Electronic supplementary information

Computational Elucidation of the Reaction Mechanism for Synthesis of Pyrrolidinedione Derivatives via Nef-type Rearrangement – Cyclization Reaction

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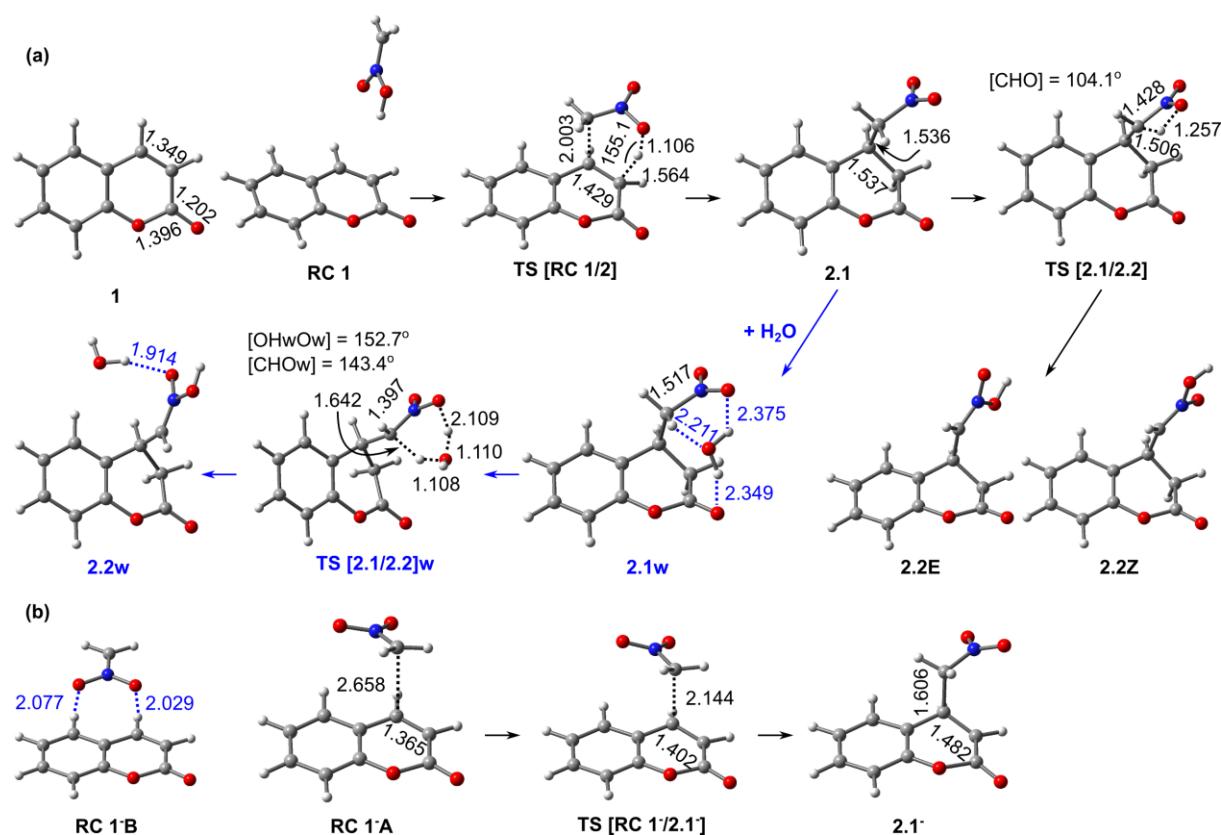
Figure S1. Structures of reaction complexes, transition states and intermediates for Michael addition of nitromethane, CH_3NO_2 (a), and deprotonated nitromethane, $CH_2NO_2^-$ (b), to coumarin **1** (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
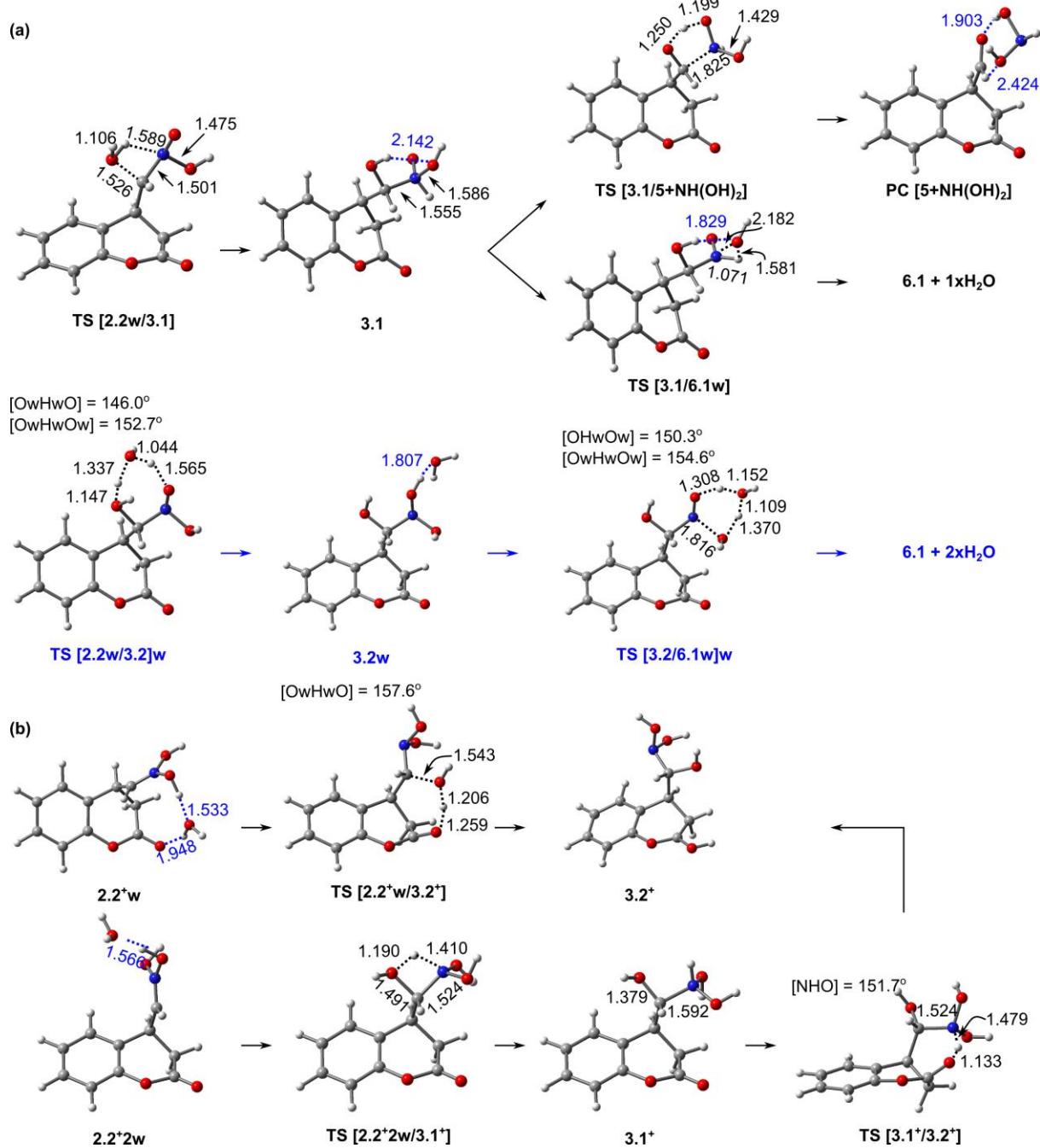
Figure S2. Structures of reaction complexes, transition states and intermediates for O-atom migration assisted by a water molecule (a) and assisted by a water molecule in acidic solution (b). (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
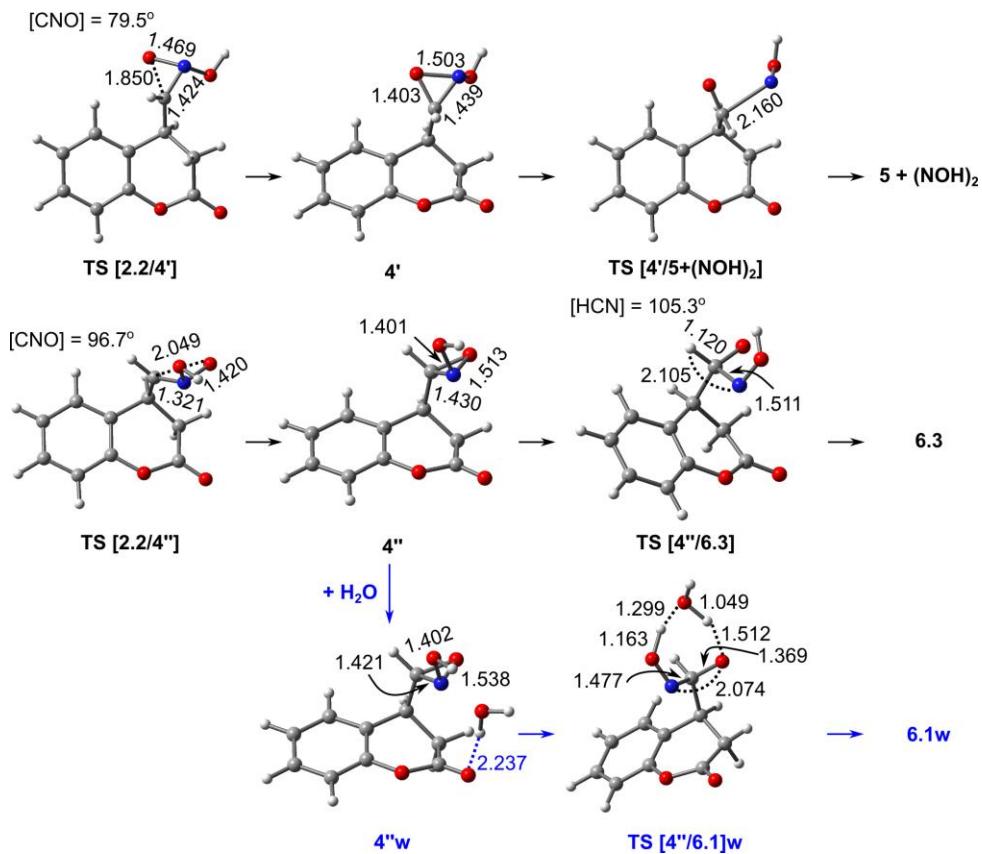
**Figure S3.** Structures of reaction complexes, transition states and intermediates for O-atom migration via formation of a three-membered oxaziridine cycle. (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
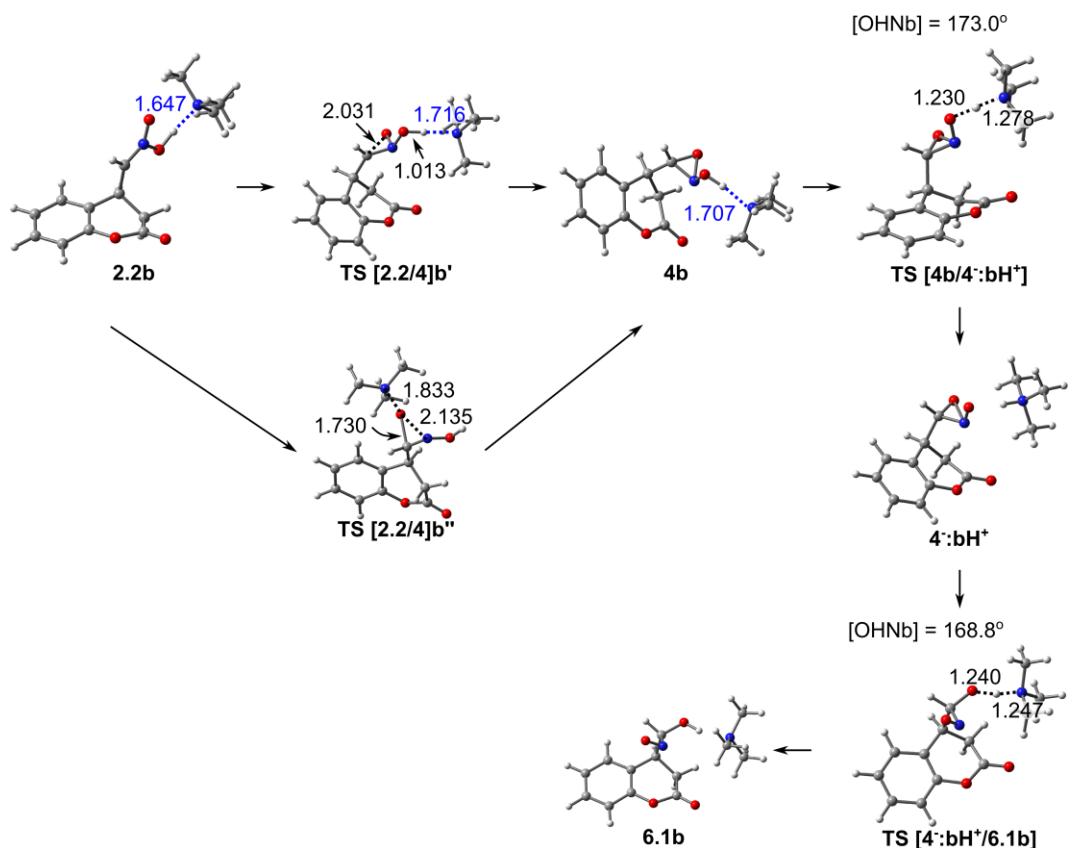
Figure S4. Structures of reaction complexes, transition states and intermediates for O-atom migration via formation of a three-membered oxaziridine cycle, assisted by trimethylamine. (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
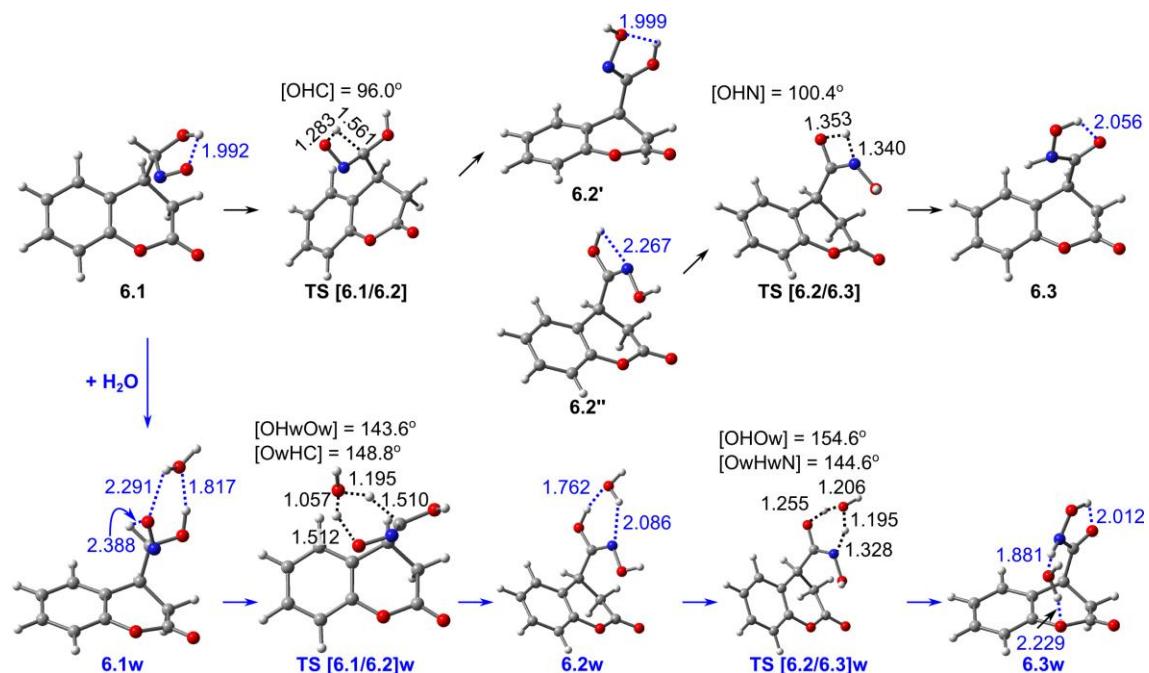
Figure S5. Structures of reaction complexes, transition states and intermediates for the transformation between different tautomeric forms of the nitrosohydroxymethyl group in intermediate **6**. (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
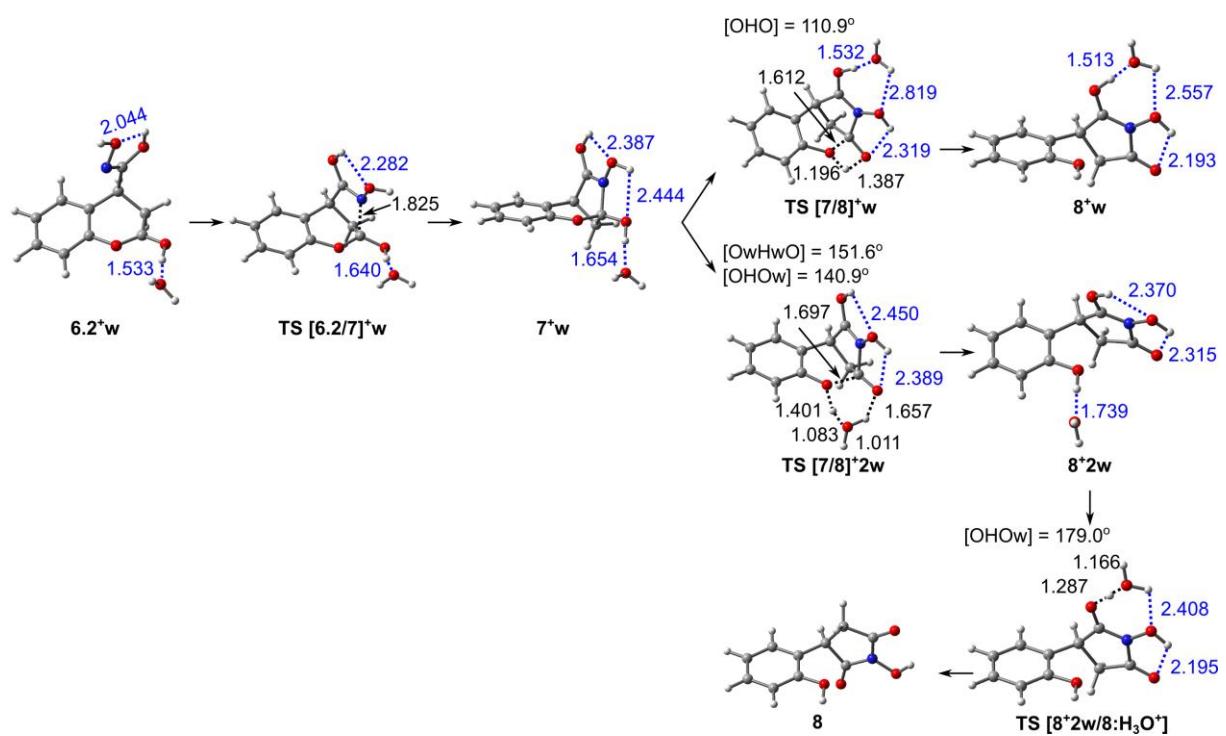
**Figure S6.** Structures of reaction complexes, transition states and intermediates for formation of pyrrolidine ring from intermediate **6.2**. (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
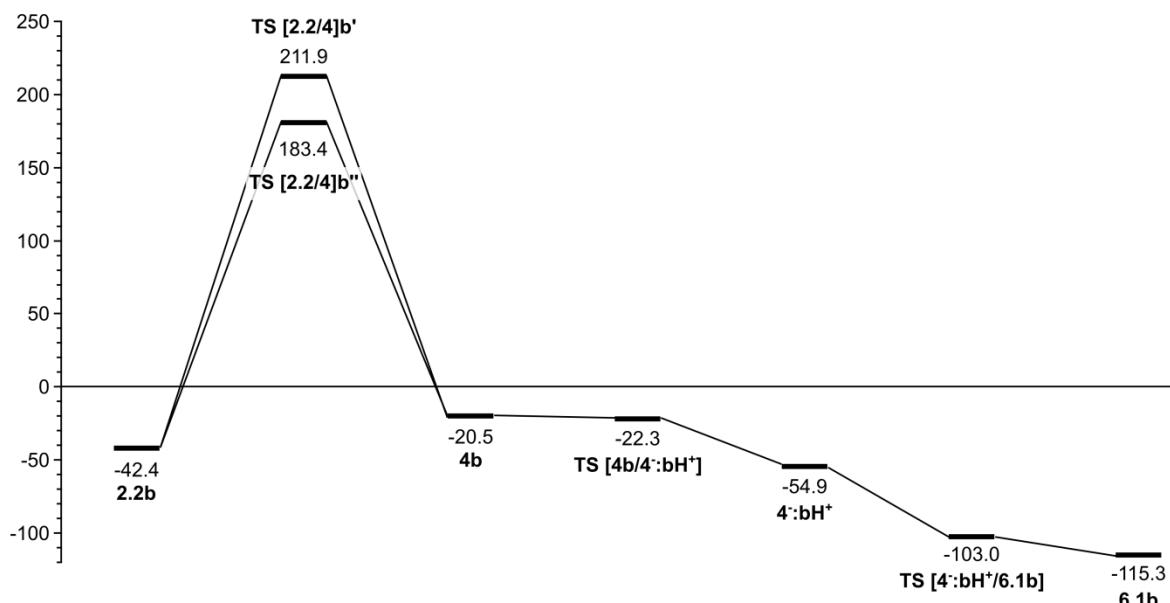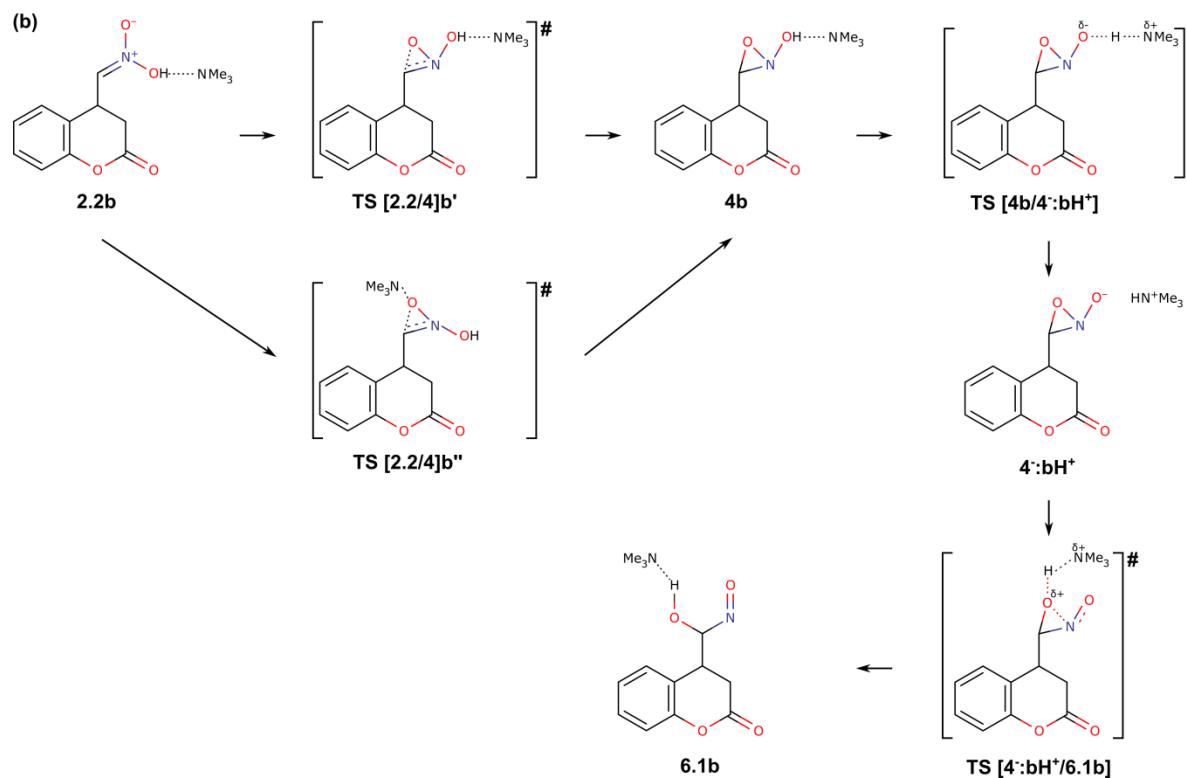
Figure S7. (a) Energy diagram of the mechanism for O-atom migration assisted by trimethylamine. (b) Schematic representation of the reaction paths.

Tables

Table S1. Reaction and activation energies, E_{rea} and E_{act} (in kJ/mol), for various reaction steps calculated as single point energy at MP2/6-311+G* level accounting the solvent effect by PCM. The corrections for the zero-point vibrational energy, ZPE (in kJ/mol), and entropy corrections, S_{tot} and S_{vib}, are obtained from frequency calculations at B3LYP/6-311+G* level. T is equal to 298.15 K.

Structure	E_{rea} or E_{act}	ZPE	$T*S_{tot}$	$T*S_{vib}$	ZPE-TΔS	E+ZPE-TΔS
Michael addition						
Neutral system						
TS [RC 1/2]	69.6	-5.3	-25.5	-24.5	20.1	89.7
2.1	-166.7	13.3	-20.0	-19.1	33.2	-133.4
TS [2.1/2.2]	307.6	-17.1	-3.4	-3.4	-13.7	293.9
2.2E	97.3	-3.7	-0.5	-0.6	-3.3	94.0
2.2Z	90.0	-4.0	-0.5	-0.5	-3.5	86.5
TS [2.1/2.2]w	197.8	-14.6	-13.1	-13.1	-1.5	196.3
2.2w	88.9	-3.5	1.5	1.2	-5.0	83.9
Negatively charged system						
TS [RC 1-/2.1-]	21.7	1.8	-14.7	-13.9	16.4	38.2
2.1-	-46.1	6.3	-14.9	-14.1	21.2	-24.9
Oxygen migration						
Neutral system						
TS [2.2w/3.1]	241.9	-6.9	-14.5	-14.1	7.6	249.5
3.1	16.6	11.1	-13.5	-13.0	24.5	41.1
TS [3.1/6.1w]	73.5	-26.1	-12.7	-12.8	-13.4	60.1
TS [3.1/5+NH(OH)2]	58.7	-12.6	-6.4	-6.5	-6.2	52.5
6.1w	-104.2	-11.6	12.3	12.1	-23.9	-128.2
TS [2.2w/3.2]w	130.8	58.1	-22.3	-22.8	80.5	211.3
3.2w	-36.6	73.9	7.0	6.3	66.8	30.3
TS [3.2/6.1w]w	142.4	-9.0	-30.0	-29.8	21.1	163.5
Protonated system						
TS [2.2+2w/3.1+]	149.2	7.1	-10.2	-9.4	17.3	166.6
3.1+	1.3	15.2	-19.0	-18.2	34.2	35.4
TS [3.1+/3.2+]	90.1	-13.7	-5.6	-5.5	-8.2	81.9
TS [2.2+w/3.2+]	101.5	-1.0	-20.6	-20.4	19.6	121.2
3.2+	27.0	9.9	-7.6	-7.5	17.5	44.5
Nef reaction						
TS [2.2/4']	164.0	-6.9	-6.0	-6.0	-0.8	163.2
TS [2.2/4'']	261.8	-8.4	-1.3	-1.0	-7.1	254.8
4'	35.5	-0.2	-2.7	-2.5	2.5	38.0
4''	29.0	0.0	-2.7	-2.5	2.7	31.8
TS [4'/5+(NOH)2]	149.5	-8.5	-4.8	-5.0	-3.6	145.8
TS [4''/6.3]	151.8	-8.3	-2.0	-1.7	-6.3	145.5

TS [4"/6.1]w	99.5	-10.6	-3.8	-3.6	-6.8	92.6
6.3	-220.8	2.1	3.0	3.1	-0.9	-221.7
Base assisted Nef reaction						
TS [2.2/4]b'	254.3	-6.6	-0.4	0.1	-6.2	248.1
TS [2.2/4]b"	225.8	-2.0	-8.9	-8.3	6.9	232.7
4b	21.8	0.3	-1.0	-0.6	1.3	23.2
TS [4b/4-:bH+]	-1.8	-9.1	-5.9	-5.7	-3.1	-4.9
4-:bH+	-34.4	3.7	-21.9	-21.7	25.7	-8.7
TS [4-:bH+/6.1b]	-48.1	-14.2	19.5	19.8	-33.7	-81.8
TS [4-:bH+/6.2-:bH+]	276.8	-17.2	18.0	17.7	-35.2	241.5
6.1b	-60.4	-5.0	25.5	25.7	-30.5	-90.9
Tautomerisation of 6						
TS [6.1/6.2]	335.9	-19.6	-11.2	-11.3	-8.5	327.4
6.2'	-88.4	3.8	0.9	0.8	2.9	-85.5
6.2"	-69.2	4.3	-0.9	-0.8	5.3	-63.9
TS [6.2/6.3]	174.5	-17.3	-6.3	-6.3	-11.0	163.4
6.3	-39.6	-0.8	3.2	3.0	-4.1	-43.6
TS [6.1/6.2]w	178.4	-27.1	-28.2	-27.7	1.1	179.5
6.2w	-79.9	4.8	-5.5	-5.4	10.3	-69.7
TS [6.2/6.3]w	87.4	-31.7	-22.9	-22.6	-8.9	78.6
6.3w	-37.8	-1.4	2.3	2.6	-3.8	-41.6
Cyclization						
TS [6.2/7]+w	11.9	-1.5	-16.4	-16.0	15.0	26.9
7+w	-2.1	3.7	-9.1	-8.6	12.8	10.7
TS [7/8]+w	199.4	-15.5	-24.1	-23.8	8.5	208.0
TS [7/8]+2w	84.8	-7.9	-9.8	-9.6	1.9	86.8
8+w	-36.2	-2.0	-8.4	-8.4	6.4	-29.8
8+2w	-18.6	-4.6	10.3	10.0	-14.9	-33.5
TS [8+2w/8:H3O+]	-12.6	-11.4	-5.9	-5.8	-5.5	-18.1
8	-62.9	-96.8	-22.6	-21.3	-74.2	-137.2

[a] Activation energy, E_{act}, and reaction energy, E_{rea}, of the corresponding reaction step.
[b] In entropy S_{tot} all degrees of freedom are included, while in S_{vib} only vibrational degrees of freedom are taken into account.

Table S2. Reaction and activation energies, E_{rea} and E_{act} (in kJ/mol), for various reaction steps in the case of the *ethyl ester of 3-coumarin-carboxylic acid* calculated as single point energy at MP2/6-311+G* level accounting the solvent effect by PCM.

Structure	Erel [a]	Erea [b]	Eact [b]
I. Michael addition			
2.1	-88.7		-
TS [2.1/2.2]	218.0		306.7
2.2E	5.8		*94.5*
2.2Z	-1.4		*87.3*
2.1w	-107.4		
TS [2.1/2.2]w	87.4		194.8
2.2w	-		-
II. Oxygen migration			
Protonated system			
2.2⁺w	58.5		
2.2⁺2w	50.1		
TS [2.2⁺2w/3.1⁺]	208.4		158.4
3.1⁺	62.0		*11.9*
TS [3.1⁺/3.2⁺]	164.1		102.1
TS [2.2⁺w/3.2⁺]	144.7		86.2
3.2⁺	90.1		*31.6*
Nef reaction			
TS [2.2/4']	277.1		271.4
TS [2.2/4'']	264.9		266.3
4'	43.8		*38.1*
4''	31.2		*32.6*
Tautomerisation of 6			
6.1	-80.7		
TS [6.1/6.2]	252.5		333.2
6.2'	-171.1		*-90.3*
6.2''	-146.4		*-65.7*
TS [6.2/6.3]	24.9		171.3
6.3	-190.7		*-44.2*
6.1w	-104.2		
TS [6.1/6.2]w	69.9		174.1
6.2w	-182.5		*-78.2*
TS [6.2/6.3]w	-94.9		87.5
6.3w	-223.5		*-41.0*
III. Cyclization			
6.2⁺w	-108.0		
TS [6.2/7]⁺w	-116.1		-
7⁺w	-116.8		*-8.8*
TS [7/8]⁺w	85.1		201.9

TS [7/8]⁺2w	-49.9	67.0
8⁺w	-	-
8⁺2w	-123.9	*-7.1*
TS [8⁺2w/8:H₃O⁺]	-134.4	-
8	-199.4	*-75.5*

[a] Relative energy of the species, E_{rel}, with respect to the energy of **1** and nitromethane at the corresponding level.

[b] Activation energy, E_{act}, and reaction energy, E_{rea}, of the corresponding reaction step.

Description of the results obtained for the mechanism of the Nef rearrangement assisted by triethylamine

In recent experimental studies, we showed that the final product of the new rearrangement, pyrrolidinedion derivative, could be synthesized also in basic media in presence of triethylamine. By this reason, we modeled O-migration, in which such a base (with trimethymamine as a model) can influence the process of oxygen migration in the three-membered transition state **TS [2.2/4]b** (Fig. S4, S7):

- forming hydrogen bonds between the NOH group and the base in the transition state **TS [2.2/4]b'**;

- coordination of the nitrogen atom from the amine to the migrating oxygen atom from CH_2NO_2H in the transition state **TS [2.2/4]b''**.

The former approach is based on the basic properties of trialkylamine, while the latter one is connected with the possible formation of trialkylamino N-oxide. The formation of hydrogen bond stabilizes the starting compound **2.2b** by 57.1 kJ mol^{-1} with respect to **2.2Z**, while the stabilization of the transition state **TS [2.2/4]b'** is weaker and the energy barrier of the reaction step, 254.3 kJ mol^{-1}, increases compared to the reaction without amine, 167.5 (164.1) kJ mol^{-1}. The transfer of O atom coordinated to N atom from Me$_3$N through **TS [2.2/4]b''** has a slightly lower energy barrier, 225.8 kJ mol^{-1}, which is still by ~ 60 kJ mol^{-1} higher than the barrier of the reaction without amine.

The reaction step via the presumed transition state **pseudoTS [4b/4$^-$:bH$^+$]** (which has lower energy than the preceding intermediate) instead of the neutral complex **4b** spontaneously leads to formation of the ionic couple **4$^-$:bH$^+$**, in which the NOH group of **4** is deprotonated and the amine is protonated. The formation of the ionic couple leads to the opening of the three-centered ring and complete migration of the oxygen atom to the carbon atom, which was not possible to achieve in absence of the base (see above). The intermediate **6.1** can be easily obtained from **[4]$^-$:bH$^+$** by reverse protonation of **4$^-$** from the protonated base. This process is spontaneous via the structure denoted as **TS [4$^-$:bH$^+$/6.1b]** (Figs. S4, S7).

Intermediate	E_{rel} [a]		E_{act} [b] or E_{rea} [b]	
Transition state	L1	L2|PCM	L1	L2|PCM
Base assisted Nef reaction				
2.2b	-9.4	-42.4		
TS [2.2/4]b'	234.6	211.9	243.9	254.3
TS [2.2/4]b''	232.9	183.4	242.3	225.8
4b	36.3	-20.5	45.6	21.8

pseudoTS [4b/4⁻:bH⁺]	49.2	-22.3	12.9	-1.8
4⁻:bH⁺	37.5	-54.9	1.2	-34.4
pseudoTS [4⁻:bH⁺/6.1b]	-24.6	-103.0	-62.1	-48.1
TS [4⁻:bH⁺/6.2⁻:bH⁺]	323.3	221.8	285.8	276.8
6.1b	-49.0	-115.3	-86.4	-60.4

[a] Relative energy of the species, E_{rel}, with respect to the energy of **1** and nitromethane at the corresponding level.

[b] Activation energy, E_{act}, and reaction energy, E_{rea}, of the corresponding reaction step.

TS structures (Energies at L1)

TS [RC 1/2]

-742.1602358   ImgFreq/IR Inten: -851.5222/12.3334

O	-0.91305	1.77920	-0.37935
C	0.29198	2.09008	0.26751
O	0.62625	3.24331	0.28722
C	1.03737	0.96203	0.81543
C	0.49231	-0.35913	0.81706
C	-0.91502	-0.50894	0.41735
C	-1.64923	-1.68757	0.61692
H	-1.17036	-2.53408	1.10083
C	-2.97341	-1.77691	0.21294
H	-3.53217	-2.69128	0.37821
C	-3.58424	-0.67988	-0.40529
H	-4.61850	-0.74483	-0.72586
C	-2.88090	0.50124	-0.60122
H	-3.33971	1.36916	-1.06033
C	-1.55200	0.58382	-0.18457
C	1.38266	-1.44969	-0.60819
H	0.90799	-1.05713	-1.49523
N	2.68510	-1.06404	-0.45595
O	2.90174	0.19732	-0.84144
O	3.52146	-1.65182	0.22209
H	1.76679	1.23321	1.57142
H	0.83484	-1.01504	1.61442
H	1.19675	-2.48151	-0.34092
H	2.17026	0.77539	-0.24679

TS [2.1/2.2]

-742.1354092   ImgFreq/IR inten: -2172.6740/541.3399

O	-0.93507	1.76505	-0.38671
C	0.26798	2.03500	0.22386
O	0.81958	3.06676	-0.02672
C	0.76377	0.98993	1.20026
H	1.81734	1.19002	1.39487
H	0.22714	1.13886	2.14496
C	0.51107	-0.44375	0.69795
H	0.73051	-1.13868	1.51859
C	-0.95024	-0.56222	0.32723
C	-1.68598	-1.74050	0.47044
H	-1.19747	-2.62198	0.87642
C	-3.02946	-1.79540	0.10852
H	-3.58639	-2.71823	0.22826
C	-3.65518	-0.65702	-0.40127
H	-4.70202	-0.68998	-0.68358
C	-2.94243	0.52875	-0.54609

H	-3.40495	1.42712	-0.93846
C	-1.59919	0.56355	-0.18255
C	1.38161	-0.78999	-0.49738
O	3.38314	-1.17242	0.76573
N	2.77604	-0.96737	-0.24740
O	3.36489	-0.73586	-1.41052
H	1.04620	-1.64942	-1.08034
H	2.20515	-0.32454	-1.66911

TS [2.1/2.2]w
-818.6264588   ImgFreq/IR inten: -1393.6794/102.5452

O	1.14768	1.75540	0.29575
C	0.03690	2.05236	-0.46764
O	-0.50648	3.10406	-0.29021
C	-0.37106	1.00513	-1.47838
H	-1.38849	1.22155	-1.79920
H	0.27915	1.12046	-2.35426
C	-0.22315	-0.42561	-0.92521
H	-0.37086	-1.12202	-1.75860
C	1.18395	-0.57685	-0.39264
C	1.89989	-1.77497	-0.44065
H	1.43425	-2.64880	-0.88758
C	3.19439	-1.85896	0.06656
H	3.73643	-2.79712	0.01763
C	3.79179	-0.73031	0.62921
H	4.80139	-0.78550	1.02226
C	3.09859	0.47503	0.68333
H	3.54039	1.36748	1.11180
C	1.80437	0.53731	0.17447
C	-1.22917	-0.74303	0.16940
O	-2.90162	-0.90904	-1.40709
N	-2.53355	-1.01985	-0.24705
O	-3.40185	-1.31705	0.68610
H	-0.91988	-1.47335	0.91370
H	-1.72260	0.25790	1.37339
H	-3.10688	-0.41850	1.69101
O	-2.52133	0.41952	2.12461
H	-2.19818	0.23309	3.01520

TS [RC 1⁻/2.1⁻]
-741.6739479   ImgFreq/IR inten: -271.0039/625.5705

O	-2.30114	-0.60008	0.39959
C	-1.86759	-1.89151	-0.03477
O	-2.67164	-2.79038	0.14735
C	-0.58470	-1.94884	-0.62933
C	0.29418	-0.85764	-0.68196
C	-0.28475	0.46315	-0.41935
C	0.38019	1.67012	-0.68385

H	1.38970	1.63524	-1.07700
C	-0.22082	2.89416	-0.41517
H	0.31508	3.81607	-0.61809
C	-1.50695	2.93111	0.13184
H	-1.98143	3.88438	0.34799
C	-2.18730	1.74911	0.40070
H	-3.18895	1.75005	0.81756
C	-1.57981	0.52119	0.12351
C	1.78323	-1.07227	0.84527
H	1.35299	-0.64073	1.73858
N	2.89423	-0.39996	0.36870
O	3.57808	-0.94457	-0.54179
O	3.11813	0.78186	0.74273
H	-0.26915	-2.92858	-0.96867
H	1.11813	-0.89708	-1.38962
H	1.86258	-2.14574	0.76395

TS [2.2w/3.1]

-818.5707078   ImgFreq/IR inten: -811.7078/529.1724

O	-1.23896	1.76540	-0.60328
C	-0.09207	2.24717	-0.00874
O	0.32308	3.31461	-0.35253
C	0.53024	1.36696	1.05444
H	-0.00419	1.56128	1.99130
H	1.56373	1.67220	1.19691
C	0.41234	-0.13677	0.73799
H	0.71917	-0.70413	1.62138
C	-1.03414	-0.43836	0.40860
C	-1.66596	-1.63913	0.74200
H	-1.09841	-2.41116	1.25259
C	-3.00523	-1.85515	0.43154
H	-3.47863	-2.79358	0.69857
C	-3.73523	-0.85901	-0.21855
H	-4.77985	-1.01902	-0.46299
C	-3.13062	0.34979	-0.54698
H	-3.67624	1.14455	-1.04249
C	-1.79045	0.54762	-0.22802
C	1.36866	-0.50816	-0.38946
N	2.76579	-0.90564	-0.01262
O	3.24154	-0.00877	1.05793
O	3.55772	-0.85650	-1.06593
H	1.35100	0.12339	-1.27696
H	4.06540	0.30857	0.64899
O	1.05941	-1.93234	-0.84229
H	1.36676	-2.01521	-1.76487
H	1.92324	-2.23647	-0.22220

TS [3.1/6.1]w

-818.6414856 ImgFreq/IR inten: -752.8107/81.5313

O	-1.35687	1.72360	-0.62448
C	-0.24951	2.26070	-0.02374
O	0.16926	3.31463	-0.40952
C	0.33810	1.45447	1.11586
H	-0.28782	1.63583	1.99693
H	1.32248	1.86363	1.34019
C	0.34118	-0.05841	0.83804
H	0.62200	-0.59102	1.74969
C	-1.05746	-0.45917	0.42311
C	-1.61125	-1.71043	0.70427
H	-1.00502	-2.44724	1.21961
C	-2.91163	-2.01893	0.31754
H	-3.32491	-2.99607	0.54203
C	-3.67881	-1.07066	-0.36074
H	-4.69340	-1.30475	-0.66483
C	-3.14701	0.18102	-0.65205
H	-3.71824	0.93520	-1.18094
C	-1.84432	0.47039	-0.25951
C	1.35147	-0.47925	-0.23870
N	2.77682	-0.03210	0.18164
O	3.57954	-1.10807	-1.53866
O	3.17865	-0.20706	1.30294
H	1.21402	0.05631	-1.18605
H	4.41599	-1.53966	-1.31310
O	1.34422	-1.84391	-0.39229
H	2.08115	-2.02235	-1.02591
H	3.43293	0.18294	-0.63743

TS [3.1/5+NH(OH)₂]

-818.6452361 ImgFreq/IR inten: -1142.8770/826.7598

O	-1.39874	1.79977	-0.42400
C	-0.23620	2.23703	0.14844
O	0.17411	3.32826	-0.12640
C	0.42079	1.29042	1.13443
H	-0.09382	1.42689	2.09273
H	1.44305	1.64600	1.27278
C	0.32466	-0.18992	0.72980
H	0.60685	-0.82219	1.57865
C	-1.11253	-0.49242	0.36328
C	-1.69101	-1.75274	0.53364
H	-1.08263	-2.55805	0.93057
C	-3.01805	-1.98365	0.18555
H	-3.44934	-2.96918	0.32305
C	-3.78859	-0.94677	-0.34256
H	-4.82423	-1.11929	-0.61543

C	-3.23210	0.31488	-0.52319
H	-3.80448	1.13784	-0.93546
C	-1.90244	0.52534	-0.17245
C	1.25197	-0.57052	-0.43784
N	2.94728	-0.38843	0.21179
O	3.66053	0.48563	-0.66475
O	3.40616	-1.63819	0.18479
H	1.31960	0.18398	-1.23338
H	4.49569	0.01432	-0.82750
O	1.30268	-1.81604	-0.78827
H	2.45192	-2.09338	-0.38127
H	3.04947	0.00680	1.14707

TS [2.2w/3.2]w

-895.0662618   ImgFreq/IR inten: -784.3438/640.9200

O	-1.83800	1.63691	-0.45776
C	-0.84715	2.30122	0.23886
O	-0.70208	3.47054	0.04190
C	-0.05150	1.47029	1.22423
H	-0.62514	1.45038	2.15826
H	0.88241	1.99263	1.41599
C	0.15977	0.01549	0.76338
H	0.56903	-0.55063	1.60653
C	-1.18226	-0.55699	0.36283
C	-1.54612	-1.89059	0.56307
H	-0.83675	-2.57003	1.02598
C	-2.80007	-2.35815	0.18114
H	-3.06404	-3.39730	0.34427
C	-3.71400	-1.48448	-0.40928
H	-4.69348	-1.84065	-0.71003
C	-3.37825	-0.14924	-0.60677
H	-4.07190	0.55314	-1.05439
C	-2.11983	0.29989	-0.21650
C	1.18725	-0.07822	-0.36449
N	2.56259	0.32998	0.05459
O	2.62278	1.74601	-0.17236
O	3.44785	-0.28516	-0.83293
H	0.88094	0.44140	-1.27924
H	3.02925	1.81289	-1.05662
O	1.35272	-1.48937	-0.76321
H	2.08864	-1.35379	-1.43341
H	2.01352	-2.02178	0.00889
H	3.65624	-1.55583	0.05575
O	3.19966	-2.37470	0.51533
H	3.32267	-2.31942	1.46920

TS [3.2/6.1w]w				
-895.0882589	ImgFreq/IR inten: -1326.5756/194.2267			
O		-1.48825	1.78215	-0.57039
C		-0.31750	2.11766	0.06492
O		0.28456	3.08227	-0.31896
C		0.09435	1.20919	1.20043
H		-0.56392	1.42516	2.05020
H		1.11430	1.45374	1.47898
C		-0.08867	-0.27162	0.82358
H		0.11606	-0.89007	1.70152
C		-1.53610	-0.44677	0.40838
C		-2.28467	-1.59609	0.66944
H		-1.80269	-2.43350	1.16200
C		-3.62265	-1.68059	0.29480
H		-4.18707	-2.58274	0.50497
C		-4.23391	-0.60488	-0.35052
H		-5.27672	-0.66395	-0.64391
C		-3.50904	0.55193	-0.61821
H		-3.95660	1.40341	-1.11802
C		-2.17304	0.61561	-0.23583
C		0.86782	-0.77131	-0.27462
N		2.29988	-0.85002	0.22790
O		2.84120	0.88298	0.21210
O		3.00879	-1.42818	-0.69996
H		0.85589	-0.14045	-1.17620
H		2.57601	1.28489	-0.63179
O		0.49683	-2.08587	-0.58100
H		1.14618	-2.43834	-1.20610
H		4.21485	-1.08506	-0.32812
O		4.94743	-0.30107	0.09120
H		4.14204	0.45416	0.19975
H		5.61862	-0.03409	-0.54661
TS [2.2$^+$2w/3.1$^+$]				
-818.9474032	ImgFreq/IR inten: -1487.8898/1295.6481			
O		-1.11566	1.83089	-0.47678
C		0.04886	2.18125	0.15878
O		0.59509	3.20183	-0.12798
C		0.56187	1.19052	1.19283
H		0.00035	1.34044	2.12032
H		1.59752	1.46111	1.40391
C		0.35415	-0.27268	0.75347
H		0.62309	-0.95370	1.56382
C		-1.10603	-0.44790	0.38187
C		-1.82230	-1.62554	0.62004
H		-1.32576	-2.46890	1.08998

C	-3.16875	-1.71265	0.27948
H	-3.71814	-2.62599	0.47591
C	-3.81183	-0.61630	-0.29855
H	-4.86240	-0.67848	-0.55874
C	-3.11841	0.56721	-0.53262
H	-3.60015	1.43378	-0.96996
C	-1.77326	0.63938	-0.18946
C	1.21741	-0.60487	-0.45022
N	2.70824	-0.85723	-0.26222
O	3.14975	-0.99463	1.04385
O	3.42057	0.12860	-0.94396
H	1.10531	0.06219	-1.30313
H	3.26225	-0.09887	1.41615
O	1.03074	-2.01634	-0.89329
H	0.52177	-2.15688	-1.70936
H	2.21889	-2.04646	-0.83979
H	4.28554	-0.26088	-1.16196

TS [3.1⁺/3.2⁺]

-818.9847008   ImgFreq/IR inten: -790.2056/1952.7991

O	-0.88616	1.83313	-0.36178
C	0.27450	1.75721	0.21731
O	1.28439	2.21150	-0.38698
C	0.41588	0.88812	1.41642
H	-0.37291	1.09468	2.14204
H	1.38492	1.00944	1.88939
C	0.18713	-0.51735	0.80402
H	0.33997	-1.27948	1.56857
C	-1.25950	-0.48516	0.32770
C	-2.13958	-1.56318	0.40072
H	-1.78042	-2.51918	0.76726
C	-3.47772	-1.41404	0.02973
H	-4.14893	-2.26226	0.09742
C	-3.95677	-0.18233	-0.41011
H	-4.99760	-0.06908	-0.68964
C	-3.10033	0.91646	-0.49809
H	-3.44091	1.88186	-0.85311
C	-1.78322	0.73458	-0.12876
C	1.18455	-0.81044	-0.35991
N	2.47555	-0.01764	-0.19098
O	3.33413	-0.29883	-1.24724
O	3.06353	-0.45020	1.02359
H	0.80166	-0.41951	-1.30653
H	3.49187	-1.26396	-1.21847
O	1.47596	-2.16603	-0.45459
H	1.21921	-2.52498	-1.31264
H	2.06745	1.40283	-0.25442

H		3.86240	0.09337	1.12889

TS [2.2⁺w/3.2⁺]

-818.9805439	ImgFreq/IR inten: -1126.4281/2592.9207		

O	-1.40383	1.81772	-0.30938
C	-0.22882	2.05621	0.21438
O	0.58681	2.76695	-0.40433
C	0.19405	1.23805	1.39307
H	-0.58407	1.21746	2.15753
H	1.11336	1.62393	1.82670
C	0.32699	-0.17677	0.78394
H	0.64066	-0.86778	1.56517
C	-1.07151	-0.53019	0.29225
C	-1.59882	-1.82074	0.32963
H	-0.97016	-2.64309	0.65525
C	-2.92665	-2.05561	-0.02792
H	-3.32096	-3.06438	0.00893
C	-3.74906	-0.99981	-0.41574
H	-4.78288	-1.18336	-0.68408
C	-3.24973	0.30184	-0.46528
H	-3.86218	1.13851	-0.77981
C	-1.92895	0.50270	-0.11402
C	1.40460	-0.21815	-0.33980
N	2.24356	-1.36803	-0.24042
O	2.87272	-1.47424	1.00485
O	3.22626	-1.21078	-1.24854
H	0.97946	-0.21240	-1.34147
H	3.52669	-0.75330	1.08057
H	3.44291	-2.10641	-1.54853
O	2.28222	1.04891	-0.27308
H	2.94264	0.99603	-0.98604
H	1.62353	2.05728	-0.33038

TS [2.2/4']

-742.1531741	ImgFreq/IR inten: -106.9246/73.8740		

O	1.63521	1.67808	-0.23923
C	0.48239	2.35135	0.05631
O	0.43611	3.53451	-0.11618
C	-0.65024	1.52364	0.62899
H	-1.57025	2.09403	0.51745
H	-0.45003	1.40975	1.70220
C	-0.75716	0.12878	-0.04307
H	-1.11317	0.25933	-1.06771
C	0.60883	-0.52709	-0.03366
C	0.80697	-1.90988	0.01753
H	-0.05697	-2.56481	0.04224
C	2.09190	-2.44706	0.01218

H	2.22573	-3.52256	0.04958
C	3.19987	-1.60257	-0.04818
H	4.20306	-2.01508	-0.05300
C	3.02388	-0.22403	-0.11178
H	3.86513	0.45665	-0.17357
C	1.73459	0.29653	-0.10691
C	-1.78458	-0.63916	0.70611
N	-3.15396	-0.72851	0.32624
O	-3.40095	0.25041	-0.68479
O	-2.62327	-1.94979	-0.29455
H	-4.36318	0.23477	-0.77085
H	-1.57817	-1.06110	1.68295

TS [2.2/4'']
-742.1249367   ImgFreq/IR inten: -914.2135/43.8485

O	0.49836	1.65963	0.58338
C	-0.63987	1.89507	-0.17301
O	-1.31415	2.83917	0.10627
C	-0.88889	0.94736	-1.32687
H	-0.33674	1.34084	-2.18776
H	-1.95145	0.97078	-1.55856
C	-0.41206	-0.48333	-1.05771
H	-0.42184	-1.05413	-1.99385
C	1.00522	-0.45683	-0.50415
C	1.94641	-1.46274	-0.74056
H	1.67345	-2.31012	-1.36325
C	3.22443	-1.38371	-0.19750
H	3.94666	-2.16853	-0.39269
C	3.57244	-0.28610	0.59289
H	4.56745	-0.21657	1.01912
C	2.65223	0.72771	0.83354
H	2.90141	1.59199	1.43822
C	1.37379	0.63387	0.28742
C	-1.23512	-1.25756	-0.07698
N	-2.30925	-0.76228	0.51158
O	-2.73606	-1.55987	1.59977
O	-3.15332	-0.79610	-0.63028
H	-3.28990	-0.96359	2.12412
H	-0.87442	-2.23961	0.23810

TS [4'/5+(NOH)₂]
-742.1536390   ImgFreq/IR inten: -170.4202/2.0477

O	1.08385	1.81242	0.34357
C	-0.17588	2.15954	-0.08158
O	-0.59639	3.24504	0.19834
C	-0.90942	1.12950	-0.91333
H	-0.55001	1.24445	-1.94294
H	-1.96677	1.38901	-0.90416

C	-0.66429	-0.31765	-0.46616
H	-1.04241	-1.01040	-1.22145
C	0.82533	-0.53069	-0.28391
C	1.44458	-1.77027	-0.46670
H	0.83615	-2.62441	-0.74655
C	2.81670	-1.91752	-0.28867
H	3.28078	-2.88659	-0.43603
C	3.59062	-0.81571	0.07911
H	4.66115	-0.92224	0.21827
C	2.99401	0.42603	0.27017
H	3.57031	1.29720	0.55978
C	1.61966	0.55426	0.09234
C	-1.36548	-0.66617	0.84794
N	-3.48198	-0.48570	0.45796
O	-3.73104	-0.88929	-0.71862
O	-1.71667	-1.81003	1.13080
H	-4.43835	-1.58056	-0.72399
H	-1.34998	0.12041	1.62329

TS [4''/6.3]
-742.1545510   ImgFreq/IR inten: -593.5718/183.6230

O	0.30364	1.75450	0.50909
C	-0.89761	1.91598	-0.15770
O	-1.61976	2.80030	0.19533
C	-1.15424	0.99566	-1.33055
H	-0.74045	1.50099	-2.21137
H	-2.23288	0.92727	-1.47034
C	-0.53632	-0.39966	-1.20136
H	-0.51161	-0.86480	-2.19020
C	0.84523	-0.33445	-0.62288
C	1.81640	-1.31855	-0.85527
H	1.57349	-2.15160	-1.50872
C	3.07812	-1.23541	-0.28053
H	3.81709	-2.00447	-0.47702
C	3.39218	-0.15146	0.54576
H	4.37596	-0.07809	0.99697
C	2.45069	0.83963	0.78950
H	2.67024	1.69142	1.42272
C	1.18657	0.74147	0.20868
C	-1.43227	-1.36793	-0.34640
N	-1.31381	-0.87066	1.07574
O	-2.05089	-1.51019	1.89173
O	-2.72942	-1.35119	-0.55024
H	-2.55297	-2.21966	1.39935
H	-0.92324	-2.36543	-0.35427

TS [4''/6.1]w

-818.6381640	ImgFreq/IR inten: -1006.4768/581.8438		
O	-1.35245	1.57632	-0.65636
C	-0.37710	2.26192	0.03711
O	-0.06970	3.35149	-0.34798
C	0.16608	1.59510	1.28193
H	-0.49665	1.89725	2.10175
H	1.14882	2.01739	1.48599
C	0.22069	0.06232	1.22472
H	0.32745	-0.31266	2.24833
C	-1.04999	-0.48236	0.61801
C	-1.54687	-1.75654	0.91249
H	-1.01235	-2.37765	1.62626
C	-2.71235	-2.23230	0.31977
H	-3.08141	-3.22245	0.56412
C	-3.40602	-1.42419	-0.58271
H	-4.31757	-1.78331	-1.04858
C	-2.93674	-0.15101	-0.88460
H	-3.45848	0.49851	-1.57807
C	-1.76486	0.30796	-0.28601
C	1.46845	-0.46756	0.49673
N	1.53765	0.05668	-0.88240
O	2.22571	-0.62631	-1.68639
O	2.65138	0.11441	0.86665
H	2.97476	-1.34641	-1.16342
H	1.46552	-1.57184	0.50266
O	3.90433	-1.66855	-0.31508
H	4.80486	-1.54244	-0.63560
H	3.63958	-0.91207	0.36201

TS [2.2/4]b'

-916.6616805	ImgFreq/IR inten: -894.6979/67.2922		
O	-1.39132	1.65929	0.22523
C	-0.58332	1.33600	1.30198
O	0.26157	2.11850	1.62393
C	-0.89149	0.03203	2.00234
H	-1.70060	0.23197	2.71431
H	-0.00539	-0.27282	2.55367
C	-1.34823	-1.06949	1.04066
H	-1.73051	-1.92162	1.61397
C	-2.45500	-0.52816	0.14841
C	-3.50394	-1.30897	-0.34383
H	-3.55482	-2.35974	-0.07277
C	-4.48104	-0.75506	-1.16500
H	-5.29134	-1.37221	-1.53704
C	-4.41485	0.59842	-1.50126
H	-5.17341	1.03823	-2.13989

C	-3.38209	1.39371	-1.01675
H	-3.31220	2.44748	-1.26071
C	-2.40823	0.82430	-0.19976
C	-0.27782	-1.59275	0.12976
N	0.95670	-1.12822	0.13236
O	1.70625	-1.48920	-0.97925
O	1.31590	-1.75978	1.37704
H	2.49672	-0.85581	-0.95518
H	-0.56711	-2.29749	-0.65443
N	3.81118	0.22047	-0.71349
C	4.37740	-0.19610	0.57612
C	4.79005	0.08750	-1.79402
C	3.28229	1.58784	-0.64123
H	2.81066	1.85052	-1.59063
H	4.07609	2.32237	-0.43250
H	2.53089	1.65759	0.14590
H	4.32992	0.35948	-2.74649
H	5.12983	-0.94809	-1.86080
H	5.66967	0.73224	-1.63792
H	3.59887	-0.18525	1.34005
H	5.20434	0.45962	0.89061
H	4.75170	-1.21841	0.49771

TS [2.2/4]b''

-916.6623065   ImgFreq/IR inten: -623.7936/365.4912

O	3.04867	-0.12165	0.84069
C	2.85927	-1.44705	0.50974
O	3.57226	-2.26553	1.01503
C	1.74981	-1.73007	-0.47627
H	1.49152	-2.78241	-0.39193
H	2.14337	-1.55795	-1.48607
C	0.52870	-0.81799	-0.22394
H	0.15738	-1.02962	0.78474
C	1.02147	0.61393	-0.28419
C	0.32992	1.68271	-0.85998
H	-0.64539	1.50020	-1.29446
C	0.87070	2.96793	-0.88056
H	0.31562	3.78085	-1.33728
C	2.12515	3.20437	-0.32071
H	2.55234	4.20157	-0.33171
C	2.84135	2.15326	0.24421
H	3.82476	2.30058	0.67601
C	2.28776	0.87731	0.24854
C	-0.61126	-1.11825	-1.17882
N	-1.16692	-2.31671	-1.32756
O	-0.90302	-3.12603	-0.21193
O	-2.09936	-0.60157	-0.46276

H	-1.46457	-3.89596	-0.35935
H	-0.60052	-0.58036	-2.12286
N	-3.10331	0.55232	0.54768
C	-3.53325	1.65652	-0.30560
C	-4.19966	-0.34201	0.91284
C	-2.30456	0.97107	1.69661
H	-3.79019	-1.20840	1.42905
H	-4.69667	-0.68256	0.00649
H	-4.92422	0.16902	1.56295
H	-2.67232	2.26555	-0.57624
H	-4.26740	2.29259	0.20937
H	-3.97868	1.24970	-1.21215
H	-1.94442	0.08456	2.21703
H	-2.90052	1.57949	2.39126
H	-1.44933	1.55180	1.35488

TS [4b/4·:bH⁺]

-916.7322648 ImgFreq/IR inten: -860.8006/6016.3728

O	1.18397	-1.31140	1.06682
C	0.48519	-0.46830	1.90035
O	-0.38370	-0.94334	2.57896
C	0.92689	0.97629	1.91939
H	1.76840	1.04148	2.61989
H	0.10841	1.57028	2.32217
C	1.36394	1.49871	0.54272
H	1.86747	2.46192	0.68166
C	2.31601	0.51387	-0.08774
C	3.32760	0.88299	-0.97867
H	3.45423	1.93407	-1.22262
C	4.17105	-0.06726	-1.54867
H	4.94994	0.24188	-2.23750
C	4.01350	-1.41482	-1.22394
H	4.66856	-2.16256	-1.65861
C	3.01691	-1.80651	-0.33541
H	2.87400	-2.84625	-0.06343
C	2.17926	-0.84229	0.21775
C	0.15395	1.79229	-0.36791
N	-0.86590	0.77344	-0.33508
O	-1.48392	0.61103	-1.46171
O	-0.87687	2.49441	0.19068
H	-2.50880	0.03355	-1.10169
H	0.45349	2.09137	-1.38114
N	-3.54199	-0.51826	-0.59118
C	-3.09648	-1.72614	0.14128
C	-4.14013	0.47872	0.32619
C	-4.45959	-0.85845	-1.69557
H	-4.71686	0.04746	-2.24546

H	-5.37709	-1.32072	-1.31610
H	-3.96593	-1.55284	-2.37636
H	-4.38601	1.38013	-0.23529
H	-3.41229	0.73873	1.09224
H	-5.04718	0.07921	0.79227
H	-2.59300	-2.40031	-0.55248
H	-3.95287	-2.24348	0.58735
H	-2.39374	-1.44051	0.92242

TS [4·:bH⁺/6.1]b

-916.7603690   ImgFreq/IR inten: -820.5050/5432.8938

O	1.18397	-1.31140	1.06682
C	0.48519	-0.46830	1.90035
O	-0.38370	-0.94334	2.57896
C	0.92689	0.97629	1.91939
H	1.76840	1.04148	2.61989
H	0.10841	1.57028	2.32217
C	1.36394	1.49871	0.54272
H	1.86747	2.46192	0.68166
C	2.31601	0.51387	-0.08774
C	3.32760	0.88299	-0.97867
H	3.45423	1.93407	-1.22262
C	4.17105	-0.06726	-1.54867
H	4.94994	0.24188	-2.23750
C	4.01350	-1.41482	-1.22394
H	4.66856	-2.16256	-1.65861
C	3.01691	-1.80651	-0.33541
H	2.87400	-2.84625	-0.06343
C	2.17926	-0.84229	0.21775
C	0.15395	1.79229	-0.36791
N	-0.86590	0.77344	-0.33508
O	-1.48392	0.61103	-1.46171
O	-0.87687	2.49441	0.19068
H	-2.50880	0.03355	-1.10169
H	0.45349	2.09137	-1.38114
N	-3.54199	-0.51826	-0.59118
C	-3.09648	-1.72614	0.14128
C	-4.14013	0.47872	0.32619
C	-4.45959	-0.85845	-1.69557
H	-4.71686	0.04746	-2.24546
H	-5.37709	-1.32072	-1.31610
H	-3.96593	-1.55284	-2.37636
H	-4.38601	1.38013	-0.23529
H	-3.41229	0.73873	1.09224
H	-5.04718	0.07921	0.79227
H	-2.59300	-2.40031	-0.55248
H	-3.95287	-2.24348	0.58735

H		-2.39374	-1.44051	0.92242

TS [4·:bH⁺/6.2]⁻:bH⁺

-916.6279092   ImgFreq/IR inten: -1485.9711/2006.5186

O	-2.06978	1.48418	-0.89267
C	-1.23231	2.16121	-0.03979
O	-0.70629	3.16397	-0.43594
C	-1.11213	1.60333	1.35923
H	-1.97168	1.99022	1.92203
H	-0.21063	2.02012	1.80398
C	-1.11754	0.06377	1.42054
H	-1.28352	-0.23042	2.46290
C	-2.26313	-0.45205	0.58093
C	-2.91958	-1.65727	0.84237
H	-2.59673	-2.25157	1.69187
C	-3.96236	-2.10272	0.03465
H	-4.45815	-3.04199	0.25659
C	-4.36593	-1.33545	-1.05885
H	-5.17916	-1.67198	-1.69370
C	-3.72652	-0.13256	-1.33981
H	-4.01647	0.48262	-2.18420
C	-2.68204	0.29329	-0.52274
C	0.18024	-0.62093	0.99140
N	0.88129	-0.06545	-0.14484
O	1.54764	-1.27662	-0.56881
O	1.38821	0.17782	1.25110
H	3.00039	-0.84830	-0.45486
H	0.93403	-1.77729	0.29112
N	4.00473	-0.42730	-0.36907
C	3.87091	1.04087	-0.59720
C	4.48007	-0.72618	1.00928
C	4.84054	-1.07735	-1.40995
H	4.85349	-2.15279	-1.23694
H	5.85839	-0.68554	-1.37204
H	4.40447	-0.87914	-2.38789
H	4.53574	-1.80675	1.13692
H	3.75274	-0.32050	1.70897
H	5.46553	-0.28348	1.16547
H	3.44333	1.20591	-1.58449
H	4.85345	1.51157	-0.52834
H	3.19319	1.44592	0.15012

TS [6.1/6.2]

-742.1181135   ImgFreq/IR inten: -2359.5993/442.3123

O	0.42755	1.76403	0.60656
C	-0.77569	2.01984	-0.00956
O	-1.45177	2.91531	0.40569

C	-1.10618	1.16702	-1.21536
H	-0.60007	1.62863	-2.07209
H	-2.17804	1.23782	-1.39116
C	-0.64165	-0.29912	-1.09019
H	-0.68648	-0.74526	-2.08917
C	0.78676	-0.32640	-0.59663
C	1.68196	-1.35222	-0.91545
H	1.34213	-2.16759	-1.54767
C	2.98797	-1.34213	-0.43818
H	3.66759	-2.14678	-0.69691
C	3.41908	-0.28950	0.37254
H	4.43608	-0.27239	0.74970
C	2.54907	0.74359	0.69840
H	2.85746	1.57206	1.32557
C	1.24276	0.71587	0.21341
C	-1.55008	-1.15656	-0.21619
O	-2.92581	-0.97337	-0.54957
N	-1.38468	-0.99295	1.18149
O	-1.75613	-2.09627	1.67493
H	-3.28654	-1.77623	-0.93747
H	-1.77404	-2.53961	0.47121

TS [6.2/6.3]

-742.2090475   ImgFreq/IR inten: -1884.4039/398.1168

O	-0.12819	-1.83583	0.25735
C	1.05676	-1.79696	-0.43943
O	1.81981	-2.70914	-0.32106
C	1.25744	-0.63030	-1.38393
H	0.86249	-0.95891	-2.35248
H	2.33145	-0.49941	-1.51264
C	0.54203	0.68189	-1.00741
H	0.44453	1.28860	-1.91017
C	-0.84493	0.38349	-0.46810
C	-1.88549	1.31441	-0.53609
H	-1.69463	2.28342	-0.98678
C	-3.14571	1.01614	-0.02870
H	-3.94169	1.75011	-0.08861
C	-3.37914	-0.23100	0.55333
H	-4.35974	-0.47426	0.94830
C	-2.35802	-1.17145	0.62617
H	-2.51389	-2.14879	1.06833
C	-1.09904	-0.85574	0.11969
C	1.29765	1.55358	-0.03733
O	1.40832	2.83195	-0.17108
N	1.92257	1.26709	1.07929
O	2.24011	-0.05191	1.43425
H	2.12097	2.58602	0.95222

H	1.92282	-0.16138	2.34187

TS [6.1/6.2]w

-818.6277658   ImgFreq/IR inten: -1607.8191/738.1699

O	-0.17672	-1.92095	0.65956
C	1.00489	-2.10932	-0.01706
O	1.77664	-2.93073	0.38556
C	1.19975	-1.25564	-1.25135
H	0.63631	-1.72099	-2.06874
H	2.25402	-1.27360	-1.51368
C	0.67100	0.18514	-1.05687
H	0.70638	0.68574	-2.02832
C	-0.76489	0.07350	-0.60191
C	-1.78192	0.92900	-1.03225
H	-1.53290	1.75804	-1.68687
C	-3.09855	0.74325	-0.62041
H	-3.87316	1.42251	-0.95972
C	-3.41726	-0.32270	0.22193
H	-4.44058	-0.47390	0.54874
C	-2.42632	-1.20719	0.63429
H	-2.64703	-2.05172	1.27676
C	-1.11675	-1.00596	0.21205
C	1.65049	0.95176	-0.12461
O	2.93870	0.85745	-0.64084
N	1.60611	1.05087	1.21370
O	0.46352	1.28364	1.77341
H	3.55795	1.00147	0.09110
H	1.03227	2.32781	-0.18048
H	-0.08834	2.40681	0.92537
O	0.13864	3.05983	0.12535
H	0.50355	3.87696	0.49282

TS [6.2/6.3]w

-818.7069622   ImgFreq/IR inten: -1711.7737/149.2402

O	-1.55031	1.58862	-0.32618
C	-0.51589	2.25439	0.28275
O	-0.34387	3.40888	0.02013
C	0.25164	1.49666	1.34413
H	-0.30897	1.64930	2.27439
H	1.21065	1.99747	1.47452
C	0.40406	-0.02295	1.12946
H	0.54826	-0.48052	2.11007
C	-0.85634	-0.59849	0.51629
C	-1.16147	-1.96026	0.61622
H	-0.46608	-2.61585	1.13214
C	-2.32992	-2.47907	0.06933
H	-2.54662	-3.53804	0.15732
C	-3.22241	-1.62796	-0.58512

H	-4.14011	-2.02014	-1.01051
C	-2.94129	-0.27120	-0.69173
H	-3.61711	0.41245	-1.19287
C	-1.76157	0.23248	-0.14499
C	1.66267	-0.43662	0.37246
O	2.50533	-1.18167	1.00490
N	1.94228	-0.09643	-0.86479
O	1.08016	0.84969	-1.44761
H	3.47864	-1.33604	0.22825
H	0.78689	0.45506	-2.28042
H	3.16646	-0.51171	-1.16774
O	4.08394	-1.18486	-0.80379
H	4.91311	-0.70410	-0.70410

TS [6.2/7]⁺w

-819.0805505   ImgFreq/IR inten: -164.8451/83.6549

O	-0.54915	-1.09261	0.13240
C	-1.24055	-0.12272	0.77942
O	-2.48773	-0.42659	1.00717
C	-0.47822	0.64732	1.83680
H	-0.09265	-0.04521	2.58759
H	-1.14299	1.36581	2.31375
C	0.65632	1.30580	1.03219
H	1.23802	2.04202	1.58430
C	1.51139	0.18696	0.45112
C	2.89674	0.25362	0.30298
H	3.42661	1.14291	0.62819
C	3.59618	-0.81662	-0.24855
H	4.67369	-0.76099	-0.35004
C	2.91208	-1.95868	-0.66600
H	3.45651	-2.79180	-1.09544
C	1.52806	-2.04165	-0.53388
H	0.97993	-2.92094	-0.85134
C	0.84932	-0.96883	0.02257
C	-0.05796	1.90068	-0.15266
O	0.49542	2.80552	-0.91622
N	-1.19049	1.30788	-0.35300
O	-1.76824	1.49263	-1.59681
H	-0.04448	2.98320	-1.70746
H	-2.72628	1.53329	-1.44991
O	-3.66463	-2.21265	-0.52750
H	-2.84883	-1.14925	0.41683
H	-3.25017	-2.94789	-0.99255
H	-4.58148	-2.45189	-0.34904

TS [7/8]⁺w

-819.0097791	ImgFreq/IR inten: -1840.9797/1056.4662			
O		-0.52154	1.39577	-0.71800
C		0.65838	1.67540	0.34352
O		0.95958	2.81888	-0.14980
C		0.09893	1.29243	1.69782
H		-0.83302	1.80879	1.91870
H		0.83403	1.51569	2.47333
C		-0.07923	-0.22991	1.46393
H		-0.13298	-0.83102	2.37007
C		-1.30317	-0.44144	0.57109
C		-2.24073	-1.45062	0.78941
H		-2.08869	-2.15675	1.59918
C		-3.37769	-1.54176	-0.01169
H		-4.10456	-2.32357	0.17463
C		-3.58543	-0.62694	-1.04275
H		-4.47252	-0.69772	-1.66160
C		-2.65686	0.38362	-1.29437
H		-2.79600	1.09188	-2.10289
C		-1.53877	0.45311	-0.48394
C		1.17662	-0.56177	0.66673
O		1.64525	-1.74037	0.54088
N		1.61161	0.54699	0.11159
O		2.54083	0.59816	-0.89119
H		2.45033	-1.87402	-0.07498
H		2.69841	1.55530	-1.02112
H		-0.18799	2.53398	-0.87487
O		3.66270	-2.24535	-0.93414
H		4.07266	-1.66461	-1.58366
H		4.07208	-3.11634	-0.97852

TS [7/8]⁺2w

-819.0457766	ImgFreq/IR inten: -392.6944/79.8358			
O		0.36530	1.16578	-0.10171
C		1.56486	0.18478	0.59102
O		2.63578	0.81430	0.57014
C		0.82979	-0.43639	1.77256
H		0.38480	0.31984	2.41605
H		1.53924	-1.03252	2.35050
C		-0.22730	-1.31856	1.06351
H		-0.61779	-2.13372	1.67122
C		-1.32993	-0.44444	0.48424
C		-2.67339	-0.82390	0.47852
H		-2.96074	-1.77592	0.91352
C		-3.64112	0.01334	-0.06676
H		-4.68327	-0.28314	-0.05600

C	-3.26291	1.23432	-0.62582
H	-4.01185	1.88910	-1.05707
C	-1.92664	1.62462	-0.64112
H	-1.63084	2.56685	-1.09045
C	-0.96386	0.78695	-0.08353
C	0.55259	-1.83613	-0.12316
O	0.22547	-2.89280	-0.80726
N	1.51991	-1.01459	-0.38205
O	2.26922	-1.07937	-1.51738
H	0.77776	-3.02099	-1.59910
H	3.09376	-0.60279	-1.29803
H	2.50841	2.40621	0.12971
H	0.97212	2.41909	-0.25917
O	1.84158	3.06489	-0.24887
H	1.75771	3.86004	0.29705

TS [8⁺2w/8:H₃O⁺]

TS [8$^+$2w/8:H$_3$O$^+$]

-819.0948271   ImgFreq/IR inten: -565.7872/3670.1894

O	-0.58889	-0.26831	1.67487
C	1.74675	-1.76937	-0.06437
O	2.57743	-2.50008	0.39216
C	0.37404	-1.97313	-0.64597
H	-0.25903	-2.44515	0.10617
H	0.43487	-2.65413	-1.49722
C	-0.13575	-0.55352	-1.04088
H	-0.16889	-0.46308	-2.13145
C	-1.49526	-0.16365	-0.49862
C	-2.57603	0.06144	-1.35249
H	-2.43303	-0.01821	-2.42587
C	-3.83302	0.38226	-0.84624
H	-4.66327	0.55052	-1.52184
C	-4.01342	0.48437	0.53098
H	-4.98776	0.73255	0.93673
C	-2.94541	0.27031	1.39999
H	-3.08738	0.35302	2.47408
C	-1.69463	-0.05023	0.88299
C	0.97830	0.37561	-0.59009
O	0.96132	1.62113	-0.67983
N	1.98944	-0.36407	-0.12788
O	3.15433	0.17124	0.36554
H	1.94193	2.34136	-0.25947
H	3.65266	-0.60919	0.68697
H	-0.81049	-0.18153	2.61029
O	2.82185	2.99373	0.14086
H	3.65066	2.52692	0.30803
H	2.96195	3.88924	-0.19189

Ethyl ester of 3-coumarin-carboxylic acid

TS [2.1/2.2]

-1009.3959879   ImgFreq/IR inten: -2165.4786/564.3904

O	-0.42107	0.59259	1.76819
C	-0.15167	-0.72609	1.50586
O	-0.18152	-1.51689	2.40225
C	0.18679	-1.06641	0.06061
H	0.68866	-2.03723	0.08643
C	-1.05275	-1.26946	-0.82409
C	1.11172	0.00610	-0.56112
H	1.19314	-0.21324	-1.63147
C	0.45371	1.35424	-0.36938
C	0.55575	2.39653	-1.29308
H	1.12367	2.23938	-2.20539
C	-0.06778	3.61979	-1.06222
H	0.01930	4.41859	-1.79051
C	-0.81033	3.80958	0.10423
H	-1.30043	4.75932	0.29018
C	-0.93173	2.78143	1.03337
H	-1.50358	2.90221	1.94621
C	-0.29774	1.56726	0.78713
C	2.48885	0.00142	0.07696
O	3.32780	-1.87752	-1.15614
N	3.35353	-1.08627	-0.25725
O	4.21098	-1.16000	0.74978
H	3.05898	0.92106	-0.06310
H	3.37219	-0.36356	1.23960
O	-0.98673	-1.39563	-2.02068
O	-2.18164	-1.31384	-0.11122
C	-3.41651	-1.54908	-0.84518
C	-4.54999	-1.54834	0.15652
H	-3.32322	-2.50293	-1.36792
H	-3.52159	-0.76276	-1.59515
H	-4.41663	-2.33194	0.90521
H	-5.49616	-1.72808	-0.36108
H	-4.62159	-0.58845	0.67244

TS [2.1/2.2]w

-1085.8869486   ImgFreq/IR inten: -1383.0074/101.7790

O	-0.42203	0.58579	1.70505
C	-0.23935	-0.73614	1.36795
O	-0.17390	-1.54862	2.24295
C	-0.09689	-1.03163	-0.11674
H	0.37003	-2.01608	-0.19412
C	-1.44409	-1.15364	-0.84257
C	0.79053	0.03159	-0.80485
H	0.74433	-0.16170	-1.88107

C	0.19344	1.38862	-0.50412
C	0.20452	2.45348	-1.40686
H	0.65211	2.30921	-2.38565
C	-0.35879	3.68214	-1.07074
H	-0.34450	4.49817	-1.78500
C	-0.95014	3.85501	0.18148
H	-1.39467	4.80804	0.44795
C	-0.97946	2.80446	1.09375
H	-1.43472	2.91098	2.07180
C	-0.40702	1.58635	0.74029
C	2.23181	-0.01107	-0.32654
O	2.56637	-1.99594	-1.44658
N	3.01750	-1.06761	-0.79276
O	4.26854	-1.08684	-0.41006
H	2.78517	0.92174	-0.40496
H	2.75985	-0.17251	1.22208
O	-1.55177	-1.13969	-2.04221
O	-2.46228	-1.30882	0.01223
C	-3.78355	-1.49508	-0.56648
C	-4.76244	-1.66286	0.57484
H	-3.74946	-2.37109	-1.21710
H	-4.01080	-0.62514	-1.18588
H	-5.76961	-1.81028	0.17552
H	-4.77696	-0.77963	1.21713
H	-4.50850	-2.52958	1.18858
H	4.19916	-0.73043	0.92429
O	3.64422	-0.43116	1.83634
H	4.01142	0.35637	2.25743

TS [2.2⁺2w/3.1⁺]

-1086.2166867	ImgFreq/IR inten: -1423.7935/1170.4711		
O	-1.02935	-1.47900	1.70118
C	0.21885	-0.95961	1.81259
O	0.90205	-1.24335	2.74835
C	0.70014	0.04697	0.76247
C	1.94231	-0.39556	-0.01995
H	1.09104	0.85976	1.38479
C	-0.36576	0.61524	-0.23255
H	0.07365	0.69310	-1.22961
C	-1.60530	-0.24874	-0.32985
C	-2.49642	-0.11929	-1.40615
H	-2.28795	0.60590	-2.18642
C	-3.62453	-0.92500	-1.50121
H	-4.29902	-0.81416	-2.34235
C	-3.87062	-1.89069	-0.52266
H	-4.74498	-2.52765	-0.59257

C	-2.98516	-2.05524	0.53455
H	-3.13941	-2.81087	1.29575
C	-1.86137	-1.23765	0.61817
C	-0.66486	2.03199	0.21703
N	0.39426	3.08719	-0.03732
O	1.30890	2.81340	-1.02466
O	1.00880	3.38051	1.19393
H	-0.98753	2.13078	1.25158
H	1.86542	2.01421	-0.78551
O	-1.62608	2.76447	-0.66048
H	-2.52392	2.88809	-0.30867
H	-0.82157	3.61732	-0.61217
H	1.47856	4.22095	1.05697
O	2.56443	0.43805	-0.66264
O	2.22417	-1.66438	0.07067
C	3.43700	-2.18262	-0.59839
H	3.74320	-2.99760	0.05396
H	4.18761	-1.39446	-0.58117
C	3.11447	-2.65235	-2.00030
H	4.00909	-3.10345	-2.43736
H	2.81210	-1.82467	-2.64487
H	2.32806	-3.40965	-1.99442

TS [2.2⁺w/3.2⁺]

-1086.2448778   ImgFreq/IR inten: -820.6690/2136.9112

O	-0.42009	0.16650	1.78406
C	0.29870	-0.78281	1.26769
O	1.22023	-1.29170	1.96435
C	0.23783	-1.02623	-0.20531
C	-1.14990	-1.37231	-0.78435
H	0.87581	-1.87135	-0.45885
C	0.80635	0.29667	-0.76530
H	0.87067	0.22345	-1.85134
C	-0.18939	1.36460	-0.33448
C	-0.55722	2.45995	-1.11339
H	-0.08661	2.60701	-2.07967
C	-1.54213	3.34529	-0.67210
H	-1.81845	4.18982	-1.29266
C	-2.18166	3.14134	0.54897
H	-2.94966	3.82837	0.88455
C	-1.83747	2.05283	1.35122
H	-2.30558	1.87764	2.31252
C	-0.85714	1.19843	0.88760
C	2.23713	0.57909	-0.20331
N	2.94768	-0.70762	0.19969
O	4.20356	-0.40195	0.70880
O	3.09161	-1.48013	-0.98094

H	2.17772	1.11030	0.75055
H	4.66897	0.08910	0.00179
O	3.02739	1.27073	-1.11542
H	3.25521	2.14954	-0.78879
H	2.11500	-1.30005	1.26417
H	3.53137	-2.29950	-0.69783
O	-1.43624	-1.15388	-1.92789
O	-1.88127	-2.00299	0.12858
C	-3.19588	-2.53146	-0.28308
H	-3.34545	-3.37303	0.39062
H	-3.10117	-2.89457	-1.30557
C	-4.27913	-1.48325	-0.14230
H	-5.24406	-1.93431	-0.38819
H	-4.12075	-0.64615	-0.82433
H	-4.33891	-1.10828	0.88170

TS [3.1+/3.2+]

-1086.2410391   ImgFreq/IR inten:
                       -1144.7969/2716.0642

O	-0.75858	0.20111	1.85642
C	-0.13567	-0.88543	1.48553
O	0.54777	-1.51476	2.31787
C	-0.00186	-1.17710	0.01752
C	-1.31743	-1.30236	-0.77931
H	0.50326	-2.13655	-0.10214
C	0.86583	-0.00483	-0.48378
H	0.99958	-0.12225	-1.55883
C	0.06858	1.25801	-0.18529
C	0.07398	2.38302	-1.00904
H	0.72153	2.40149	-1.87927
C	-0.75993	3.46665	-0.73522
H	-0.74414	4.33256	-1.38674
C	-1.62186	3.43395	0.35964
H	-2.27405	4.27458	0.56605
C	-1.65101	2.32187	1.20043
H	-2.29821	2.27617	2.06818
C	-0.80835	1.26642	0.90762
C	2.27032	-0.01313	0.18969
N	3.32132	0.19854	-0.75012
O	3.31078	-0.72795	-1.79633
O	4.52494	0.06146	-0.01394
H	2.37477	0.73925	0.96842
H	3.53697	-1.60510	-1.43245
H	5.15648	0.66931	-0.42699
O	2.50974	-1.36178	0.90911
H	3.38726	-1.32814	1.32795
H	1.62903	-1.63744	1.68815

O	-1.37527	-1.07759	-1.95633
O	-2.28336	-1.76342	0.00594
C	-3.59102	-2.06162	-0.60815
H	-3.99125	-2.84618	0.03117
H	-3.40605	-2.46081	-1.60449
C	-4.47604	-0.83360	-0.63448
H	-5.45664	-1.11006	-1.03071
H	-4.06480	-0.05498	-1.27927
H	-4.62430	-0.42927	0.36912

TS [2.2/4']

-1009.3845499   ImgFreq/IR inten: -774.9873/21.7264

O	-1.18943	-2.29431	-0.24983
C	0.09088	-2.11347	0.17343
O	0.87363	-3.01367	0.09284
C	0.41016	-0.75205	0.79101
H	0.00767	-0.77917	1.80995
C	1.92320	-0.58410	0.93097
C	-0.28183	0.40602	0.01047
H	0.18228	0.51059	-0.97222
C	-1.76164	0.07290	-0.12385
C	-2.76576	1.04570	-0.17483
H	-2.48585	2.09361	-0.10717
C	-4.10030	0.67321	-0.31347
H	-4.86833	1.43762	-0.35264
C	-4.44552	-0.67493	-0.40310
H	-5.48433	-0.96783	-0.51095
C	-3.45814	-1.65437	-0.36112
H	-3.69469	-2.70912	-0.44005
C	-2.13008	-1.26904	-0.22331
C	-0.10399	1.67134	0.78109
N	0.46270	2.79085	0.35313
O	1.00197	2.69072	-0.95071
O	-0.73573	3.56609	0.44742
H	1.50628	3.51102	-1.04834
H	-0.43303	1.72062	1.81217
O	2.49016	-0.54793	1.99335
O	2.50540	-0.46075	-0.26304
C	3.95482	-0.33885	-0.27780
H	4.37120	-1.21424	0.22378
H	4.22870	0.54564	0.30077
C	4.39039	-0.24166	-1.72307
H	5.47862	-0.14855	-1.77252
H	3.95149	0.63161	-2.21071
H	4.09991	-1.13311	-2.28286

TS [2.2/4'']

-1009.3866489	ImgFreq/IR inten: -897.0411/42.6806		
O	0.12374	0.46193	1.71061
C	-0.32071	-0.77258	1.27250
O	-0.67531	-1.57055	2.08358
C	-0.31564	-0.99247	-0.23453
H	-0.24140	-2.07485	-0.37962
C	-1.61565	-0.53837	-0.91319
C	0.87775	-0.32134	-0.92439
H	0.70271	-0.33872	-2.00576
C	0.99118	1.12512	-0.46264
C	1.46726	2.15706	-1.27570
H	1.76770	1.93378	-2.29515
C	1.54118	3.46108	-0.79827
H	1.90743	4.25378	-1.44098
C	1.13175	3.74444	0.50661
H	1.18457	4.75973	0.88477
C	0.64722	2.73255	1.32759
H	0.31885	2.92870	2.34170
C	0.58539	1.42954	0.83885
C	2.20301	-0.95754	-0.66948
N	2.36864	-2.00054	0.12613
O	3.73346	-2.23184	0.41881
O	1.76925	-2.95827	-0.73874
H	3.71173	-2.77134	1.22229
H	3.09054	-0.47134	-1.08102
O	-1.68449	-0.26350	-2.08595
O	-2.64529	-0.52909	-0.06620
C	-3.95142	-0.19790	-0.61650
H	-4.16938	-0.90278	-1.42102
H	-3.89491	0.80230	-1.05066
C	-4.95465	-0.28264	0.51255
H	-5.95221	-0.04215	0.13502
H	-4.71324	0.42263	1.31065
H	-4.98386	-1.28707	0.93955

TS [6.1/6.2]

-1009.3803317	ImgFreq/IR inten: -2358.3760/451.6270		
O	-0.06854	0.43936	1.68772
C	-0.41342	-0.85204	1.38164
O	-0.74195	-1.59036	2.26275
C	-0.34948	-1.24175	-0.08829
C	-1.64319	-0.92246	-0.84874
H	-0.24827	-2.32896	-0.11370
C	0.85550	-0.60347	-0.82359
H	0.67244	-0.74156	-1.89308
C	0.90334	0.87263	-0.50323

C	1.40390	1.82778	-1.39334
H	1.77491	1.50101	-2.36017
C	1.42830	3.17725	-1.05907
H	1.82015	3.90380	-1.76250
C	0.94224	3.59163	0.18325
H	0.95737	4.64257	0.45191
C	0.43343	2.66130	1.08115
H	0.05082	2.95494	2.05178
C	0.41960	1.31301	0.73057
C	2.18141	-1.29023	-0.52479
O	2.06858	-2.71079	-0.56152
N	2.81917	-0.90929	0.68186
O	4.04887	-1.10431	0.46230
H	2.50184	-3.05935	-1.34674
H	3.71933	-1.28859	-0.76648
O	-1.75442	-1.08336	-2.03937
O	-2.61220	-0.47145	-0.04795
C	-3.89610	-0.17664	-0.66501
H	-4.26538	-1.09117	-1.13315
H	-3.73486	0.56314	-1.45156
C	-4.81934	0.32731	0.42239
H	-5.79940	0.55538	-0.00542
H	-4.42855	1.23747	0.88231
H	-4.95435	-0.42234	1.20475

TS [6.2/6.3]

-1009.4706740   ImgFreq/IR inten: -1882.8793/388.3928

O	-0.04427	0.29626	1.74619
C	-0.30341	-0.95570	1.26302
O	-0.56556	-1.83733	2.03035
C	-0.19444	-1.12764	-0.24575
C	-1.45031	-0.67914	-1.00602
H	-0.10378	-2.20011	-0.41966
C	1.03357	-0.38098	-0.80309
H	0.96782	-0.40479	-1.89573
C	0.96566	1.06020	-0.33394
C	1.42352	2.13817	-1.09241
H	1.87598	1.94810	-2.05977
C	1.31141	3.44036	-0.61587
H	1.67420	4.26814	-1.21507
C	0.73250	3.67708	0.63193
H	0.64234	4.69059	1.00799
C	0.26630	2.61619	1.40105
H	-0.18339	2.77059	2.37508
C	0.39039	1.32084	0.90956
C	2.36007	-1.00300	-0.44631
O	3.48247	-0.39776	-0.63062

N	2.68478	-2.16747	0.07744
O	1.80882	-3.26024	0.14928
H	3.87375	-1.59225	-0.16488
H	1.77208	-3.50534	1.08586
O	-1.46999	-0.52266	-2.20107
O	-2.50183	-0.53356	-0.19688
C	-3.76878	-0.17358	-0.81783
H	-4.03172	-0.95854	-1.52956
H	-3.62290	0.75311	-1.37582
C	-4.79252	-0.02979	0.28651
H	-5.76159	0.23513	-0.14486
H	-4.50724	0.75510	0.99011
H	-4.90972	-0.96312	0.84102

TS [6.1/6.2]w

-1085.8894675   ImgFreq/IR inten: -1591.9468/751.6748

O	-0.27101	0.20815	1.78077
C	-0.69254	-1.01883	1.33899
O	-1.09611	-1.81964	2.13022
C	-0.57786	-1.26624	-0.15893
C	-1.77683	-0.74951	-0.96300
H	-0.56897	-2.34902	-0.29058
C	0.73258	-0.66302	-0.73172
H	0.67039	-0.75294	-1.81816
C	0.75444	0.79592	-0.34169
C	1.18873	1.81571	-1.19175
H	1.57814	1.55669	-2.17061
C	1.13698	3.14865	-0.79519
H	1.48479	3.92662	-1.46624
C	0.62748	3.48006	0.46122
H	0.58565	4.51698	0.77744
C	0.15411	2.48370	1.30822
H	-0.26008	2.71248	2.28330
C	0.21331	1.15777	0.89392
C	1.92376	-1.53849	-0.25601
O	1.66393	-2.87166	-0.55637
N	2.68769	-1.36692	0.83592
O	3.09798	-0.17379	1.11440
H	2.20499	-3.41614	0.03587
H	3.02713	-0.89176	-1.06058
H	3.58101	0.33022	-0.23184
O	3.74171	0.04715	-1.23589
H	4.65591	-0.25590	-1.32731
O	-1.78679	-0.70227	-2.16793
O	-2.79972	-0.39882	-0.17791
C	-4.01476	0.04980	-0.83973
H	-4.35050	-0.74484	-1.50887

H		-3.76905	0.92166	-1.44926
C		-5.03065	0.36457	0.23620
H		-5.96236	0.70125	-0.22660
H		-4.67380	1.15651	0.89815
H		-5.24955	-0.51692	0.84233

TS [6.2/6.3]w
-1085.9655039   ImgFreq/IR inten: -1717.4712/137.0958

O		-0.61659	0.68170	1.74190
C		-0.51235	-0.67707	1.60938
O		-0.65734	-1.37194	2.57035
C		-0.28650	-1.20553	0.19804
C		-1.62110	-1.39657	-0.55656
H		0.11610	-2.21489	0.31667
C		0.65933	-0.34555	-0.67394
H		0.42496	-0.59128	-1.71061
C		0.37587	1.12462	-0.44512
C		0.71167	2.08984	-1.40047
H		1.20738	1.77242	-2.31300
C		0.41769	3.43411	-1.19964
H		0.68772	4.16639	-1.95261
C		-0.23425	3.83168	-0.03072
H		-0.47426	4.87695	0.13291
C		-0.58295	2.88881	0.92886
H		-1.08883	3.16941	1.84571
C		-0.27246	1.54641	0.71688
C		2.13871	-0.70278	-0.55949
O		2.70051	-1.18898	-1.61302
N		2.87538	-0.54246	0.51659
O		2.18091	-0.18466	1.68508
H		3.87443	-1.47578	-1.27767
H		2.62463	0.60684	2.01981
H		4.07106	-1.07996	0.31145
O		4.80309	-1.54519	-0.51103
H		5.09003	-2.44579	-0.32377
O		-1.67276	-1.65085	-1.73354
O		-2.67672	-1.28244	0.25166
C		-3.99762	-1.49826	-0.32309
H		-4.59398	-1.83495	0.52424
H		-3.92642	-2.30044	-1.05766
C		-4.55031	-0.22274	-0.93120
H		-5.57140	-0.39859	-1.28205
H		-3.95231	0.10148	-1.78457
H		-4.58002	0.58254	-0.19378

TS [6.2/7]$^+$w
-1086.3392486   ImgFreq/IR inten: -156.1182/85.2664

O		-0.03895	0.61962	1.01697

C	0.08204	1.21589	-0.19435
O	0.78255	2.31514	-0.17355
C	0.22495	0.28862	-1.38262
C	1.44070	-0.66226	-1.36529
H	0.35559	0.87696	-2.28955
C	-1.09055	-0.50942	-1.35670
H	-1.26239	-1.13239	-2.23281
C	-1.12028	-1.29639	-0.05272
C	-1.66032	-2.57548	0.08031
H	-2.07992	-3.07127	-0.78891
C	-1.65224	-3.21604	1.31659
H	-2.06406	-4.21417	1.40893
C	-1.11225	-2.57594	2.43256
H	-1.10598	-3.07444	3.39499
C	-0.57520	-1.29562	2.32226
H	-0.15042	-0.78329	3.17743
C	-0.58685	-0.67592	1.08233
C	-2.14059	0.55690	-1.18791
O	-3.40562	0.33137	-1.42602
N	-1.62990	1.62893	-0.67406
O	-2.52376	2.53486	-0.13073
H	-3.96109	1.07937	-1.14114
H	-2.16699	3.41722	-0.31875
O	0.98496	3.65438	2.08389
H	0.85549	2.73868	0.73009
H	0.94332	3.30070	2.97929
H	1.51759	4.45788	2.10538
O	1.44703	-1.66450	-2.03015
O	2.43361	-0.20890	-0.61217
C	3.67240	-0.99818	-0.60942
H	4.01838	-1.07314	-1.64100
H	3.42650	-2.00099	-0.25767
C	4.66298	-0.29212	0.28629
H	5.59822	-0.85693	0.30584
H	4.29326	-0.21935	1.31138
H	4.88454	0.71269	-0.07898

TS [7/8]⁺w

-1086.2689347   ImgFreq/IR inten: -1839.7895/970.5662

O	0.08406	-0.18210	-1.35989
C	-0.28746	-1.37564	-0.37478
O	0.07164	-2.30311	-1.18120
C	0.22071	-0.98673	1.01350
C	1.70454	-0.69769	1.24461
H	-0.05454	-1.78843	1.69948
C	-0.69001	0.25114	1.25670
H	-0.77698	0.53895	2.30229

C	-0.19270	1.40713	0.38806
C	-0.11509	2.72247	0.84643
H	-0.44738	2.95874	1.85166
C	0.40878	3.72345	0.02974
H	0.47286	4.73992	0.40083
C	0.85841	3.41860	-1.25372
H	1.26763	4.20001	-1.88631
C	0.78350	2.11384	-1.74295
H	1.11288	1.86521	-2.74687
C	0.26119	1.14065	-0.91179
C	-2.01762	-0.24462	0.70225
O	-3.14873	0.26095	1.01149
N	-1.76152	-1.20566	-0.15642
O	-2.66400	-1.72984	-1.03926
H	-3.97845	-0.10447	0.54178
H	-2.16188	-2.44549	-1.48395
H	0.54867	-1.17193	-1.84882
O	-5.32543	-0.56003	-0.03372
H	-5.43594	-1.19739	-0.74801
H	-6.18968	-0.23300	0.24249
O	2.07253	-0.17786	2.26541
O	2.47453	-1.10819	0.24462
C	3.92581	-0.95481	0.42198
H	4.20092	-1.47367	1.34082
H	4.13295	0.10801	0.55418
C	4.60070	-1.53612	-0.79811
H	5.68416	-1.44880	-0.68617
H	4.31530	-1.00308	-1.70785
H	4.35886	-2.59345	-0.92156

TS [7/8]⁺2w

-1086.3192152   ImgFreq/IR inten: -241.5133/103.9918

O	1.12946	-0.32845	1.23109
C	1.04494	-1.39068	0.09142
O	1.32662	-2.52020	0.52634
C	-0.18667	-1.01586	-0.77318
C	-1.53165	-1.02251	-0.06197
H	-0.25155	-1.76060	-1.57295
C	0.24861	0.35502	-1.36575
H	-0.31872	0.67145	-2.23613
C	0.27109	1.39336	-0.25631
C	-0.10878	2.72419	-0.44094
H	-0.45332	3.04948	-1.41684
C	-0.05195	3.62649	0.61636
H	-0.35786	4.65561	0.46734
C	0.39782	3.20050	1.86537
H	0.44650	3.90037	2.69119

C	0.79580	1.88177	2.06552
H	1.16621	1.54967	3.02949
C	0.72880	0.98223	1.00505
C	1.69573	0.07247	-1.71632
O	2.34889	0.74196	-2.62840
N	2.14074	-0.84886	-0.93741
O	3.42832	-1.26955	-0.88320
H	3.29221	0.50633	-2.67057
H	3.37496	-2.11070	-0.38158
H	0.53154	-2.80744	2.42565
H	0.60697	-1.26384	2.51646
O	0.04590	-2.05032	2.80338
H	-0.77994	-1.92991	2.20961
O	-1.74127	-1.45660	1.06538
O	-2.47668	-0.54769	-0.83575
C	-3.86303	-0.53566	-0.32463
H	-3.86647	0.06146	0.58754
H	-4.12253	-1.56351	-0.07029
C	-4.74169	0.04068	-1.40812
H	-5.77578	0.05853	-1.05556
H	-4.70723	-0.56446	-2.31592
H	-4.45414	1.06438	-1.65529

TS [8⁺2w/8:H₃O⁺]

-1086.3464809   ImgFreq/IR inten: -104.2035/161.0798

O	0.84579	0.90551	1.45784
C	1.09635	-1.93547	0.02528
O	1.28568	-2.90840	0.70111
C	-0.12253	-1.32698	-0.62093
C	-1.34129	-1.30988	0.31559
H	-0.37555	-1.96054	-1.47510
C	0.36048	0.08689	-1.14785
H	0.22617	0.12211	-2.23224
C	-0.34045	1.29120	-0.54810
C	-1.27778	2.02020	-1.28600
H	-1.47004	1.75683	-2.32216
C	-1.98545	3.06456	-0.69726
H	-2.71679	3.61806	-1.27582
C	-1.74970	3.39308	0.63755
H	-2.29492	4.20712	1.10234
C	-0.80710	2.68763	1.38199
H	-0.60850	2.95155	2.41636
C	-0.11116	1.64000	0.78741
C	1.86881	0.08940	-0.88648
O	2.67072	0.99953	-1.12165
N	2.18315	-1.11810	-0.35624
O	3.43940	-1.46087	0.11094

H	3.93901	1.00447	-0.53374
H	3.27435	-2.27699	0.63278
H	0.58282	0.75597	2.37450
O	4.80041	0.75920	0.09365
H	4.59312	-0.16152	0.38487
H	5.67203	0.80771	-0.32973
O	-2.45079	-1.45929	-0.39987
O	-1.27683	-1.17520	1.50946
C	-3.72170	-1.43995	0.33299
C	-4.83078	-1.66448	-0.66834
H	-3.79861	-0.47491	0.83613
H	-3.67691	-2.22109	1.09285
H	-5.79330	-1.64531	-0.15130
H	-4.73301	-2.63382	-1.16111
H	-4.84311	-0.88402	-1.43189