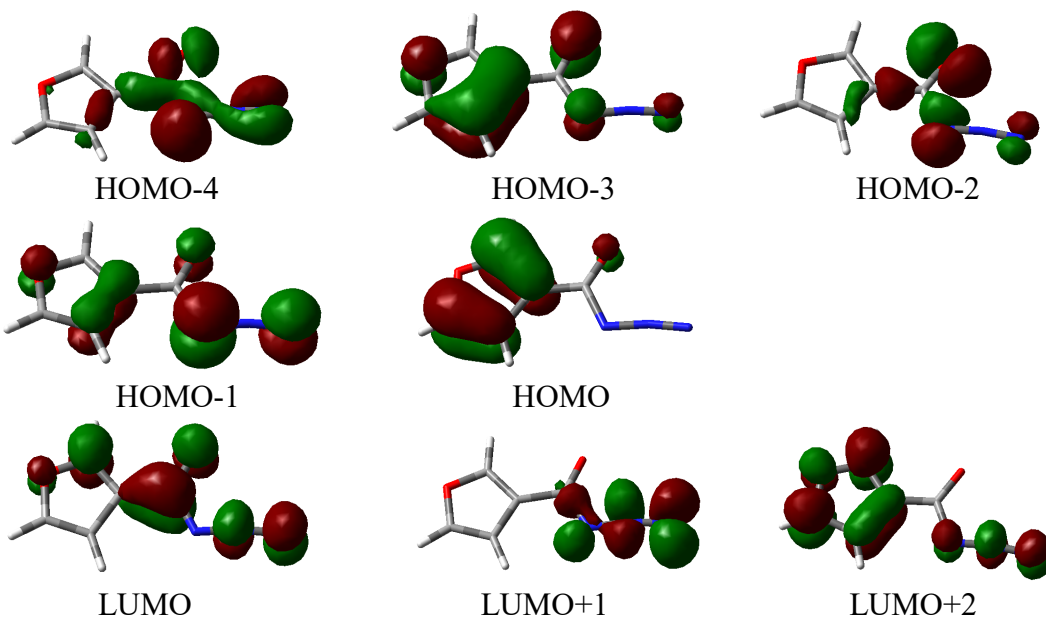
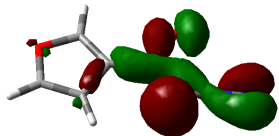


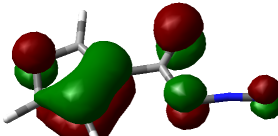


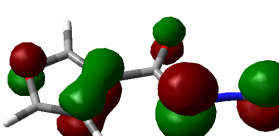
Table S7. Relative TD- $\omega$ B97XD vertical excitation energy ( $\Delta E$ ) and wavelength ( $\lambda$ ) at  $\mathbf{5-S_0}$  together with the electronic configuration (weight in the parenthesis, orbitals below the table) and oscillator strength ( $f$ )

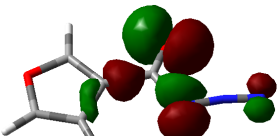
State	Configuration and weight	$\Delta E/eV$	$\lambda/nm$	Oscillator strength
S <sub>0</sub>	-	0.00	-	-
S <sub>1</sub>	HOMO-1 $\rightarrow$ LUMO(0.69)	4.59	270	0.0001
S <sub>2</sub>	HOMO-2 $\rightarrow$ LUMO+1(0.61)	4.99	248	0.0004
S <sub>3</sub>	HOMO $\rightarrow$ LUMO(0.63)	5.38	230	0.1310
S <sub>4</sub>	HOMO-1 $\rightarrow$ LUMO+1(0.45)	5.48	226	0.0012
S <sub>5</sub>	HOMO-3 $\rightarrow$ LUMO(0.41)	6.34	196	0.3184
S <sub>6</sub>	HOMO $\rightarrow$ LUMO+1(0.67)	6.55	189	0.0000
S <sub>7</sub>	HOMO-3 $\rightarrow$ LUMO(0.47)	6.59	188	0.0677
S <sub>8</sub>	HOMO-4 $\rightarrow$ LUMO(0.60)	6.62	187	0.0004
S <sub>9</sub>	HOMO $\rightarrow$ LUMO+2(0.60)	7.17	173	0.2305
S <sub>10</sub>	HOMO-4 $\rightarrow$ LUMO+1(0.44)	7.64	162	0.1129

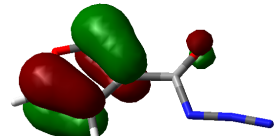
  

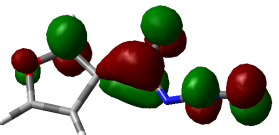
  
HOMO-4

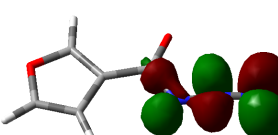
  
HOMO-3

  
HOMO-2

  
HOMO-1

  
HOMO

  
LUMO

  
LUMO+1

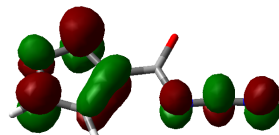
  
LUMO+2

Table S8. Relative energies (in brackets), key bond lengths(B), angles(A) and Mayer bond orders(in parentheses) of furoylnirene **2** and **6**. Relative energies are shown in eV. Bond lengths are given in Å and angles are in °.

	<b>2-S<sub>0</sub></b>	<b>2-S<sub>1</sub></b>	<b>2-T<sub>1</sub></b>	<b>6-S<sub>0</sub></b>	<b>6-S<sub>1</sub></b>	<b>6-T<sub>1</sub></b>
Relative energies	[0.00]	[1.06]	[-0.10]	[-0.09]	[0.93]	[-0.14]
B (C6-O11)	1.29 (1.04)	1.34 (1.10)	1.21 (1.77)	1.30 (1.06)	1.35 (1.00)	1.22 (1.74)
B (C6-N10)	1.28 (1.63)	1.30 (1.66)	1.40 (1.01)	1.26 (1.63)	1.27 (1.70)	1.39 (1.04)
B (O11-N10)	1.84 (0.85)	2.24 (0.57)	2.26 (0.09)	1.86 (0.84)	2.24 (0.47)	2.24 (0.12)
A (N10-C6-O11)	91	115	120	93	118	118

Table S9. Relative energies (in brackets), key bond lengths(B) and Mayer bond orders(in parentheses) of furylnirene **4** and **8**. Relative energies are shown in eV. Bond lengths are given in Å.

	<b>4-S<sub>0</sub></b>	<b>4-S<sub>2</sub></b>	<b>4-T<sub>1</sub></b>	<b>8-S<sub>0</sub></b>	<b>8-S<sub>1</sub></b>	<b>8-S<sub>2</sub></b>	<b>8-T<sub>1</sub></b>
Relative energies	[0.00]	[2.63]	[-0.56]	[0.45]	[1.03]	[2.66]	[-0.32]
B (O1-C2)	1.40 (0.93)	1.40 (0.93)	1.39 (0.96)	1.35 (0.95)	1.31 (1.14)	1.34 (1.07)	1.34 (0.96)
B (C2-N10) or B (C3-N10)	1.26 (1.66)	1.28 (1.58)	1.30 (1.31)	1.26 (1.84)	1.30 (1.56)	1.33 (1.45)	1.33 (1.22)

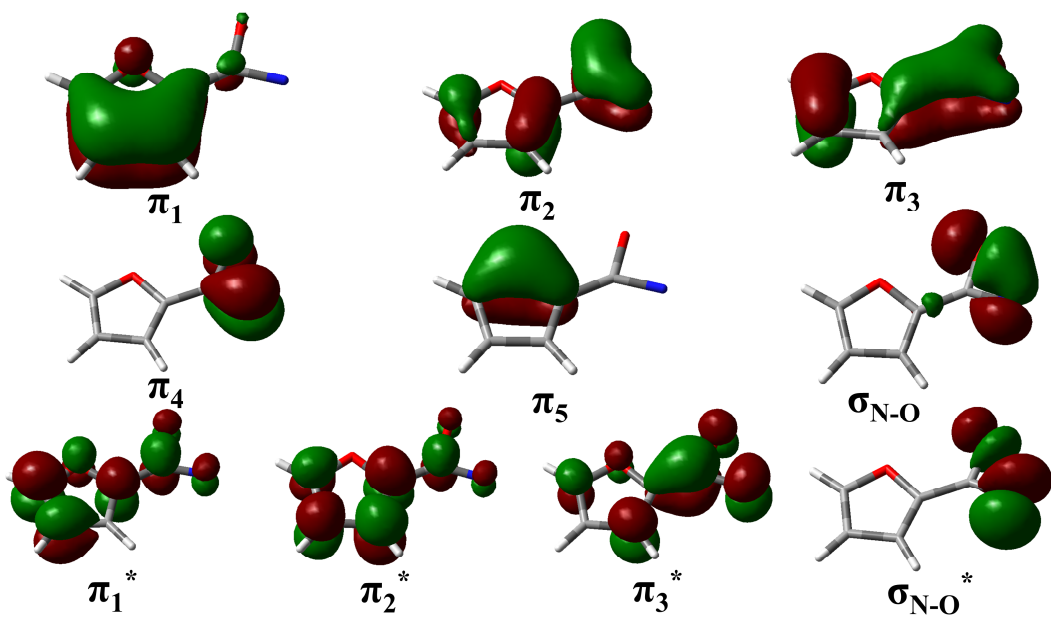


Figure S1. The (12,10) active orbitals of **2** in the CASPT2 calculations.

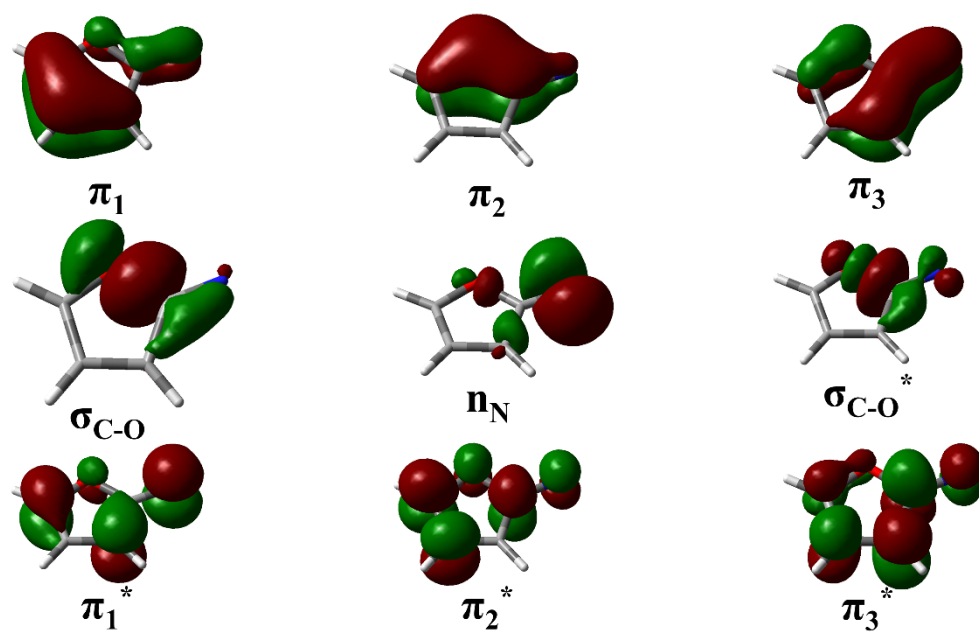


Figure S2. The (10,9) active orbitals of **4** in the CASPT2 calculations.

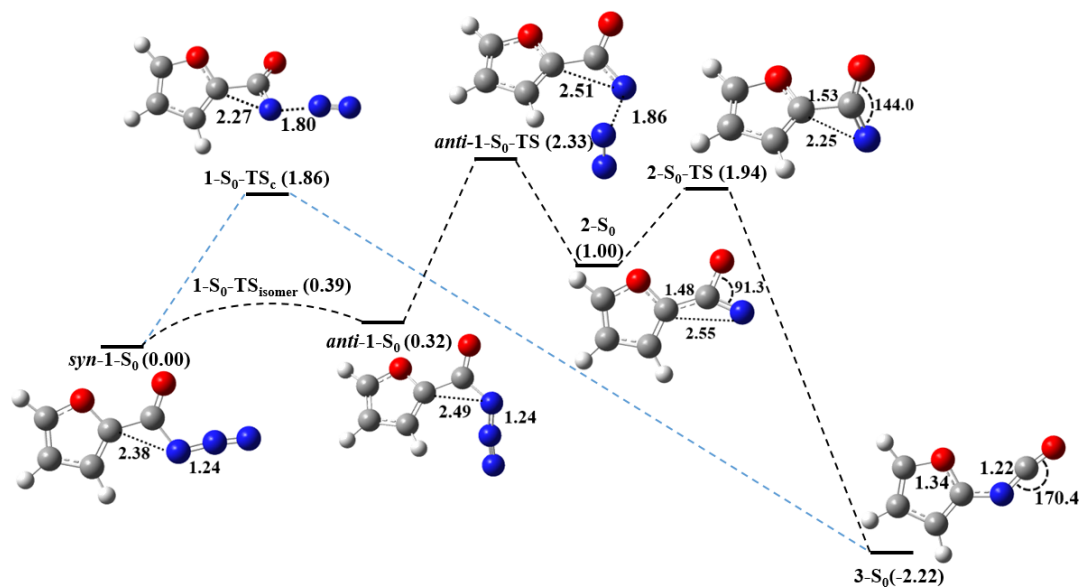


Figure S3. CASPT2//CASSCF energy profiles for the pyrolysis of **1**. Energies are given in eV. Bond lengths are given in Å and angles are in °.

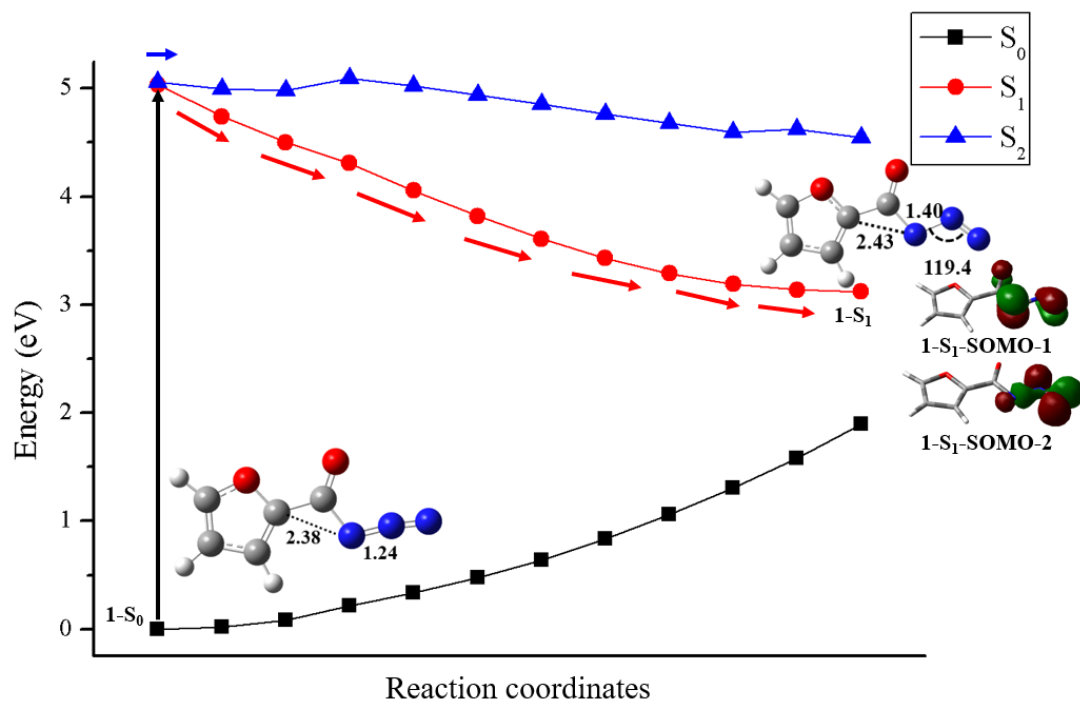


Figure S4. Energy plot from  $1-S_0$  to  $1-S_1$ . Bond lengths are given in Å and angles are in  $^\circ$ .

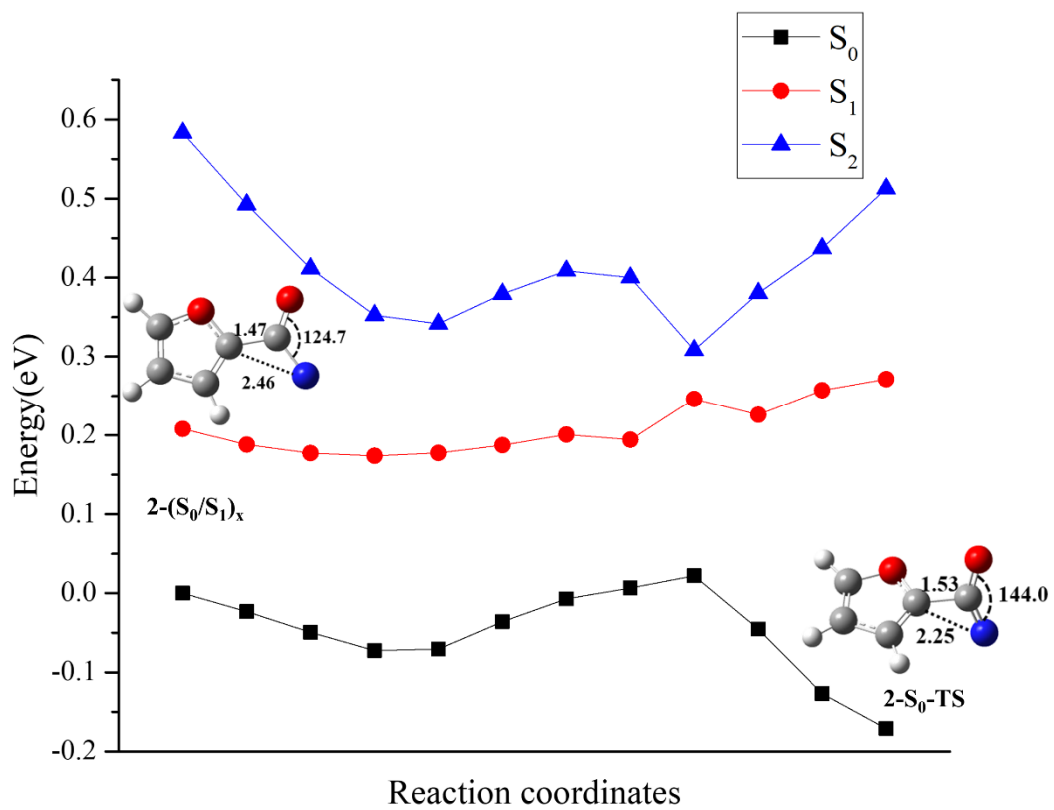


Figure S5. Energy plot from  $2-(S_0/S_1)_x$  to  $2-S_0-TS$ . Bond lengths are given in Å and angles are in °.



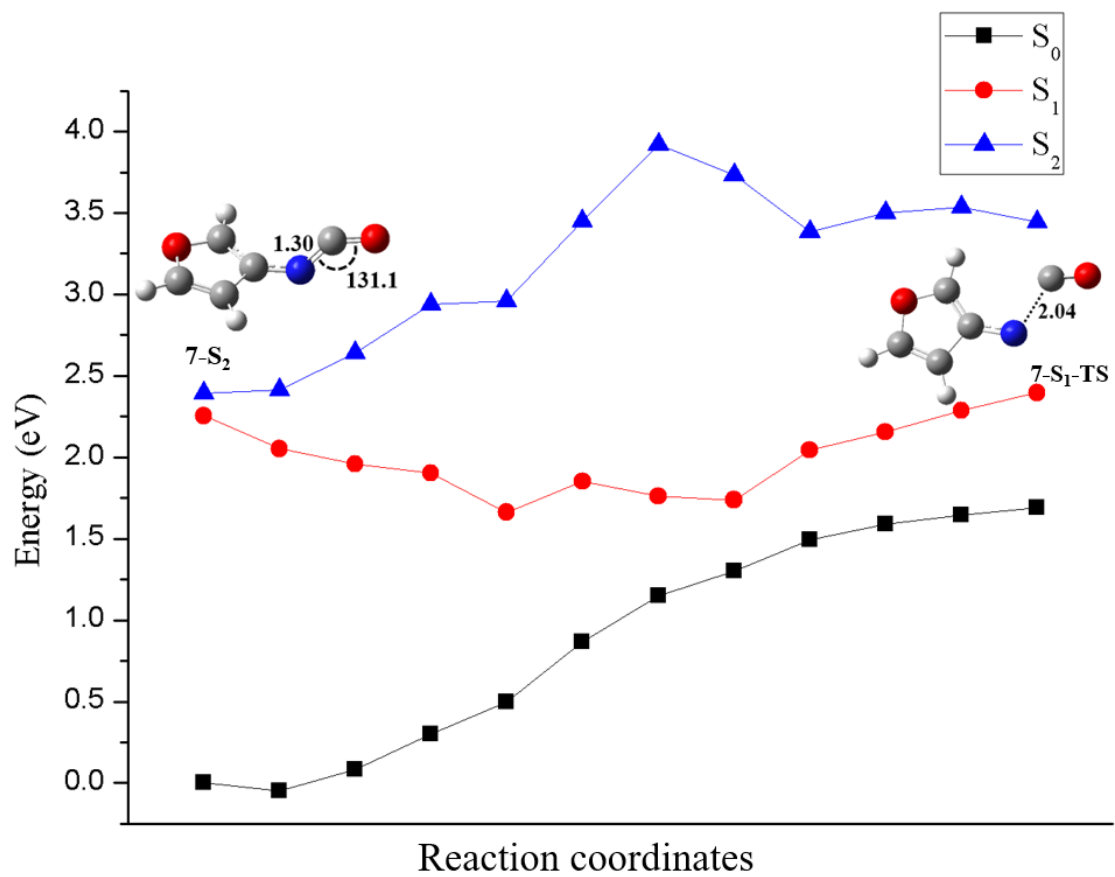


Figure S6. Energy plot from 7- $S_2$  to 7- $S_1$ -TS. Bond lengths are given in Å and angles are in °.

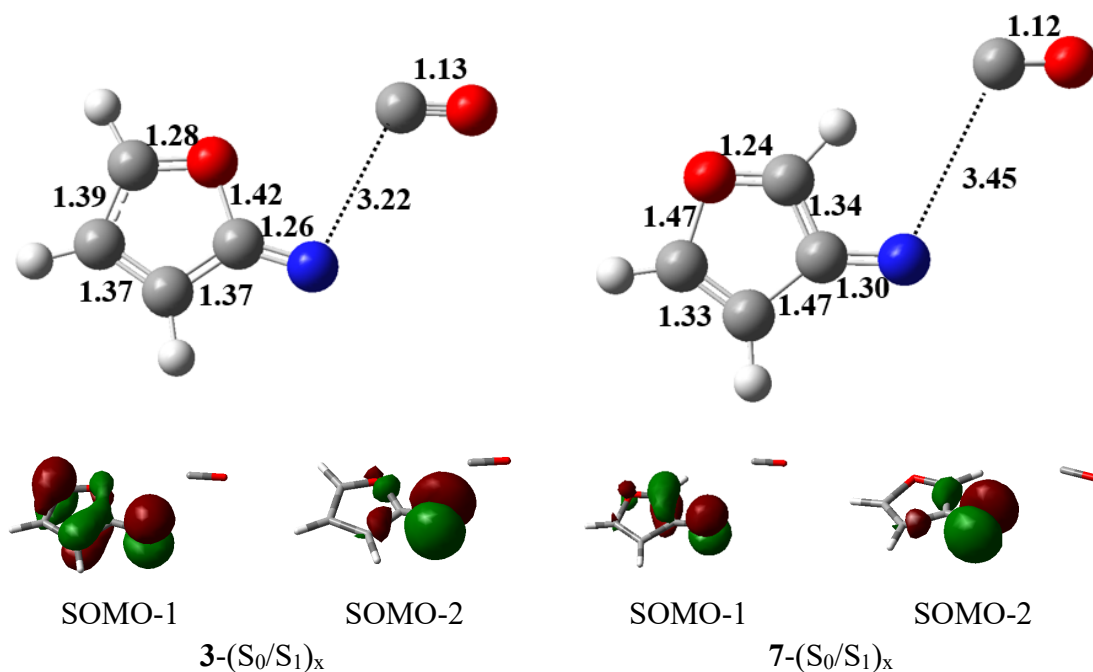


Figure S7. CASSCF optimized structures and SOMOs of conical intersections  $3-(S_0/S_1)_x$  and  $7-(S_0/S_1)_x$ . Bond lengths are given in Å.

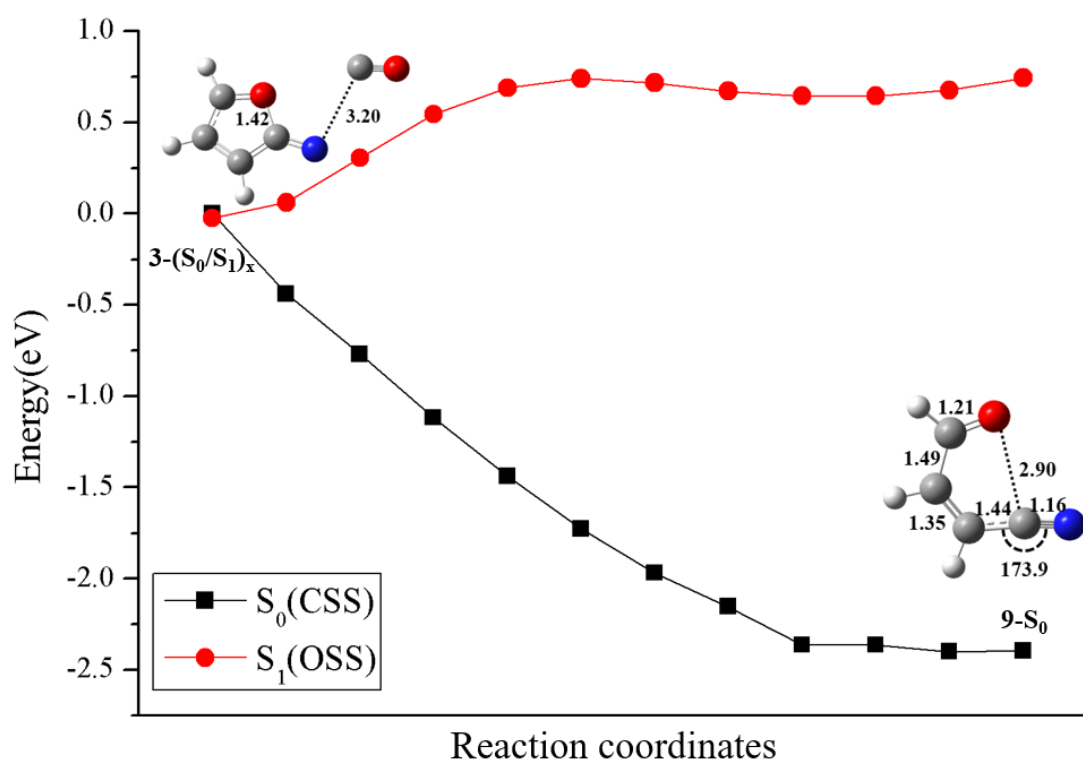


Figure S8. Energy plot from  $3-(S_0/S_1)_x$  to  $9-S_0$ . Bond lengths are given in Å and angles are in °.

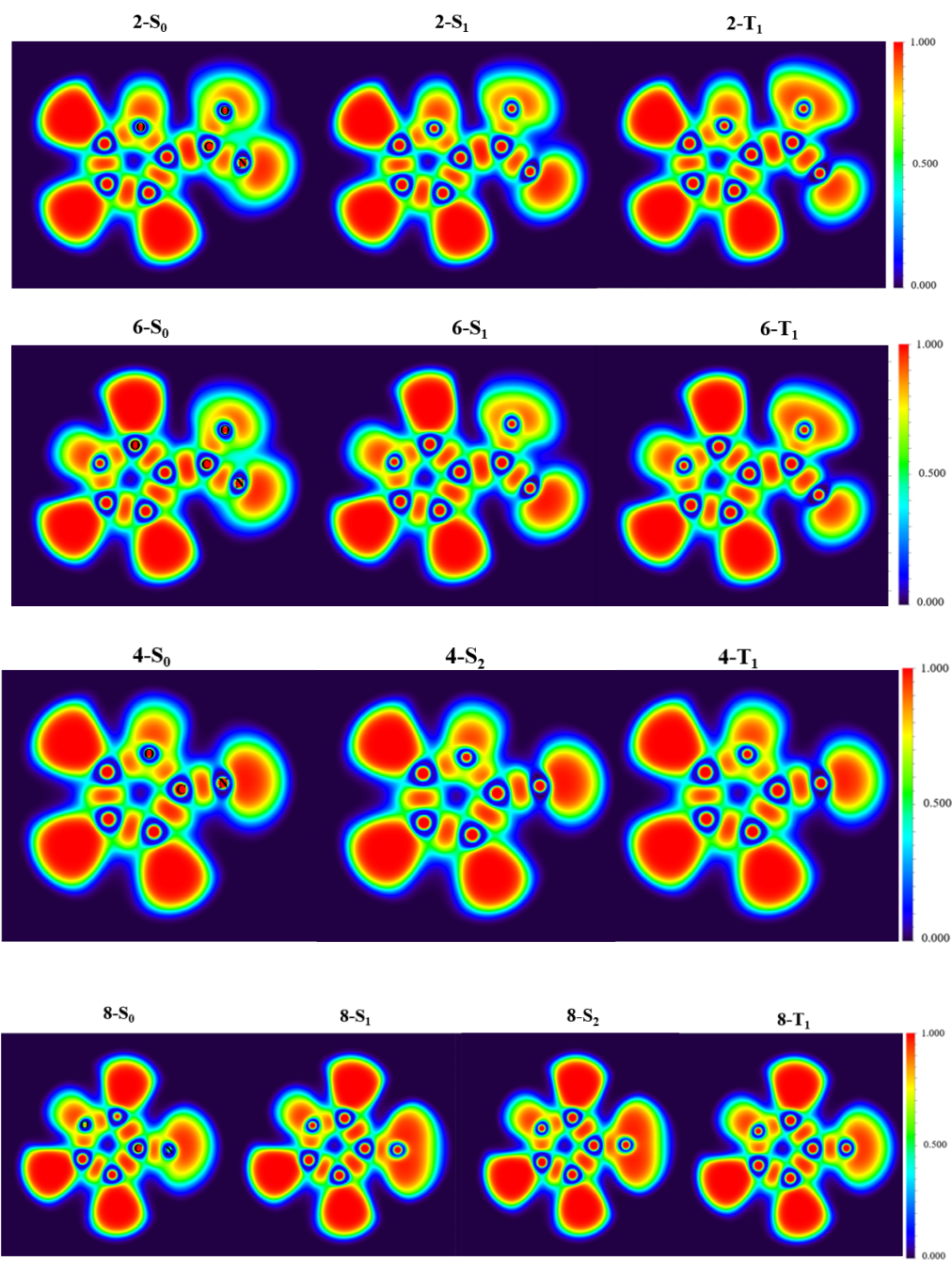


Figure S9. Electron localization of furoylnitrene 2, 6 and furylnitrene 4, 8.

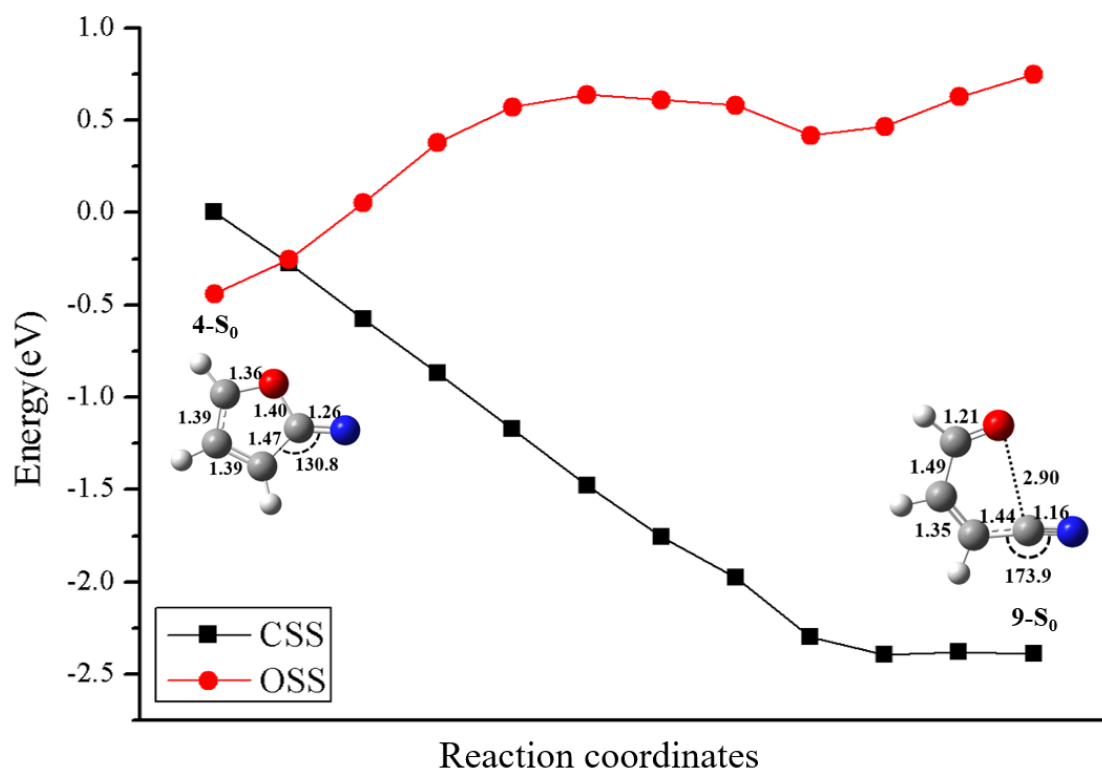


Figure S10. Energy plot from 4-S<sub>0</sub> to 9-S<sub>0</sub>. Bond lengths are given in Å and angles are in °.

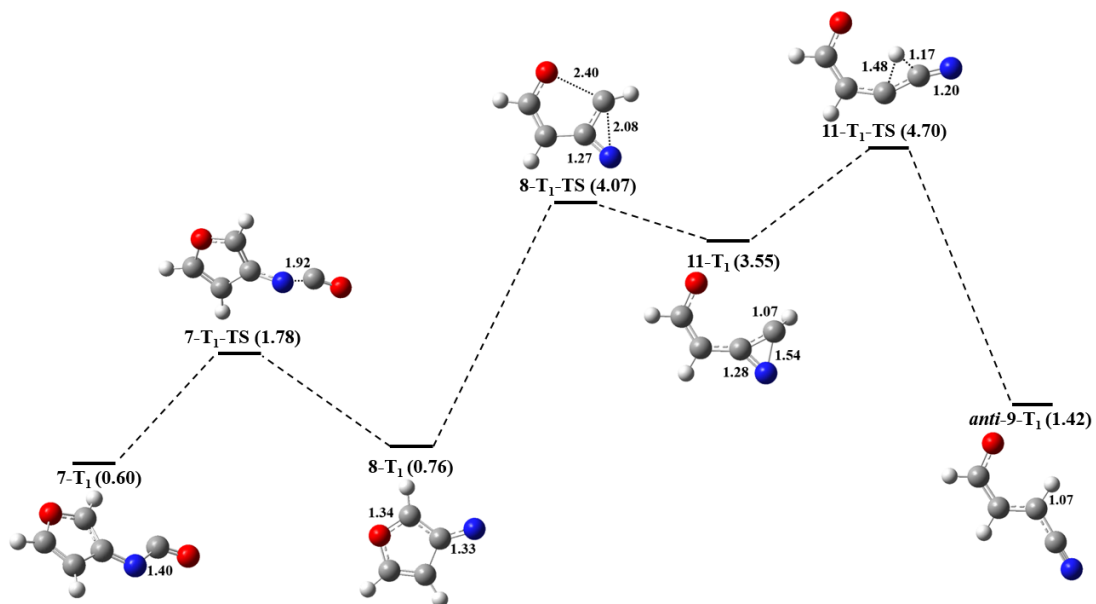


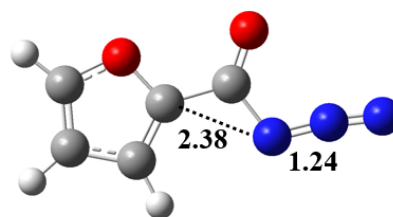
Figure S11. CASPT2//CASSCF energy profiles for the reaction from **7** to **9** in the  $T_1$  state. Energies are given in eV and bond lengths are in Å.

**Molecular structures, Cartesian coordinates, CASPT2 absolute energies (in Hartree) and relative energies in parentheses (in eV) of critical points**

The following relative energies in parentheses are relative to *syn-1-S<sub>0</sub>*.

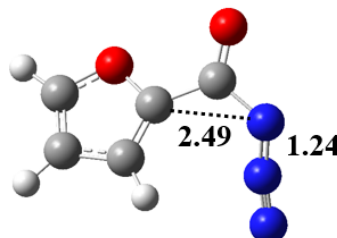
*syn-1-S<sub>0</sub>* -506.0560020 (0.00)

C	-2.886262	0.395057	-0.000355
C	-2.773246	-0.943941	0.000054
C	-1.364973	-1.206915	0.000437
C	-0.768146	-0.000929	-0.000169
H	-3.729328	1.051062	-0.000528
H	-3.571073	-1.656498	0.000281
H	-0.874003	-2.156803	0.001001
C	0.641926	0.408793	-0.000940
O	1.016454	1.548263	-0.006264
O	-1.687568	0.980443	-0.000659
N	1.503738	-0.704170	0.004990
N	2.708830	-0.401512	0.002051
N	3.836111	-0.271215	-0.000185



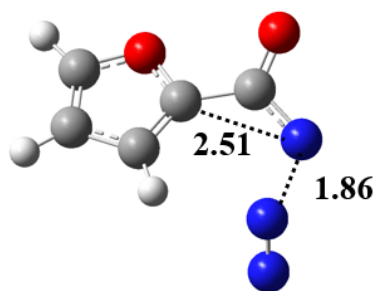
*anti-1-S<sub>0</sub>* -506.0441577 (0.32)

C	-2.943816	0.476716	-0.206718
C	-2.972994	-0.826998	0.112769
C	-1.602981	-1.203743	0.297872
C	-0.880120	-0.089887	0.072328
H	-3.709512	1.184440	-0.438425
H	-3.837825	-1.448850	0.208931
H	-1.238107	-2.170113	0.575592
C	0.559684	0.237111	0.157036
O	0.955757	1.356436	0.290448
O	-1.692198	0.937140	-0.232186
N	1.507215	-0.816387	0.157157
N	1.221871	-1.874275	-0.453048
N	1.157657	-2.883362	-0.953901



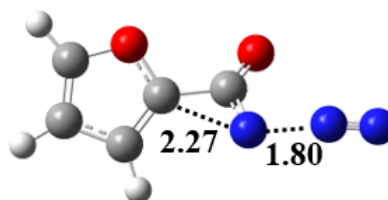
*anti-1-S<sub>0</sub>-TS* -505.97024748 (2.33)

C	0.024544	-0.102739	0.021117
C	-0.007312	0.048442	1.354418
C	1.366035	0.108808	1.763349
C	2.091918	-0.010926	0.637116
H	-0.740760	-0.200165	-0.717534
H	-0.876339	0.114201	1.974693
H	1.739941	0.252976	2.755317
C	3.537636	0.060640	0.335594
O	3.958777	0.508532	-0.711032
O	1.281937	-0.137183	-0.427625
N	4.520342	-0.217794	1.241214
N	3.859515	-1.517132	2.388432
N	3.902232	-2.291588	3.170647



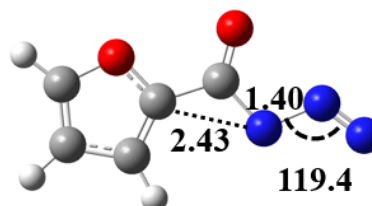
**1-S<sub>0</sub>-TSc** -505.9874926 (1.86)

C	2.890281	0.378713	-0.416387
C	2.878044	-0.816550	0.222364
C	1.495814	-1.078876	0.523351
C	0.810465	-0.009750	0.039080
H	3.673349	0.980337	-0.822035
H	3.724194	-1.427945	0.455668
H	1.081053	-1.922637	1.032697
C	-0.638162	0.347115	0.037156
O	-1.063238	1.459710	0.185916
O	1.643961	0.873803	-0.535217
N	-1.290301	-0.829043	-0.193674
N	-3.002435	-0.319249	0.024546
N	-4.081237	-0.210894	0.080401



**1-S<sub>1</sub>** -505.9413757 (3.12)

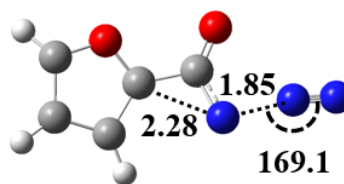
C	-2.910620	0.380273	-0.014143
C	-2.778514	-0.965557	0.023571
C	-1.355933	-1.211833	0.024154
C	-0.783423	-0.000722	-0.012760
H	-3.756287	1.031999	-0.031951
H	-3.566794	-1.688100	0.047867
H	-0.855490	-2.156911	0.049178
C	0.617594	0.452940	-0.029968
O	0.925733	1.620904	-0.066030
O	-1.704185	0.977342	-0.036953
N	1.568762	-0.598597	-0.001313
N	2.858924	-0.043457	0.015468
N	3.792694	-0.756650	0.032599





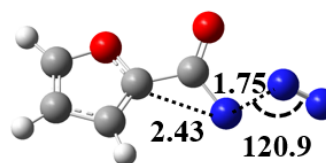
**1-S<sub>1</sub>-TSc** -505.8935451 (4.42)

C	2.915137	0.423091	-0.518087
C	2.900162	-0.901466	0.162246
C	1.518156	-1.143591	0.540709
C	0.789655	0.092389	0.153383
H	3.700004	1.151171	-0.476985
H	3.722227	-1.578898	0.237271
H	1.105700	-1.986538	1.046440
C	-0.639898	0.342215	-0.080884
O	-1.097993	1.425340	-0.344837
O	1.653835	0.953053	-0.422729
N	-1.281119	-0.864274	0.057481
N	-3.043316	-0.306994	0.115837
N	-4.120764	-0.180764	0.164023



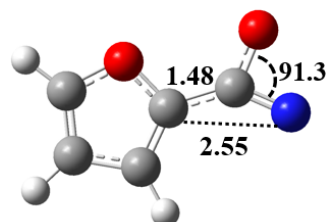
**1-S<sub>1</sub>-TS** -505.9395484 (3.17)

C	0.039346	-0.052249	-0.013823
C	0.009840	0.062641	1.333128
C	1.392026	0.022577	1.751289
C	2.104217	-0.105056	0.624471
H	-0.721414	-0.076034	-0.762511
H	-0.856440	0.175946	1.950307
H	1.775694	0.103163	2.746729
C	3.558391	-0.062763	0.349186
O	3.979831	0.295313	-0.742465
O	1.308411	-0.154038	-0.456599
N	4.387475	-0.424687	1.394228
N	5.894652	0.355054	0.982556
N	6.865707	-0.024343	1.386037



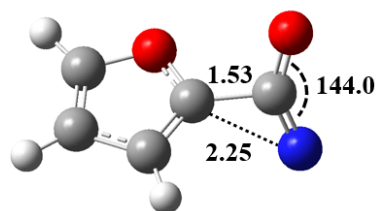
**2-S<sub>0</sub>** -396.6706297 (1.00)

C	-2.117557	-0.283360	0.000000
C	-2.030899	1.057287	0.000000
C	-0.628761	1.352572	0.000000
C	-0.010140	0.159673	0.000000
H	-2.945807	-0.957506	0.000000
H	-2.842716	1.753478	0.000000
H	-0.160550	2.314972	0.000000
C	1.389775	-0.206937	0.000000
O	1.929511	-1.383489	0.000000
N	2.537142	0.351961	0.000000
O	-0.904345	-0.843819	0.000000

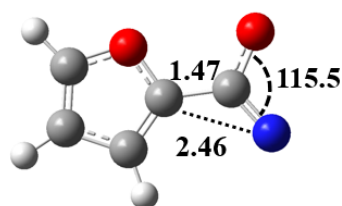


**2-S<sub>0</sub>-TS** -396.6362143 (1.94)

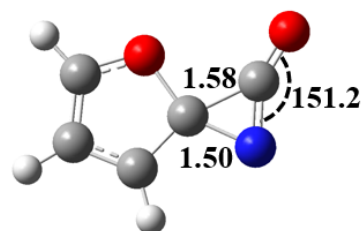
C	-2.139931	-0.191562	0.181984
C	-2.083645	1.128572	-0.102336
C	-0.677921	1.453250	-0.210547
C	-0.039730	0.283506	0.004813
H	-2.944347	-0.872216	0.349773
H	-2.911774	1.795947	-0.216245
H	-0.227875	2.401843	-0.409398
C	1.447147	-0.059986	0.044884
O	1.679117	-0.943392	-0.845529
N	1.975119	0.637908	0.950664
O	-0.891494	-0.722873	0.250637



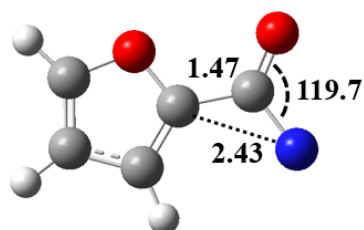
<b>2-S<sub>1</sub></b>	<b>-396.6315037 (2.06)</b>		
C	-2.099242	-0.285273	-0.004086
C	-2.000973	1.052852	-0.002896
C	-0.594327	1.335549	0.004638
C	0.016972	0.139086	0.008739
H	-2.931523	-0.954335	-0.006746
H	-2.806497	1.756590	-0.003661
H	-0.120418	2.295049	0.009564
C	1.433607	-0.241847	-0.000786
O	1.784805	-1.536501	0.010368
N	2.421319	0.608366	-0.017912
O	-0.888073	-0.854709	0.002776



<b>2-S<sub>1</sub>-TS</b>	<b>-396.5980592 (2.97)</b>		
C	-1.927193	-0.209426	-0.002020
C	-2.021852	1.159957	-0.001445
C	-0.716897	1.650711	0.007179
C	0.259433	0.572325	0.011906
H	-2.678927	-0.973203	-0.008756
H	-2.926225	1.733954	-0.007020
H	-0.403884	2.675298	0.009851
C	1.661009	-0.159238	0.020350
O	2.238118	-1.176644	0.024146
N	1.644139	1.162761	0.020059
O	-0.657833	-0.624613	0.005816



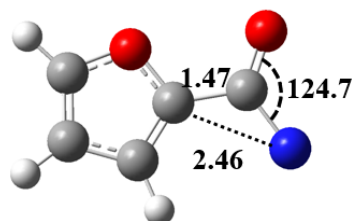
<b>2-T<sub>1</sub></b>	<b>-396.6744102 (0.90)</b>		
C	-2.118466	-0.287535	-0.000527
C	-1.988235	1.060301	-0.000581
C	-0.570017	1.311218	0.000714
C	0.017122	0.084629	-0.000311
H	-2.966532	-0.935841	-0.001207



H	-2.777307	1.782474	-0.001543
H	-0.072703	2.258616	0.000964
C	1.428794	-0.320028	0.000110
O	1.809218	-1.470271	0.000144
N	2.365344	0.721717	0.001302
O	-0.911568	-0.890451	0.000934

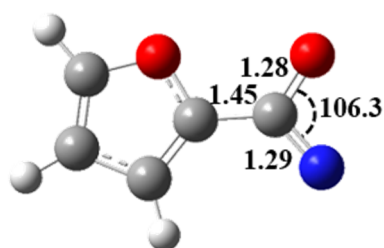
**2-(S<sub>0</sub>/S<sub>1</sub>)<sub>x</sub>** -396.6261043 (2.21)

C	-2.104059	-0.282144	-0.005115
C	-1.972117	1.054725	-0.003867
C	-0.580095	1.292068	0.007981
C	0.019807	0.086774	0.015745
H	-2.955804	-0.925737	-0.011620
H	-2.755032	1.782910	-0.017209
H	-0.068636	2.232986	0.003842
C	1.436690	-0.300914	-0.011747
O	1.714666	-1.497224	-0.028987
N	2.392492	0.751896	0.040882
O	-0.912261	-0.880515	0.010094



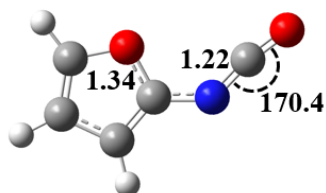
**2-(S<sub>0</sub>/T<sub>1</sub>)<sub>x</sub>** -396.6653040 (1.14)

C	-2.118128	-0.286355	-0.004736
C	-2.009802	1.065513	-0.000757
C	-0.599673	1.342440	0.002451
C	0.006712	0.124787	0.000397
H	-2.953059	-0.951217	-0.008248
H	-2.812276	1.772620	-0.000335
H	-0.116195	2.296948	0.005666
C	1.412613	-0.252939	0.002319
O	1.856242	-1.450327	-0.006224
N	2.450744	0.518527	0.013367
O	-0.901529	-0.865167	-0.003903



**3-S<sub>0</sub>** -396.7890558 (-2.22)

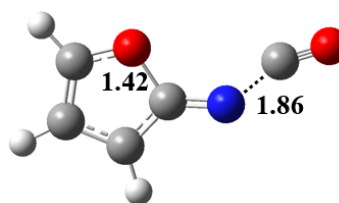
C	-2.116026	-0.158672	-0.003129
C	-2.088053	1.177700	-0.001204
C	-0.695224	1.549017	0.002077
C	-0.025716	0.390747	0.001805
H	-2.902771	-0.879774	-0.005620
H	-2.933007	1.834087	-0.001884
H	-0.269530	2.529595	0.004459
C	1.995432	-0.880627	0.000955
O	2.779707	-1.734753	-0.001248
N	1.328480	0.145093	0.004954



O -0.857638 -0.657583 -0.001168

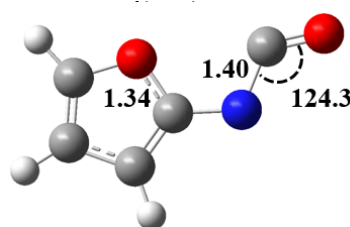
**3-S<sub>0</sub>-TS** -396.6656085 (1.14)

C	-2.193121	-0.104803	-0.272153
C	-2.141878	1.208285	0.117491
C	-0.779976	1.506398	0.168620
C	-0.051433	0.392278	-0.235052
H	-3.041021	-0.746346	-0.406667
H	-2.975334	1.839027	0.343456
H	-0.318870	2.430965	0.448451
C	2.195989	-0.886830	0.595563
O	3.183335	-1.397689	0.363811
N	1.191749	0.225278	-0.499061
O	-1.026019	-0.614223	-0.498518



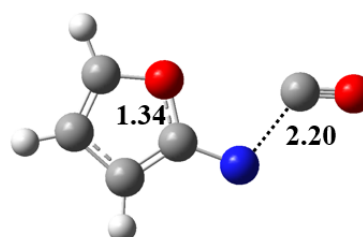
**3-S<sub>1</sub>** -396.6914817 (0.43)

C	0.126441	0.095845	-0.030954
C	0.034882	-0.072197	1.295830
C	1.384177	-0.026426	1.790527
C	2.156273	0.167554	0.707093
H	-0.596131	0.133724	-0.817124
H	-0.863059	-0.214010	1.860683
H	1.725465	-0.121385	2.801035
C	4.069126	0.498229	-0.631851
O	5.231924	0.624592	-0.884051
N	3.559303	0.286553	0.652417
O	1.410843	0.245473	-0.405851



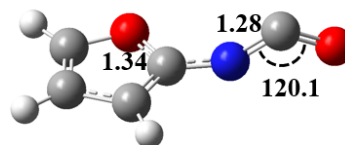
**3-S<sub>1</sub>-TS** -396.6170643 (2.46)

C	-2.086014	-0.141499	0.013323
C	-2.139750	1.195903	-0.013024
C	-0.779326	1.644526	-0.014672
C	-0.027535	0.523344	0.012328
H	-2.832791	-0.901673	0.022030
H	-3.020789	1.801305	-0.031888
H	-0.416602	2.647032	-0.031662
C	1.948343	-1.466304	0.007393
O	3.005971	-1.871289	-0.020925
N	1.370106	0.451941	0.027035
O	-0.805968	-0.568455	0.030056



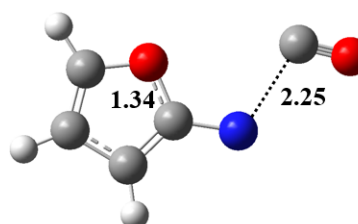
**3-S<sub>2</sub>** -396.6177663 (2.44)

C	-2.289742	-0.082737	0.035749
C	-2.056544	1.233960	-0.034664
C	-0.626898	1.383841	-0.013247
C	-0.139585	0.131714	0.060780
H	-3.181279	-0.669794	0.051862
H	-2.789198	2.011735	-0.090499
H	-0.053534	2.286198	-0.040586
C	2.157299	-0.752492	-0.449557
O	3.205201	-1.120000	0.193445
N	1.121733	-0.338027	0.188856
O	-1.131799	-0.769569	0.097859



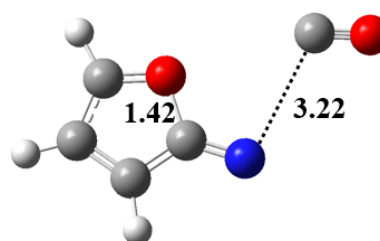
**3-S<sub>2</sub>-TS** -396.5809899 (3.44)

C	-2.164783	-0.066914	0.032121
C	-2.153378	1.269737	-0.014732
C	-0.773965	1.654028	-0.047898
C	-0.080226	0.496771	-0.017189
H	-2.948037	-0.785905	0.068090
H	-3.001947	1.918885	-0.025291
H	-0.367915	2.636001	-0.087909
C	2.085092	-1.773469	0.045580
O	3.216055	-1.814127	0.046552
N	1.311022	0.337034	-0.030827
O	-0.906273	-0.557211	0.031496



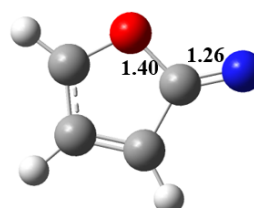
**3-(S<sub>0</sub>/S<sub>1</sub>)<sub>x</sub>** -396.6603287 (1.26)

C	-1.948410	-0.148666	-0.037754
C	-2.205880	1.212893	0.097245
C	-0.968249	1.782533	-0.026350
C	-0.020966	0.812142	-0.217840
H	-2.631556	-0.997690	-0.003296
H	-3.167656	1.664763	0.265271
H	-0.603909	2.817475	0.009553
C	2.037162	-2.096205	0.262076
O	3.151438	-2.287425	0.210347
N	1.225033	0.959565	-0.342414
O	-0.715541	-0.423896	-0.221584



**4-S<sub>0</sub>** -283.5347533 (0.93)

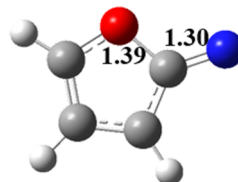
C	-2.109388	-0.177765	-0.003512
C	-2.064507	1.208593	-0.001413
C	-0.730706	1.583298	0.002373
C	0.049129	0.340011	0.002825
H	-2.920048	-0.870910	-0.005035



H	-2.919114	1.853269	-0.002452
H	-0.303083	2.562428	0.004579
N	1.294815	0.149020	0.004687
O	-0.862219	-0.726656	-0.001367

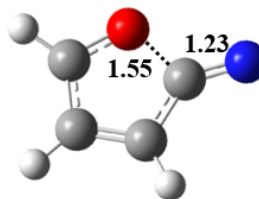
4-T<sub>1</sub> -283.555481 (0.37)

C	-2.108988	-0.170654	-0.002997
C	-2.075321	1.196481	-0.000886
C	-0.713051	1.568618	0.002202
C	0.025523	0.363310	0.002637
H	-2.913362	-0.872174	-0.006158
H	-2.926097	1.845428	-0.002102
H	-0.290329	2.550501	0.003989
N	1.305602	0.144573	0.004822
O	-0.869099	-0.704795	-0.000821



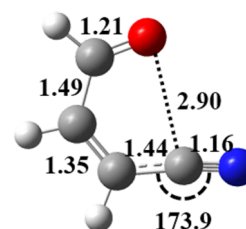
4-(S<sub>0</sub>/T<sub>1</sub>)<sub>x</sub> -283.5347533 (0.95)

C	-2.101028	-0.199419	0.060252
C	-2.050547	1.204081	0.069177
C	-0.729442	1.571391	-0.025665
C	0.097442	0.394653	-0.006287
H	-2.932999	-0.841996	-0.159305
H	-2.906162	1.848100	0.056011
H	-0.316964	2.555291	-0.131802
N	1.304359	0.149086	-0.006022
O	-0.929781	-0.759899	0.144326



*syn-9*-S<sub>0</sub> -283.6070294 (-1.03)

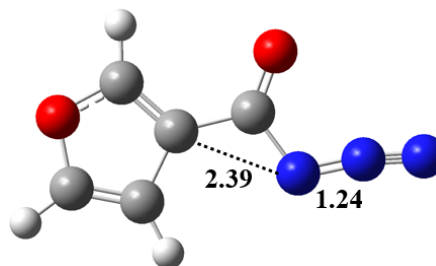
C	-2.424125	-0.242432	-0.295305
C	-2.072225	1.123412	0.172388
C	-0.845176	1.677545	0.144562
C	0.356730	1.051786	-0.346676
H	-3.479207	-0.502940	-0.237298
H	-2.882353	1.712387	0.563889
H	-0.709494	2.677976	0.511196
N	1.380768	0.655295	-0.719150
O	-1.621623	-1.037287	-0.716513



The following energies in parentheses are relative to **5-S<sub>0</sub>**.

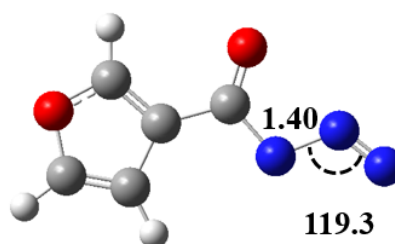
**5-S<sub>0</sub>** -506.0566588 (0.00)

C	-2.691790	-0.958463	0.000808
C	-1.381472	-1.202676	-0.000541
C	-0.749385	0.104016	-0.000663
C	-1.765270	1.000955	-0.000060
H	-3.546567	-1.598969	0.001302
H	-0.898246	-2.156075	-0.001314
H	-1.784078	2.067861	-0.000113
O	-2.948704	0.366127	0.000027
C	0.677818	0.453651	0.000225
O	1.093175	1.581632	-0.000530
N	1.514751	-0.678882	0.000302
N	2.728281	-0.419862	0.000447
N	3.849241	-0.361586	0.000401



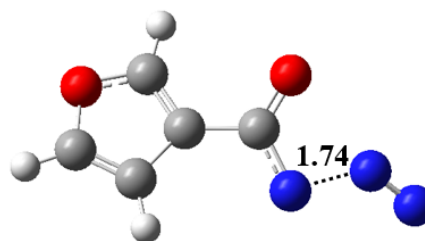
**5-S<sub>1</sub>** -505.9416567 (3.13)

C	-2.698315	-0.976684	-0.002808
C	-1.386715	-1.217690	0.000732
C	-0.759548	0.092131	0.003412
C	-1.780518	0.984958	0.001207
H	-3.552324	-1.618131	-0.005741
H	-0.905388	-2.172465	0.001754
H	-1.802583	2.052405	-0.000296
O	-2.959969	0.346347	-0.002707
C	0.654771	0.483863	0.006558
O	1.004191	1.647050	0.007590
N	1.586383	-0.581992	0.002818
N	2.889991	-0.054344	-0.002329
N	3.807781	-0.787714	-0.009900



**5-S<sub>1</sub>-TS** -505.9400714 (3.17)

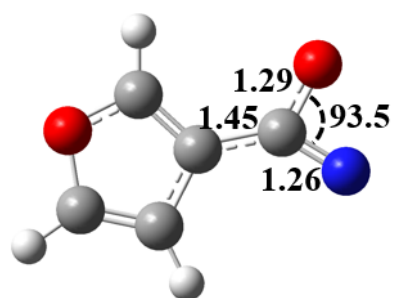
C	0.023030	0.064064	0.015720
C	-0.006923	0.017992	1.348190
C	1.382425	-0.084714	1.757845
C	2.100748	-0.093774	0.608287
H	-0.743547	0.155234	-0.722534
H	-0.871526	0.065041	1.975913
H	3.148590	-0.150531	0.413773
O	1.283960	-0.010000	-0.454377
C	1.989377	-0.061338	3.102047
O	3.173375	0.243675	3.248010
N	1.180734	-0.391661	4.167378



N	2.015854	0.291715	5.539286
N	1.848387	-0.105452	6.570843

**6-S<sub>0</sub>** -396.6737993 (0.93)

C	-2.751613	-0.962297	0.000756
C	-1.427534	-1.233674	-0.000103
C	-0.777885	0.057349	-0.000933
C	-1.777111	0.977709	-0.000494
H	-3.621862	-1.579493	0.001667
H	-0.963322	-2.197015	-0.000115
H	-1.775644	2.045229	-0.000721
O	-2.968019	0.372031	0.000418
C	0.640923	0.340383	-0.001247
O	1.242894	1.487631	0.000187
N	1.717181	-0.311236	0.000116



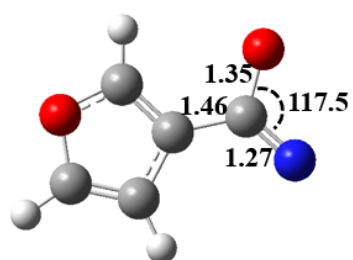
**6-S<sub>0</sub>-TS** -396.6390867 (1.87)

C	-2.774778	-0.934402	-0.015302
C	-1.440824	-1.138716	0.013259
C	-0.868488	0.187922	0.025379
C	-1.901649	1.060823	0.002857
H	-3.609190	-1.599471	-0.033480
H	-0.916898	-2.069024	0.024999
H	-1.948176	2.125920	0.002133
O	-3.064508	0.389411	-0.021728
C	0.630260	0.586317	0.057155
O	0.683108	1.849545	0.055763
N	1.306106	-0.473714	0.074616



**6-S<sub>1</sub>** -396.6364104 (1.95)

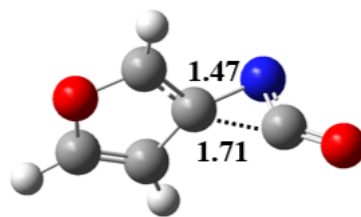
C	-2.727671	-0.952333	-0.001963
C	-1.405943	-1.238404	0.005928
C	-0.739559	0.044846	0.006188
C	-1.731537	0.974633	0.001765
H	-3.604531	-1.560739	-0.005752
H	-0.956578	-2.208738	0.010345
H	-1.713513	2.041822	-0.002680
O	-2.932617	0.383201	-0.002599
C	0.688749	0.352164	-0.002750
O	1.023738	1.659922	0.009113
N	1.637468	-0.499760	-0.018066



**6-S<sub>1</sub>-TS** -396.5956134 (3.06)

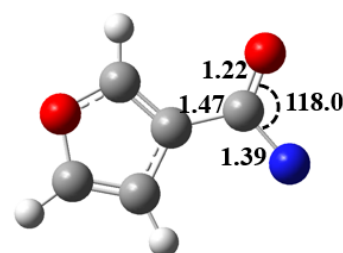


C	-2.572739	-0.995996	0.099883
C	-1.235984	-0.951967	-0.014339
C	-0.882900	0.473203	-0.104641
C	-2.136937	1.129663	-0.151172
H	-3.253692	-1.811381	0.211932
H	-0.555792	-1.776834	0.000785
H	-2.398233	2.160111	-0.196849
O	-3.138122	0.240772	0.053219
C	0.552995	1.144358	0.549565
O	1.462192	1.618382	1.194544
N	0.336565	0.970898	-0.768641



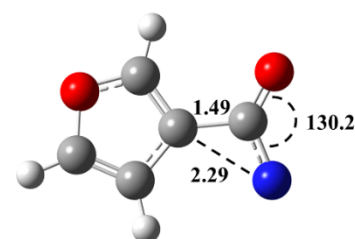
**6-T<sub>1</sub>** -396.6756552 (0.88)

C	-2.711890	-0.960281	0.000778
C	-1.381873	-1.203987	0.000039
C	-0.754374	0.099085	-0.000021
C	-1.774814	0.997432	-0.000355
H	-3.569552	-1.595431	0.001292
H	-0.903174	-2.160542	-0.000035
H	-1.791776	2.064593	-0.000778
O	-2.955067	0.369125	0.000311
C	0.677043	0.432044	-0.000342
O	1.109741	1.570215	0.000665
N	1.593744	-0.615636	-0.002022



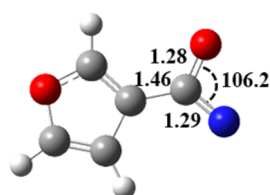
**6-(S<sub>0</sub>/S<sub>1</sub>)<sub>x</sub>** -396.6216974 (2.35)

C	-2.704548	-0.959216	0.008916
C	-1.375157	-1.232024	0.029364
C	-0.720681	0.051890	-0.017224
C	-1.732101	0.977520	-0.056394
H	-3.575113	-1.578747	0.038150
H	-0.927319	-2.202279	0.102824
H	-1.705655	2.044613	-0.103301
O	-2.921363	0.377491	-0.050697
C	0.706081	0.492904	0.051726
O	1.037583	1.619859	0.276933
N	1.456278	-0.595399	-0.280767



**6-(S<sub>0</sub>/T<sub>1</sub>)<sub>x</sub>** -396.667051 (1.11)

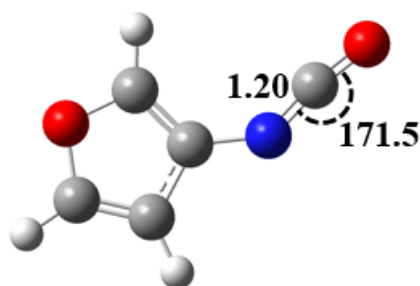
C	-2.731311	-0.962330	0.000465
C	-1.406210	-1.218922	0.000193
C	-0.766796	0.082803	-0.000538
C	-1.774228	0.990381	-0.000184
H	-3.593087	-1.591921	0.000957



H	-0.931680	-2.177571	0.000619
H	-1.783835	2.057789	-0.000202
O	-2.966089	0.371996	0.000236
C	0.661270	0.368198	-0.000608
O	1.177552	1.539098	0.001211
N	1.652423	-0.462904	-0.002616

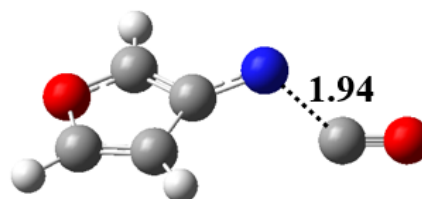
7-S<sub>0</sub> -396.7845272 (-2.08)

C	-2.838330	-1.083074	0.000459
C	-1.521498	-1.383774	0.000355
C	-0.844440	-0.109177	-0.001333
C	-1.812238	0.838820	-0.002419
H	-3.719220	-1.685873	0.001569
H	-1.068494	-2.352448	0.001313
H	-1.784044	1.906042	-0.004505
O	-3.029770	0.254905	-0.001250
C	1.355119	0.922123	0.002230
O	2.265794	1.644902	0.006091
N	0.535127	0.044168	-0.002979



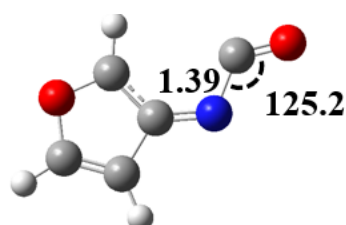
7-S<sub>0</sub>-TS -396.6350867 (1.98)

C	0.019577	-0.240034	0.155530
C	0.264815	-0.167034	1.473561
C	1.643612	0.329871	1.600739
C	2.060016	0.485236	0.307151
H	-0.819015	-0.527093	-0.437968
H	-0.404154	-0.418096	2.269805
H	2.992189	0.842432	-0.077961
O	1.124171	0.184741	-0.559436
C	2.344541	0.752547	2.659267
O	3.048603	-0.637527	3.822471
N	3.423210	-0.599546	4.889891



7-S<sub>1</sub> -396.6831102 (0.68)

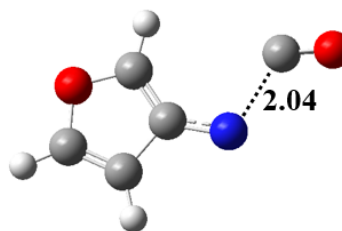
C	-2.811634	-1.068432	-0.001709
C	-1.512986	-1.419953	0.001448
C	-0.760154	-0.166137	0.002506
C	-1.746968	0.835987	0.003168
H	-3.714284	-1.640844	-0.006198
H	-1.099279	-2.406689	0.000116
H	-1.682930	1.904344	0.002262
O	-2.972547	0.283157	0.000323
C	1.064632	1.229039	-0.003691
O	2.216032	1.513888	-0.005211



N 0.558126 -0.067747 0.006516

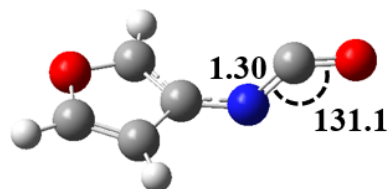
7-S<sub>1</sub>-TS -396.6087942 (2.70)

C	-0.007783	0.002063	-0.015260
C	0.014989	-0.001835	1.333878
C	1.429793	-0.003673	1.693903
C	2.103599	-0.000540	0.519491
H	-0.810941	0.004947	-0.718032
H	-0.817498	-0.002807	2.004472
H	3.142242	-0.000290	0.290774
O	1.239587	0.002687	-0.526109
N	1.797971	-0.006686	3.015740
C	3.825593	-0.008261	3.278796
O	4.376756	-0.012262	4.256858



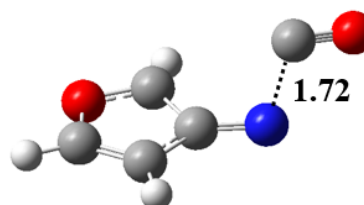
7-S<sub>2</sub> -396.6079240 (2.72)

C	-2.754446	-1.109290	0.114583
C	-1.435410	-1.294063	-0.106790
C	-0.861116	0.039231	-0.214047
C	-1.954514	0.908221	-0.067710
H	-3.558613	-1.794632	0.279567
H	-0.905637	-2.221675	-0.169403
H	-2.024661	1.974641	-0.097930
O	-3.082776	0.206366	0.142826
C	1.289653	0.756497	0.378210
O	2.433965	1.154743	0.223122
N	0.391562	0.376582	-0.482900



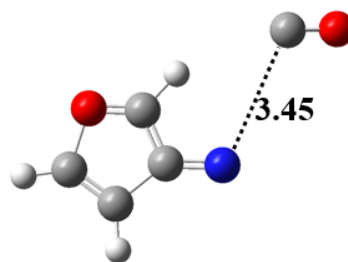
7-S<sub>2</sub>-TS -396.5914412 (2.70)

C	0.080441	0.020371	-0.017368
C	-0.137614	-0.066832	1.320261
C	1.158668	-0.018701	1.944537
C	2.088887	0.170528	0.835339
H	-0.584443	0.027373	-0.854344
H	-1.082402	-0.167989	1.813447
H	3.155218	0.084040	0.787679
O	1.409143	0.112153	-0.319683
N	1.501459	0.031212	3.217917
C	2.814058	1.135861	3.398990
O	3.401692	1.100159	4.393537

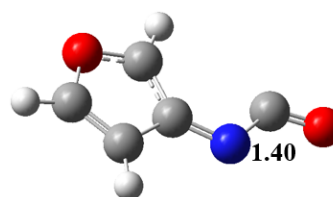


7-(S<sub>0</sub>/S<sub>1</sub>)<sub>x</sub> -396.6091355 (2.52)

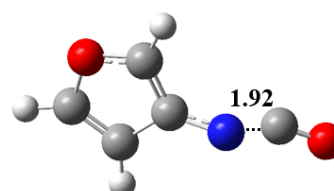
C	-0.048492	-0.029780	-0.240673
C	-0.381280	-0.004828	1.044931
C	0.904536	0.035106	1.762289
C	1.839388	0.031274	0.803422
H	-0.578246	-0.060328	-1.159183
H	-1.349925	-0.010149	1.513263
H	2.903909	0.061074	1.206780
O	1.419094	-0.004281	-0.364234
N	1.354377	0.072177	2.986395
C	4.802922	-0.017092	3.177272
O	5.254990	-0.100245	4.200495



7-T <sub>1</sub>	-396.6860605 (0.60)		
C	-2.810427	-1.070536	0.000124
C	-1.513233	-1.416814	-0.000078
C	-0.761372	-0.163434	-0.000314
C	-1.750763	0.837790	-0.000095
H	-3.712442	-1.641585	-0.000024
H	-1.095258	-2.400658	-0.000775
H	-1.691145	1.902354	0.000349
O	-2.973225	0.285159	0.000220
C	1.073604	1.226205	-0.000638
O	2.218985	1.514738	0.001046
N	0.553284	-0.076605	-0.000286

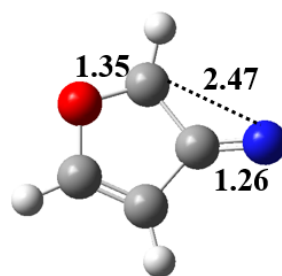


7-T <sub>1</sub> -TS	-396.6424244 (1.78)		
C	0.160798	-0.262620	0.127599
C	0.425085	-0.168823	1.445356
C	1.780141	0.369588	1.540540
C	2.179810	0.528227	0.236549
H	-0.684883	-0.592702	-0.433981
H	-0.220809	-0.434684	2.255870
H	3.080613	0.925649	-0.178840
O	1.217505	0.182333	-0.611500
N	2.477729	0.825761	2.609782
C	3.208436	-0.601735	3.661201
O	3.712382	-0.768910	4.657127



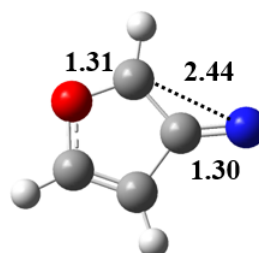
8-S<sub>0</sub> -283.5181120 (1.53)

C	1.330534	0.554152	0.009703
C	0.147179	1.177190	-0.075008
C	-0.887101	0.127161	-0.055950
C	-0.058076	-1.143316	-0.149226
H	2.328009	0.935887	0.042869
H	-0.024769	2.230902	-0.128206
H	-0.358044	-2.106966	0.214690
O	1.224762	-0.806200	0.110527
N	-2.126193	0.179687	0.154602



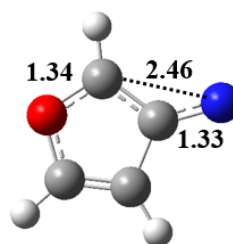
**8-S<sub>1</sub>** -283.4968104 (2.11)

C	1.352160	0.567207	-0.014095
C	0.152469	1.169884	-0.025843
C	-0.861969	0.107944	-0.005171
C	-0.067922	-1.081810	0.012648
H	2.358765	0.917650	-0.017630
H	-0.042428	2.221770	-0.040951
H	-0.359699	-2.114379	0.033316
O	1.210917	-0.803099	0.006674
N	-2.165992	0.163331	-0.011949



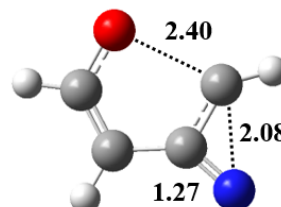
**8-T<sub>1</sub>** -283.5464855 (0.76)

C	0.672143	-1.287324	0.000172
C	1.164289	-0.033482	-0.000569
C	0.004680	0.851465	-0.000278
C	-1.103010	-0.021793	-0.000392
H	1.143514	-2.245421	0.000835
H	2.192353	0.260365	-0.000594
H	-2.155960	0.149958	-0.000207
O	-0.682345	-1.297683	-0.000073
N	-0.016804	2.183087	0.001106



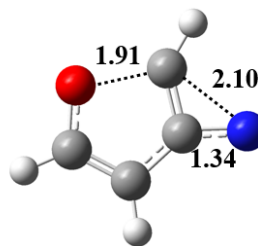
**8-T<sub>1</sub>-TS** -283.4249124 (4.07)

C	0.656106	-1.287833	-0.008487
C	1.012272	0.005635	-0.018267
C	-0.086239	0.956978	0.015218
C	-1.433528	0.549510	0.176237
H	1.343928	-2.114152	-0.018575
H	2.037358	0.315750	-0.036924
H	-2.345904	1.001065	-0.157824
O	-0.616214	-1.698076	0.023573
N	-0.209249	2.219859	0.024036



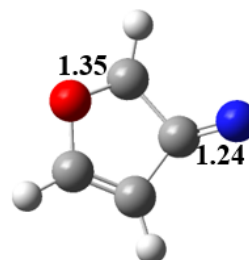
**8-(S<sub>0</sub>/S<sub>1</sub>)<sub>x</sub>** -283.4269377 (4.01)

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.3785019
C	1.3506868	0.0000000	1.8566353
C	2.3857500	0.0011477	0.9480884
H	-0.8394076	-0.0000811	-0.6693808
H	-0.8717871	-0.0001863	1.9997956
O	1.2026913	0.0002389	-0.5547916
N	2.0104145	0.0000098	3.0195217
H	3.4568360	0.0016879	0.9882861



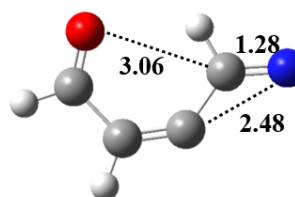
**8-(S<sub>0</sub>/T<sub>1</sub>)<sub>x</sub>** -283.5107680 (1.73)

C	0.006773	0.004398	0.003578
C	-0.000767	-0.013081	1.344962
C	1.423108	-0.011374	1.759032
C	2.142563	-0.269481	0.444365
H	-0.795959	0.072709	-0.698969
H	-0.849007	0.041544	1.995145
H	3.192460	-0.128693	0.236718
O	1.280675	0.051661	-0.541120
N	2.044998	0.634752	2.617360



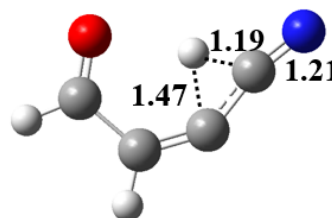
**10-S<sub>0</sub>** -283.4843219 (2.45)

C	-1.529270	-0.217352	0.007665
C	-0.505570	-1.299411	-0.013397
C	0.818208	-1.110694	-0.015429
C	1.657058	0.097843	0.001179
H	-2.562895	-0.568770	0.000516
H	-0.877686	-2.309509	-0.029138
H	1.107508	1.026628	0.023784
O	-1.287150	0.947176	0.030383
N	2.939770	0.178513	-0.008709



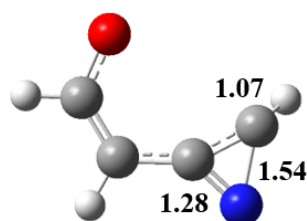
**10-S<sub>0</sub>-TS** -283.4824179 (2.50)

C	-1.509976	-0.186269	-0.000229
C	-0.380954	-1.158125	-0.000490
C	0.904647	-0.783395	-0.000383
C	1.772912	0.325214	0.001016
H	-2.516939	-0.598490	0.001211
H	-0.610023	-2.207973	-0.000729
H	0.633759	0.665997	-0.000370
O	-1.321295	0.989670	-0.001251
N	2.717618	1.078739	0.000927



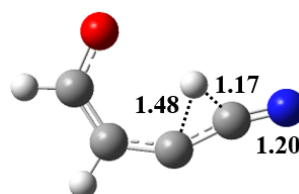
**11-T<sub>1</sub>** -283.4437189 (3.55)

C	0.743393	-1.399010	-0.030385
C	0.941052	-0.072979	-0.028384
C	-0.142791	0.882925	0.050554
C	-1.492736	1.172566	0.189899
H	1.543608	-2.115127	-0.089074
H	1.943098	0.304623	-0.091625
H	-2.319637	1.113763	-0.493029
O	-0.446996	-2.002569	0.031065
N	-0.303994	2.148723	0.044364



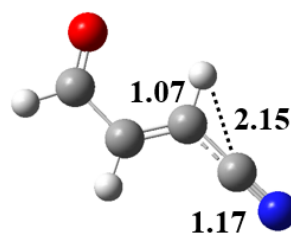
**11-T<sub>1</sub>-TS** -283.4016698 (4.70)

C	-1.549481	-0.302020	-0.021973
C	-0.438893	-1.095209	-0.006003
C	0.920645	-0.727231	0.086508
C	1.825889	0.311799	-0.063191
H	-2.552958	-0.681053	-0.059704
H	-0.613933	-2.154121	-0.044946
H	0.799584	0.731382	0.304194
O	-1.504978	1.037585	0.006422
N	2.803874	1.004237	-0.201606



*anti-9*-S<sub>0</sub> -283.6106201 (-0.99)

C	1.890415	0.431308	0.000180
C	0.422176	0.685349	0.000111
C	-0.449418	-0.339067	-0.000236
C	-1.876865	-0.143353	0.000012
H	2.522489	1.321020	-0.000716
H	0.086011	1.706460	0.000292
H	-0.094803	-1.352333	-0.000484
O	2.368143	-0.656734	0.000711
N	-3.041452	0.004932	0.000155



*anti-9*-T<sub>1</sub> -283.522256 (1.42)

C	1.823483	0.518307	-0.000307
C	0.456830	0.678052	0.001155
C	-0.463713	-0.375963	0.001202
C	-1.870644	-0.142355	-0.000111
H	2.525054	1.330189	-0.002077
H	0.093049	1.688361	0.001527
H	-0.141943	-1.399261	-0.000052
O	2.423791	-0.679359	0.000235
N	-3.019212	0.039611	-0.001547

