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).

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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	Erea or Eact	ZPE	T*Stot	T*S _{vib}	ΖΡΕ-ΤΔ	Ε+ΖΡΕ-ΤΔ
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.

Structure	Erel ^a	<i>Erea</i> ^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	1	
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

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.

TS [7/8]+2w	-49.9	67.0
8 ⁺ w	-	-
$8^{+}2w$	-123.9	-7.1
TS [8 ⁺ 2w/8:H ₃ O ⁺]	-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 CH₂NO₂H 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 Me₃N 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	Eact b	or E_{rea} ^b
Tra	nsition 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
4 b		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

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 [RC 1/2]			
-742.1602358	ImgFreq/IR Inten: -851.5222/12.3334		
0	-0.91305	1.77920	-0.37935
С	0.29198	2.09008	0.26751
0	0.62625	3.24331	0.28722
С	1.03737	0.96203	0.81543
С	0.49231	-0.35913	0.81706
С	-0.91502	-0.50894	0.41735
С	-1.64923	-1.68757	0.61692
Н	-1.17036	-2.53408	1.10083
С	-2.97341	-1.77691	0.21294
Н	-3.53217	-2.69128	0.37821
С	-3.58424	-0.67988	-0.40529
Н	-4.61850	-0.74483	-0.72586
С	-2.88090	0.50124	-0.60122
Н	-3.33971	1.36916	-1.06033
С	-1.55200	0.58382	-0.18457
С	1.38266	-1.44969	-0.60819
Н	0.90799	-1.05713	-1.49523
Ν	2.68510	-1.06404	-0.45595
0	2.90174	0.19732	-0.84144
0	3.52146	-1.65182	0.22209
Н	1.76679	1.23321	1.57142
Н	0.83484	-1.01504	1.61442
Н	1.19675	-2.48151	-0.34092
Н	2.17026	0.77539	-0.24679
TS [2.1/2.2]			
-742.1354092	ImgFreq/IR inten: -2172.6740/541.3399		
0	-0.93507	1.76505	-0.38671
С	0.26798	2.03500	0.22386
0	0.81958	3.06676	-0.02672
С	0.76377	0.98993	1.20026
Н	1.81734	1.19002	1.39487
Н	0.22714	1.13886	2.14496
С	0.51107	-0.44375	0.69795
Н	0.73051	-1.13868	1.51859
С	-0.95024	-0.56222	0.32723
С	-1.68598	-1.74050	0.47044
Н	-1.19747	-2.62198	0.87642
С	-3.02946	-1.79540	0.10852
Н	-3.58639	-2.71823	0.22826
С	-3.65518	-0.65702	-0.40127
Н	-4.70202	-0.68998	-0.68358
С	-2.94243	0.52875	-0.54609

TS structures (Energies at L1)

Н	-3.40495	1.42712	-0.93846
С	-1.59919	0.56355	-0.18255
С	1.38161	-0.78999	-0.49738
0	3.38314	-1.17242	0.76573
Ν	2.77604	-0.96737	-0.24740
0	3.36489	-0.73586	-1.41052
Н	1.04620	-1.64942	-1.08034
Н	2.20515	-0.32454	-1.66911
TS [2.1/2.2]w			
-818.6264588	ImgFreq/IR inten: -1393.6794/102.5452		
0	1.14768	1.75540	0.29575
С	0.03690	2.05236	-0.46764
0	-0.50648	3.10406	-0.29021
С	-0.37106	1.00513	-1.47838
Н	-1.38849	1.22155	-1.79920
Н	0.27915	1.12046	-2.35426
С	-0.22315	-0.42561	-0.92521
Н	-0.37086	-1.12202	-1.75860
С	1.18395	-0.57685	-0.39264
С	1.89989	-1.77497	-0.44065
Н	1.43425	-2.64880	-0.88758
С	3.19439	-1.85896	0.06656
Н	3.73643	-2.79712	0.01763
С	3.79179	-0.73031	0.62921
Н	4.80139	-0.78550	1.02226
С	3.09859	0.47503	0.68333
Н	3.54039	1.36748	1.11180
С	1.80437	0.53731	0.17447
С	-1.22917	-0.74303	0.16940
0	-2.90162	-0.90904	-1.40709
Ν	-2.53355	-1.01985	-0.24705
0	-3.40185	-1.31705	0.68610
Н	-0.91988	-1.47335	0.91370
Н	-1.72260	0.25790	1.37339
Н	-3.10688	-0.41850	1.69101
0	-2.52133	0.41952	2.12461
Н	-2.19818	0.23309	3.01520
TS [RC 1 ⁻ /2.1 ⁻]			
-741.6739479	ImgFreq/IR inten: -271.0039/625.5705		
0	-2.30114	-0.60008	0.39959
С	-1.86759	-1.89151	-0.03477
0	-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

Н	1.38970	1.63524	-1.07700
С	-0.22082	2.89416	-0.41517
Н	0.31508	3.81607	-0.61809
С	-1.50695	2.93111	0.13184
Н	-1.98143	3.88438	0.34799
С	-2.18730	1.74911	0.40070
Н	-3.18895	1.75005	0.81756
С	-1.57981	0.52119	0.12351
С	1.78323	-1.07227	0.84527
Н	1.35299	-0.64073	1.73858
Ν	2.89423	-0.39996	0.36870
0	3.57808	-0.94457	-0.54179
0	3.11813	0.78186	0.74273
Н	-0.26915	-2.92858	-0.96867
Н	1.11813	-0.89708	-1.38962
Н	1.86258	-2.14574	0.76395
TS [2.2w/3.1]			
-818.5707078	ImgFreq/IR inten: -811.7078/529.1724		
0	-1.23896	1.76540	-0.60328
С	-0.09207	2.24717	-0.00874
0	0.32308	3.31461	-0.35253
С	0.53024	1.36696	1.05444
Н	-0.00419	1.56128	1.99130
Н	1.56373	1.67220	1.19691
С	0.41234	-0.13677	0.73799
Н	0.71917	-0.70413	1.62138
С	-1.03414	-0.43836	0.40860
С	-1.66596	-1.63913	0.74200
Н	-1.09841	-2.41116	1.25259
С	-3.00523	-1.85515	0.43154
Н	-3.47863	-2.79358	0.69857
С	-3.73523	-0.85901	-0.21855
Н	-4.77985	-1.01902	-0.46299
С	-3.13062	0.34979	-0.54698
Н	-3.67624	1.14455	-1.04249
С	-1.79045	0.54762	-0.22802
С	1.36866	-0.50816	-0.38946
Ν	2.76579	-0.90564	-0.01262
0	3.24154	-0.00877	1.05793
0	3.55772	-0.85650	-1.06593
Н	1.35100	0.12339	-1.27696
Н	4.06540	0.30857	0.64899
0	1.05941	-1.93234	-0.84229
Н	1.36676	-2.01521	-1.76487
Н	1.92324	-2.23647	-0.22220

-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 1.1186 H -0.28782 1.63583 1.99693 H 0.32248 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 -1.05746 -0.45917 0.42311 C -1.05746 -0.45917 0.42314 H -3.32491 -2.99607 0.54203 C -2.91163 -2.01163 -0.1893 0.31754 H -3.32491 -2.99607 0.54203 C -3.47701 0.18102 -0.65205 H -3.71824 0.93520 -1.18094 C -1.34747 -0.47925	TS [3.1/6.1]w			
0 -1.35687 1.72360 -0.62448 C -0.24951 2.26070 -0.02374 0 0.16926 3.31463 -0.40952 C 0.33810 1.45447 1.11586 H -0.28782 1.63583 1.99693 H 0.32814 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 -1.05746 -0.45917 0.42311 C -1.05746 -0.45917 0.42311 C -1.05746 -0.45917 0.42311 C -1.05746 -0.45917 0.54203 C -3.314701 0.18102 -0.65205 C -3.314701 0.18102 -0.65205 C -3.14701 0.18102 -0.65205 C -3.14701 0.18102 -0.65205 C -3.14701 0.18102 -0.5	-818.6414856	ImgFreq/IR inten: -752.8107/81.5313		
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0 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 -1.05746 -0.45917 0.42311 C -1.61125 -1.71043 0.70427 H -3.32491 -2.99607 0.54203 C -3.67881 -1.0766 -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 -1.84432 0.47032 -0.23870 N 2.77682 -0.0210 0.18164 O 3.57954 -1.10807 -1.5386	С	-0.24951	2.26070	-0.02374
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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 -1.01502 -2.44724 1.21961 C -2.91163 -2.01893 0.31754 H -3.32491 -2.99607 0.54203 C -3.67881 -1.07066 -0.66483 C -3.14701 0.18102 -0.65205 H -3.71824 0.93520 -1.18094 C -3.14701 0.18102 -0.65205 H -3.71824 0.93520 -1.18094 C -1.84432 0.47039 -0.25870 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 -1.18095 H 0.20215 1.414805 1.42879	С	0.33810	1.45447	1.11586
H 1.32248 1.86363 1.34019 C 0.34118 -0.05841 0.83804 H 0.62200 0.059102 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 -3.32491 -2.99607 0.54203 C -3.14701 0.18102 -0.65205 H -3.17824 0.93520 -1.18094 C -1.84432 0.47039 -0.23870 N 2.77682 -0.03210 0.18164 O 3.17865 -0.20706 1.30294 H 1.21402 0.05631 -1.53866 O 1.34422 -1.84391 -0.32229 H 2.02235 -1.02591 H 3.43293 0.18294 -0.63743 TS[3.1/5+NH(OH	Н	-0.28782	1.63583	1.99693
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 -3.6781 -1.07066 -0.36074 H -4.69340 -1.30475 -0.66483 C -3.14701 0.18102 -0.65205 H -4.69340 -1.30475 -0.66483 C -3.14701 0.18102 -0.65205 H -4.69340 -1.30475 -0.23870 N 2.77682 -0.03210 0.18164 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 -0.03210 C -0.23620 2.23703 0.14844 <	Н	1.32248	1.86363	1.34019
H 0.62200 -0.59102 1.74969 C -1.05746 -0.45917 0.42311 C -1.0125 -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 -0.66433 C -3.14701 0.18102 -0.65205 H -3.71824 0.93520 -1.18094 C -1.84332 0.47039 -0.23870 N 2.77682 -0.03210 0.18164 O 3.17865 -0.20706 1.30294 H 1.21402 0.05631 -1.53866 O 1.34422 -1.84391 -0.39229 H 2.08115 -2.02235 -1.02591 H 2.08115 -2.02235 -1.02591 H 2.08115 -2.02235 -1.02591 H 2.08115 -2.022352 -1.02591	С	0.34118	-0.05841	0.83804
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 -3.32491 -2.99607 0.54203 C -3.67881 -1.07066 -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 3.17865 -0.20706 1.30294 H 1.21402 0.05631 -1.18057 H 2.08115 -2.02235 -1.02591 H 2.08115 -2.02235 -1.02591 H 2.08115 -2.02235 -1.02591 H 2.08125 -1.02591 -1.03974 -0	Н	0.62200	-0.59102	1.74969
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 -1.34432 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 3.43293 0.18294 -0.63743 TS [3.1/5+NH(OH)2] -1.53866 -0.13210 C -0.23620 2.2733 0.14844	С	-1.05746	-0.45917	0.42311
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 -1.34432 0.47039 -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 1.21402 0.05631 -1.18605 H 2.08115 -2.02235 -1.02591 O 1.34422 -1.43431 -0.39229 H 2.08115 -2.02235 -1.02591 H 2.02373 0.14844 0.03210 0.14844 O -1.39874 1.79977 -0.42400 C 0.23620 2.23703 0.14844	С	-1.61125	-1.71043	0.70427
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 1.21402 0.05631 -1.18605 H 2.08115 -2.02235 -1.02591 S 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	Н	-1.00502	-2.44724	1.21961
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 C -3.14701 0.93520 -1.18094 C -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 -1.53866 -1.31310 O 1.34422 -1.84391 -0.39229 H 2.08115 -2.02235 -1.02591 H 3.43293 0.18294 -0.63743 TS J.1/5+NH(OH)2 - - -818.6452361 ImgFreq/IR inten: -1142.8770/826.7598 - - O 0.13441 3.32826 -0.1264	С	-2.91163	-2.01893	0.31754
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 3.57954 -1.10807 -1.53866 O 3.17865 -0.20706 1.30294 H 1.21402 0.05631 -1.18605 H 1.21402 0.05631 -1.18605 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 -0.23620 2.23703 0.14844 O 0.017411 3.32826 -0.12640 C 0.42079 1.29042 1.1343	Н	-3.32491	-2.99607	0.54203
H-4.69340-1.30475-0.66483C-3.147010.18102-0.65205H-3.718240.93520-1.18094C-1.844320.47039-0.25951C1.35147-0.47925-0.23870N2.77682-0.032100.18164O3.57954-1.10807-1.53866O3.17865-0.207061.30294H1.214020.05631-1.18605H4.41599-1.53966-1.31310O1.34422-1.84391-0.39229H2.08115-2.02235-1.02591H2.08115-2.02235-1.02591H3.432930.18294-0.63743C-0.236202.237030.14844O-1.398741.79977-0.42400C-0.236202.237030.14844O0.1714113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	С	-3.67881	-1.07066	-0.36074
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 3.17865 -0.02706 1.30294 H 1.21402 0.05631 -1.18065 H 4.41599 -1.53966 -1.31310 O 1.34422 -1.84391 -0.32292 H 2.08115 -2.02235 -1.02591 H 3.43293 0.18294 -0.63743 TS[3.1/5+NH(OH)2] - - -0.32620 2.23703 0.14844 O -1.39874 1.79977 -0.42400 C 0.17411 3.32826 -0.12640 C 0.17411 3.32826 -0.12640 C 0.42079 1.2942 1.13443 H -0.09382 1.42689 2.09273 H 1.44305 1.64600 1.27278 C 0.32466 -0.18992 <td>Н</td> <td>-4.69340</td> <td>-1.30475</td> <td>-0.66483</td>	Н	-4.69340	-1.30475	-0.66483
H-3.718240.93520-1.18094C-1.844320.47039-0.25951C1.35147-0.47925-0.23870N2.77682-0.032100.18164O3.57954-1.0807-1.53866O3.17865-0.207061.30294H1.214020.05631-1.18605H4.41599-1.53966-1.31310O1.34422-1.84391-0.39229H2.08115-2.02235-1.02591H3.432930.18294-0.63743TS [3.1/5+NH(OH)2]818.6452361ImgFreq/IR inten: -1142.8770/826.7598-O-1.398741.79977-0.42400C0.2237030.14844O0.174113.32826C0.420791.29042H0.093821.426892.09273H1.44305H0.60685-0.82219C0.32466-0.18992O0.32466-0.18992O0.32466-0.18992O0.32466-0.18992C0.32466-0.18992H0.60685-0.82219H-0.60685-0.82219C-1.69101-1.75274O-1.69101-1.75274C-3.01805-1.98365H-3.44934-2.96918O-3.78859-0.94677C-3.78859-0.94677C-3.78859-0.94677C-	С	-3.14701	0.18102	-0.65205
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]	Н	-3.71824	0.93520	-1.18094
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 3.4322 -1.84391 -0.39229 H 2.08115 -2.02235 -1.02591 H 3.4422 -1.84391 -0.39229 H 2.08115 -2.02235 -1.02591 H 3.3422 -1.84391 -0.42400 C -0.23620 2.23703 0.14844 O 0.17411 3.32826 -0.12640 C 0.42079 1.29042 1.1343 H -0.09382 1.42689 2.09273 H 1.44305 1.64600 1.27278 C 0.32466 -0.18992 0.72980 <	С	-1.84432	0.47039	-0.25951
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 0.60685 -0.82219 1.57865 C -1.11253 -0.49242 0.36328 C -1.169101 -1.75274 0.53364 H -1.08263 -2.55805 0.93057 <td>С</td> <td>1.35147</td> <td>-0.47925</td> <td>-0.23870</td>	С	1.35147	-0.47925	-0.23870
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 0.420079 1.29042 1.13433 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 </td <td>Ν</td> <td>2.77682</td> <td>-0.03210</td> <td>0.18164</td>	Ν	2.77682	-0.03210	0.18164
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	0	3.57954	-1.10807	-1.53866
H1.214020.05631-1.18605H4.41599-1.53966-1.31310O1.34422-1.84391-0.39229H2.08115-2.02235-1.02591H3.432930.18294-0.63743TS [3.1/5+NH(OH)2]-818.6452361ImgFreq/IR inten: -1142.8770/826.7598O-1.398741.79977-0.42400C-0.236202.237030.14844O0.174113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	0	3.17865	-0.20706	1.30294
H4.41599-1.53966-1.31310O1.34422-1.84391-0.39229H2.08115-2.02235-1.02591H3.432930.18294-0.63743TS [3.1/5+NH(OH)2]-818.6452361ImgFreq/IR inten: -1142.8770/826.7598O-1.398741.79977-0.42400C-0.236202.237030.14844O0.174113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	Н	1.21402	0.05631	-1.18605
O1.34422-1.84391-0.39229H2.08115-2.02235-1.02591H3.432930.18294-0.63743TS [3.1/5+NH(OH)2]-818.6452361ImgFreq/IR inten: -1142.8770/826.7598O-1.398741.79977-0.42400C-0.236202.237030.14844O0.174113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	Н	4.41599	-1.53966	-1.31310
H2.08115-2.02235-1.02591H3.432930.18294-0.63743TS [3.1/5+NH(OH)2]ImgFreq/IR inten: -1142.8770/826.7598-O-1.398741.79977-0.42400C-0.236202.237030.14844O0.174113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	0	1.34422	-1.84391	-0.39229
H3.432930.18294-0.63743TS [3.1/5+NH(OH)2]-818.6452361ImgFreq/IR inten: -1142.8770/826.7598O-1.398741.79977-0.42400C-0.236202.237030.14844O0.174113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	Н	2.08115	-2.02235	-1.02591
TS [3.1/5+NH(OH)2]-818.6452361ImgFreq/IR inten: -1142.8770/826.7598O-1.39874 1.79977 O-0.236202.23703C-0.236202.23703O0.174113.32826O0.174113.32826C0.420791.29042C0.420791.29042H-0.093821.42689C0.32466-0.18992O0.32466-0.18992H0.60685-0.82219I.57865-1.11253-0.49242C-1.69101-1.75274O-3.01805-1.98365H-3.44934-2.96918O-3.78859-0.94677H-4.82423-1.11929-0.61543	Н	3.43293	0.18294	-0.63743
-818.6452361ImgFreq/IR inten: -1142.8770/826.7598O-1.398741.79977-0.42400C-0.236202.237030.14844O0.174113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	TS [3.1/5+NH(OH)2]			
O-1.398741.79977-0.42400C-0.236202.237030.14844O0.174113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	-818.6452361	ImgFreq/IR inten: -1142.8770/826.7598		
C-0.236202.237030.14844O0.174113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	0	-1.39874	1.79977	-0.42400
O0.174113.32826-0.12640C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	С	-0.23620	2.23703	0.14844
C0.420791.290421.13443H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	0	0.17411	3.32826	-0.12640
H-0.093821.426892.09273H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	С	0.42079	1.29042	1.13443
H1.443051.646001.27278C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	Н	-0.09382	1.42689	2.09273
C0.32466-0.189920.72980H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	Н	1.44305	1.64600	1.27278
H0.60685-0.822191.57865C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	С	0.32466	-0.18992	0.72980
C-1.11253-0.492420.36328C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	Н	0.60685	-0.82219	1.57865
C-1.69101-1.752740.53364H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	С	-1.11253	-0.49242	0.36328
H-1.08263-2.558050.93057C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	С	-1.69101	-1.75274	0.53364
C-3.01805-1.983650.18555H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	Н	-1.08263	-2.55805	0.93057
H-3.44934-2.969180.32305C-3.78859-0.94677-0.34256H-4.82423-1.11929-0.61543	С	-3.01805	-1.98365	0.18555
C -3.78859 -0.94677 -0.34256 H -4.82423 -1.11929 -0.61543	Н	-3.44934	-2.96918	0.32305
Н -4.82423 -1.11929 -0.61543	С	-3.78859	-0.94677	-0.34256
	Н	-4.82423	-1.11929	-0.61543

С	-3.23210	0.31488	-0.52319
Н	-3.80448	1.13784	-0.93546
С	-1.90244	0.52534	-0.17245
С	1.25197	-0.57052	-0.43784
Ν	2.94728	-0.38843	0.21179
0	3.66053	0.48563	-0.66475
0	3.40616	-1.63819	0.18479
Н	1.31960	0.18398	-1.23338
Н	4.49569	0.01432	-0.82750
0	1.30268	-1.81604	-0.78827
Н	2.45192	-2.09338	-0.38127
Н	3.04947	0.00680	1.14707
TS [2.2w/3.2]w			
-895.0662618	ImgFreq/IR inten: -784.3438/640.9200		
0	-1.83800	1.63691	-0.45776
С	-0.84715	2.30122	0.23886
0	-0.70208	3.47054	0.04190
С	-0.05150	1.47029	1.22423
Н	-0.62514	1.45038	2.15826
Н	0.88241	1.99263	1.41599
С	0.15977	0.01549	0.76338
Н	0.56903	-0.55063	1.60653
С	-1.18226	-0.55699	0.36283
С	-1.54612	-1.89059	0.56307
Н	-0.83675	-2.57003	1.02598
С	-2.80007	-2.35815	0.18114
Н	-3.06404	-3.39730	0.34427
С	-3.71400	-1.48448	-0.40928
Н	-4.69348	-1.84065	-0.71003
С	-3.37825	-0.14924	-0.60677
Н	-4.07190	0.55314	-1.05439
С	-2.11983	0.29989	-0.21650
С	1.18725	-0.07822	-0.36449
Ν	2.56259	0.32998	0.05459
0	2.62278	1.74601	-0.17236
0	3.44785	-0.28516	-0.83293
Н	0.88094	0.44140	-1.27924
Н	3.02925	1.81289	-1.05662
0	1.35272	-1.48937	-0.76321
Н	2.08864	-1.35379	-1.43341
Н	2.01352	-2.02178	0.00889
Н	3.65624	-1.55583	0.05575
0	3.19966	-2.37470	0.51533
Н	3.32267	-2.31942	1.46920

TS [3.2/6.1w]w			
-895.0882589	ImgFreq/IR inten: -1326.5756/194.2267		
0	-1.48825	1.78215	-0.57039
С	-0.31750	2.11766	0.06492
0	0.28456	3.08227	-0.31896
С	0.09435	1.20919	1.20043
Н	-0.56392	1.42516	2.05020
Н	1.11430	1.45374	1.47898
С	-0.08867	-0.27162	0.82358
Н	0.11606	-0.89007	1.70152
С	-1.53610	-0.44677	0.40838
С	-2.28467	-1.59609	0.66944
Н	-1.80269	-2.43350	1.16200
С	-3.62265	-1.68059	0.29480
Н	-4.18707	-2.58274	0.50497
С	-4.23391	-0.60488	-0.35052
Н	-5.27672	-0.66395	-0.64391
С	-3.50904	0.55193	-0.61821
Н	-3.95660	1.40341	-1.11802
С	-2.17304	0.61561	-0.23583
С	0.86782	-0.77131	-0.27462
Ν	2.29988	-0.85002	0.22790
0	2.84120	0.88298	0.21210
0	3.00879	-1.42818	-0.69996
Н	0.85589	-0.14045	-1.17620
Н	2.57601	1.28489	-0.63179
0	0.49683	-2.08587	-0.58100
Н	1.14618	-2.43834	-1.20610
Н	4.21485	-1.08506	-0.32812
0	4.94743	-0.30107	0.09120
Н	4.14204	0.45416	0.19975
Н	5.61862	-0.03409	-0.54661
TS [2.2 ⁺ 2w/3.1 ⁺]			
-818.9474032	ImgFreq/IR inten: -1487.8898/1295.6481		
0	-1.11566	1.83089	-0.47678
С	0.04886	2.18125	0.15878
0	0.59509	3.20183	-0.12798
С	0.56187	1.19052	1.19283
Н	0.00035	1.34044	2.12032
Н	1.59752	1.46111	1.40391
С	0.35415	-0.27268	0.75347
Н	0.62309	-0.95370	1.56382
С	-1.10603	-0.44790	0.38187
С	-1.82230	-1.62554	0.62004
Н	-1.32576	-2.46890	1.08998

С	-3.16875	-1.71265	0.27948
Н	-3.71814	-2.62599	0.47591
С	-3.81183	-0.61630	-0.29855
Н	-4.86240	-0.67848	-0.55874
С	-3.11841	0.56721	-0.53262
Н	-3.60015	1.43378	-0.96996
С	-1.77326	0.63938	-0.18946
С	1.21741	-0.60487	-0.45022
Ν	2.70824	-0.85723	-0.26222
0	3.14975	-0.99463	1.04385
0	3.42057	0.12860	-0.94396
Н	1.10531	0.06219	-1.30313
Н	3.26225	-0.09887	1.41615
0	1.03074	-2.01634	-0.89329
Н	0.52177	-2.15688	-1.70936
Н	2.21889	-2.04646	-0.83979
Н	4.28554	-0.26088	-1.16196
TS [3.1 ⁺ /3.2 ⁺]			
-818.9847008	ImgFreq/IR inten: -790.2056/1952.7991		
0	-0.88616	1.83313	-0.36178
С	0.27450	1.75721	0.21731
0	1.28439	2.21150	-0.38698
С	0.41588	0.88812	1.41642
Н	-0.37291	1.09468	2.14204
Н	1.38492	1.00944	1.88939
С	0.18713	-0.51735	0.80402
Н	0.33997	-1.27948	1.56857
С	-1.25950	-0.48516	0.32770
С	-2.13958	-1.56318	0.40072
Н	-1.78042	-2.51918	0.76726
С	-3.47772	-1.41404	0.02973
Н	-4.14893	-2.26226	0.09742
С	-3.95677	-0.18233	-0.41011
Н	-4.99760	-0.06908	-0.68964
С	-3.10033	0.91646	-0.49809
Н	-3.44091	1.88186	-0.85311
С	-1.78322	0.73458	-0.12876
С	1.18455	-0.81044	-0.35991
Ν	2.47555	-0.01764	-0.19098
0	3.33413	-0.29883	-1.24724
0	3.06353	-0.45020	1.02359
Н	0.80166	-0.41951	-1.30653
Н	3.49187	-1.26396	-1.21847
0	1.47596	-2.16603	-0.45459
Н	1.21921	-2.52498	-1.31264
Н	2.06745	1.40283	-0.25442

Н	3.862	0.09337	1.12889
TS [2.2 ⁺ w/3.2 ⁺]			
-818.9805439	ImgFreq/IR inten:		
	-1126.4281/2592.9207		
0	-1.403	383 1.81772	-0.30938
С	-0.228	382 2.05621	0.21438
0	0.586	581 2.76695	-0.40433
С	0.194	1.23805	1.39307
Н	-0.584	1.21746	2.15753
Н	1.113	1.62393	1.82670
С	0.326	599 -0.17677	0.78394
Н	0.640	.0.86778	1.56517
С	-1.071	-0.53019	0.29225
С	-1.598	-1.82074	0.32963
Н	-0.970	-2.64309	0.65525
С	-2.926	-2.05561	-0.02792
Н	-3.320		0.00893
С	-3.749	-0.99981	-0.41574
Н	-4.782	-1.18336	-0.68408
С	-3.249	0.30184	-0.46528
Н	-3.862	1.13851	-0.77981
С	-1.928	0.50270	-0.11402
С	1.404	-0.21815	-0.33980
Ν	2.243	-1.36803	-0.24042
0	2.872		1.00485
0	3.226	526 -1.21078	-1.24854
Н	0.979	-0.21240	-1.34147
Н	3.526	-0.75330	1.08057
Н	3.442	-2.10641	-1.54853
0	2.282	1.04891	-0.27308
Н	2.942	0.99603	-0.98604
Н	1.623	353 2.05728	-0.33038
TS [2.2/4']			
-742.1531741	ImgFreq/IR inten: -106.9246/73.8740		
0	1.635	521 1.67808	-0.23923
С	0.482	239 2.35135	0.05631
0	0.436	511 3.53451	-0.11618
С	-0.650)24 1.52364	0.62899
Н	-1.570)25 2.09403	0.51745
Н	-0.450	003 1.40975	1.70220
С	-0.757	0.12878	-0.04307
Н	-1.113	0.25933	-1.06771
С	0.608	-0.52709	-0.03366
С	0.806	·1.90988	0.01753
Н	-0.056	·2.56481	0.04224
С	2.091	-2.44706	0.01218

Н	2.22573	-3.52256	0.04958
С	3.19987	-1.60257	-0.04818
Н	4.20306	-2.01508	-0.05300
С	3.02388	-0.22403	-0.11178
Н	3.86513	0.45665	-0.17357
С	1.73459	0.29653	-0.10691
С	-1.78458	-0.63916	0.70611
Ν	-3.15396	-0.72851	0.32624
0	-3.40095	0.25041	-0.68479
0	-2.62327	-1.94979	-0.29455
Н	-4.36318	0.23477	-0.77085
Н	-1.57817	-1.06110	1.68295
TS [2.2/4'']			
-742.1249367	ImgFreq/IR inten: -914.2135/43.8485		
0	0.49836	1.65963	0.58338
С	-0.63987	1.89507	-0.17301
0	-1.31415	2.83917	0.10627
С	-0.88889	0.94736	-1.32687
Н	-0.33674	1.34084	-2.18776
Н	-1.95145	0.97078	-1.55856
С	-0.41206	-0.48333	-1.05771
Н	-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 N	-2 30925	-0.76228	0.51158
0	-2.73606	-1.55987	1.59977
0	-3.15332	-0.79610	-0.63028
H	-3 28990	-0.96359	2.12412
Н	-0.87442	-2.23961	0.23810
TS [4'/5+(NOH) ₂]		2.207.01	0.20010
-742.1536390	ImgFrea/IR inten: -170.4202/2.0477		
0	1.08385	1.81242	0.34357
С	-0.17588	2.15954	-0.08158
0	-0.59639	3.24504	0.19834
С	-0.90942	1.12950	-0.91333
Н	-0.55001	1.24445	-1.94294
Н	-1.96677	1.38901	-0.90416

С	-0.66429	-0.31765	-0.46616
Н	-1.04241	-1.01040	-1.22145
С	0.82533	-0.53069	-0.28391
С	1.44458	-1.77027	-0.46670
Н	0.83615	-2.62441	-0.74655
С	2.81670	-1.91752	-0.28867
Н	3.28078	-2.88659	-0.43603
С	3.59062	-0.81571	0.07911
Н	4.66115	-0.92224	0.21827
С	2.99401	0.42603	0.27017
Н	3.57031	1.29720	0.55978
С	1.61966	0.55426	0.09234
С	-1.36548	-0.66617	0.84794
Ν	-3.48198	-0.48570	0.45796
0	-3.73104	-0.88929	-0.71862
0	-1.71667	-1.81003	1.13080
Н	-4.43835	-1.58056	-0.72399
Н	-1.34998	0.12041	1.62329
TS [4''/6.3]			
-742.1545510	ImgFreq/IR inten: -593.5718/183.6230		
0	0.30364	1.75450	0.50909
С	-0.89761	1.91598	-0.15770
0	-1.61976	2.80030	0.19533
С	-1.15424	0.99566	-1.33055
Н	-0.74045	1.50099	-2.21137
Н	-2.23288	0.92727	-1.47034
С	-0.53632	-0.39966	-1.20136
Н	-0.51161	-0.86480	-2.19020
С	0.84523	-0.33445	-0.62288
С	1.81640	-1.31855	-0.85527
Н	1.57349	-2.15160	-1.50872
С	3.07812	-1.23541	-0.28053
Н	3.81709	-2.00447	-0.47702
С	3.39218	-0.15146	0.54576
Н	4.37596	-0.07809	0.99697
С	2.45069	0.83963	0.78950
Н	2.67024	1.69142	1.42272
С	1.18657	0.74147	0.20868
С	-1.43227	-1.36793	-0.34640
Ν	-1.31381	-0.87066	1.07574
0	-2.05089	-1.51019	1.89173
0	-2.72942	-1.35119	-0.55024
Н	-2.55297	-2.21966	1.39935
Н	-0.92324	-2.36543	-0.35427

TS [4''/6.1]w			
-818.6381640	ImgFreq/IR inten: -1006.4768/581.8438		
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С	-0.37710	2.26192	0.03711
0	-0.06970	3.35149	-0.34798
С	0.16608	1.59510	1.28193
Н	-0.49665	1.89725	2.10175
Н	1.14882	2.01739	1.48599
С	0.22069	0.06232	1.22472
Н	0.32745	-0.31266	2.24833
С	-1.04999	-0.48236	0.61801
С	-1.54687	-1.75654	0.91249
Н	-1.01235	-2.37765	1.62626
С	-2.71235	-2.23230	0.31977
Н	-3.08141	-3.22245	0.56412
С	-3.40602	-1.42419	-0.58271
Н	-4.31757	-1.78331	-1.04858
С	-2.93674	-0.15101	-0.88460
Н	-3.45848	0.49851	-1.57807
С	-1.76486	0.30796	-0.28601
С	1.46845	-0.46756	0.49673
Ν	1.53765	0.05668	-0.88240
0	2.22571	-0.62631	-1.68639
0	2.65138	0.11441	0.86665
Н	2.97476	-1.34641	-1.16342
Н	1.46552	-1.57184	0.50266
0	3.90433	-1.66855	-0.31508
Н	4.80486	-1.54244	-0.63560
Н	3.63958	-0.91207	0.36201
TS [2.2/4]b'			
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С	-0.58332	1.33600	1.30198
0	0.26157	2.11850	1.62393
С	-0.89149	0.03203	2.00234
Н	-1.70060	0.23197	2.71431
Н	-0.00539	-0.27282	2.55367
С	-1.34823	-1.06949	1.04066
Н	-1.73051	-1.92162	1.61397
С	-2.45500	-0.52816	0.14841
С	-3.50394	-1.30897	-0.34383
Н	-3.55482	-2.35974	-0.07277
С	-4.48104	-0.75506	-1.16500
Н	-5.29134	-1.37221	-1.53704
С	-4.41485	0.59842	-1.50126
Н	-5.17341	1.03823	-2.13989

С	-3.38209	1.39371	-1.01675
Н	-3.31220	2.44748	-1.26071
С	-2.40823	0.82430	-0.19976
С	-0.27782	-1.59275	0.12976
Ν	0.95670	-1.12822	0.13236
0	1.70625	-1.48920	-0.97925
0	1.31590	-1.75978	1.37704
Н	2.49672	-0.85581	-0.95518
Н	-0.56711	-2.29749	-0.65443
Ν	3.81118	0.22047	-0.71349
С	4.37740	-0.19610	0.57612
С	4.79005	0.08750	-1.79402
С	3.28229	1.58784	-0.64123
Н	2.81066	1.85052	-1.59063
Н	4.07609	2.32237	-0.43250
Н	2.53089	1.65759	0.14590
Н	4.32992	0.35948	-2.74649
Н	5.12983	-0.94809	-1.86080
Н	5.66967	0.73224	-1.63792
Н	3.59887	-0.18525	1.34005
Н	5.20434	0.45962	0.89061
Н	4.75170	-1.21841	0.49771
TS [2.2/4]b''			
-916.6623065	ImgFreq/IR inten: -623.7936/365.4912		
-916.6623065 O	ImgFreq/IR inten: -623.7936/365.4912 3.04867	-0.12165	0.84069
-916.6623065 O C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927	-0.12165 -1.44705	0.84069 0.50974
-916.6623065 O C O	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226	-0.12165 -1.44705 -2.26553	0.84069 0.50974 1.01503
-916.6623065 O C O C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981	-0.12165 -1.44705 -2.26553 -1.73007	0.84069 0.50974 1.01503 -0.47627
-916.6623065 O C O C H	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241	0.84069 0.50974 1.01503 -0.47627 -0.39193
-916.6623065 O C O C H H	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607
-916.6623065 O C O C H H H C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394
-916.6623065 O C O C H H C H	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474
-916.6623065 O C O C H H C H C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419
-916.6623065 O C O C H H C H C C C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998
-916.6623065 O C O C H H C H C C C H	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446
-916.6623065 O C O C H H C C H C C H C C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056
-916.6623065 O C O C H H C C H C C H C H	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728
-916.6623065 O C O C H H C C H C H C H C C H C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562 2.12515	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085 3.20437	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728 -0.32071
-916.6623065 O C O C H H C C H C C H C H C H C H	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562 2.12515 2.55234	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085 3.20437 4.20157	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728 -0.32071 -0.33171
-916.6623065 O C O C H H C C H C H C H C H C H C C H C C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562 2.12515 2.55234 2.84135	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085 3.20437 4.20157 2.15326	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728 -0.32071 -0.33171 0.24421
-916.6623065 O C O O C H H C C H C C H C C H C C H C C H C C H	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562 2.12515 2.55234 2.84135 3.82476	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085 3.20437 4.20157 2.15326 2.30058	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728 -0.32071 -0.33171 0.24421 0.67601
-916.6623065 O C O C H H C C H C H C H C H C H C H C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562 2.12515 2.55234 2.84135 3.82476 2.28776	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085 3.20437 4.20157 2.15326 2.30058 0.87731	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728 -0.32071 -0.33171 0.24421 0.67601 0.24854
-916.6623065 O C O C H H C C H C C H C C H C C H C C H C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562 2.12515 2.55234 2.84135 3.82476 2.28776 -0.61126	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085 3.20437 4.20157 2.15326 2.30058 0.87731 -1.11825	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728 -0.32071 -0.33171 0.24421 0.67601 0.24854 -1.17882
-916.6623065 O C O C H H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C N C N	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562 2.12515 2.55234 2.84135 3.82476 2.28776 -0.61126 -1.16692	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085 3.20437 4.20157 2.15326 2.30058 0.87731 -1.11825 -2.31671	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728 -0.32071 -0.33171 0.24421 0.67601 0.24854 -1.17882 -1.32756
-916.6623065 O C O C H H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C C H C C C H C C C C H C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562 2.12515 2.55234 2.84135 3.82476 2.28776 -0.61126 -1.16692 -0.90302	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085 3.20437 4.20157 2.15326 2.30058 0.87731 -1.11825 -2.31671 -3.12603	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728 -0.32071 -0.32171 0.24421 0.67601 0.24854 -1.17882 -1.32756 -0.21193
-916.6623065 O C O C H H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C C H C C C C H C	ImgFreq/IR inten: -623.7936/365.4912 3.04867 2.85927 3.57226 1.74981 1.49152 2.14337 0.52870 0.15738 1.02147 0.32992 -0.64539 0.87070 0.31562 2.12515 2.55234 2.84135 3.82476 2.28776 -0.61126 -1.16692 -0.90302 -2.09936	-0.12165 -1.44705 -2.26553 -1.73007 -2.78241 -1.55795 -0.81799 -1.02962 0.61393 1.68271 1.50020 2.96793 3.78085 3.20437 4.20157 2.15326 2.30058 0.87731 -1.11825 -2.31671 -3.12603 -0.60157	0.84069 0.50974 1.01503 -0.47627 -0.39193 -1.48607 -0.22394 0.78474 -0.28419 -0.85998 -1.29446 -0.88056 -1.33728 -0.32071 -0.32071 0.24421 0.67601 0.24854 -1.17882 -1.32756 -0.21193 -0.46276

H -0.60052 -0.58036 -2.12286 N -3.10331 0.55232 0.56562 -0.30560 C -3.53325 1.65652 -0.30560 C -2.30456 0.97107 1.69661 H -3.79019 -1.20840 1.429061 H -4.69667 -0.68256 0.00649 H -4.92422 0.16902 1.56295 H -2.67232 2.26555 -0.57624 H -3.97868 1.24970 -1.21215 H -3.97868 1.24970 -1.21215 H -3.97868 1.24970 -1.21215 H -1.94422 0.08456 2.21703 H -2.90052 1.57949 2.39126 H -1.4933 1.55180 1.35488 C 0.48519 -0.46830 1.90035 O -0.38370 0.94334 2.57896 C 0.92689 0.97629 1.9139 H 0.10841 1.57028 2.32217 C 2.31601 0.51387 -0.08166	Н	-1.46457	-3.89596	-0.35935
N -3.10331 0.55232 0.54768 C -3.5325 1.65652 -0.30560 C -4.19966 -0.34201 0.9124 C -2.30456 0.97107 1.69661 H -3.70019 -1.20840 1.42905 H -4.69667 -0.68256 0.00649 H -4.9242 0.16902 1.56295 H -2.67232 2.26555 -0.57624 H -2.67032 2.2259 0.20937 H -3.97868 1.24970 -1.212115 H -2.90052 1.57949 2.39126 H -1.94442 0.08456 2.21703 St Jab/4:bHT -1.44933 1.5180 1.3548 TS Jab/4:bHT -1.44933 0.94334 2.5786 O -0.43870 -0.94337 0.94334 2.57896 C 0.92689 0.97629 1.91939 H 1.76840 1.04148 2.61989 H <td>Н</td> <td>-0.60052</td> <td>-0.58036</td> <td>-2.12286</td>	Н	-0.60052	-0.58036	-2.12286
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 -4.26732 2.26555 -0.57624 H -2.67232 2.26555 -0.57624 H -2.46732 2.26555 -0.57624 H -1.94442 0.08456 2.21703 H -1.94442 0.08456 2.21703 H -1.44933 1.55180 1.35488 TS [4b/4:bH*] -1.44933 1.55180 1.35488 O 1.18397 -1.31140 1.06682 C 0.48519 -0.46830 1.90355 O -0.33870 -0.9434 2.57896 C 0.92689 0.97629 1.9139 H 1.76840 1.04148 2.618989 H 0.108441 1.57028 <t< td=""><td>Ν</td><td>-3.10331</td><td>0.55232</td><td>0.54768</td></t<>	Ν	-3.10331	0.55232	0.54768
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 -3.97868 1.24970 -1.21215 H -3.97868 1.24970 -1.21215 H -1.94442 0.08456 2.21703 H -2.90052 1.57949 2.39126 C 0.448519 -0.46830 1.90035 O 1.18397 -1.31140 1.06682 C 0.438519 -0.46830 1.90035 O -0.38370 -0.94334 2.57896 C 0.92689 0.97629 1.9139 H 1.76840 1.04148 2.61989 H 0.10841 1.57028 2.3217 C 1.36394 1.49871 0.54272 H 0.16814 1.57028 2.3217	С	-3.53325	1.65652	-0.30560
C -2.30456 0.97107 1.69661 H -3.79019 -1.20840 1.42905 H -4.69667 -0.68256 0.00649 H -2.67232 2.26555 -0.57624 H -2.67232 2.26555 -0.57624 H -2.67232 2.22555 -0.57624 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/4:5H'] -1.41933 1.55180 1.36488 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 2.6189 O 0.1841 1.57028 2.32217 C 1.36394 1.49871 0.54272 H 0.1053137 -0.08766	С	-4.19966	-0.34201	0.91284
H -3.79019 -1.20840 1.42905 H -4.69667 -0.68256 0.00649 H -4.267032 2.26555 -0.57624 H -4.26740 2.29259 0.20937 H -4.26740 2.29259 0.20937 H -1.317868 1.24970 -1.21215 H -1.94442 0.08456 2.21703 H -2.90052 1.55180 1.35488 TS [4b/4:bH'] -2.90052 1.57949 2.39126 H -1.44933 1.55180 1.35488 TS [4b/4:bH'] -1.44933 1.55180 1.35488 TS [4b/4:bH'] -0.46830 1.90035 0 O 0.38370 -0.94334 2.57896 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 3.31601 0.51387 -0.08714 </td <td>С</td> <td>-2.30456</td> <td>0.97107</td> <td>1.69661</td>	С	-2.30456	0.97107	1.69661
H -4.69667 -0.68256 0.00649 H -4.92422 0.16902 1.56295 H -2.67232 2.26555 -0.57624 H -3.97868 1.24970 -1.21215 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 1.9035 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 2.3217 C 1.36394 1.49871 0.54272 H 1.86747 2.46192 0.68166 C 2.31601 0.51387 -0.08774	Н	-3.79019	-1.20840	1.42905
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 -2.90052 1.57949 2.39126 H -2.90052 1.57949 2.39126 H -1.44933 1.5180 1.35488 TS [4b/4:bH*] -1.44933 1.5180 1.35488 C 0.48519 -0.46830 1.90682 C 0.92689 0.97629 1.91939 H 1.76840 1.04148 2.61989 H 0.10841 1.57028 2.3217 C 1.36394 1.49871 0.54372 C 2.31601 0.51387 -0.08774 C 2.31601 0.51387 -0.08774 C 3.32760 0.88299 -0.97867 H 4.94994 0.24188 -2.23750	Н	-4.69667	-0.68256	0.00649
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 [4b4':bH'] -1.44933 1.55180 1.35488 C 0.48519 -0.46830 1.90035 O -0.38370 -0.94334 2.57896 C 0.92689 0.97629 1.91939 H 0.10841 1.57028 2.3217 C 1.36394 1.49871 0.54272 H 0.10841 1.57028 2.3217 C 1.36394 1.49871 0.54272 H 0.10841 1.57028 2.32217 C 1.36394 1.49871 0.54272 H 0.10841 1.57028 2.32217 C 1.36394 1.49871 0.54272 H 0.10841 1.57028 2.32217 <t< td=""><td>Н</td><td>-4.92422</td><td>0.16902</td><td>1.56295</td></t<>	Н	-4.92422	0.16902	1.56295
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*] - - 1.44933 1.55180 1.35488 C 0.48519 -0.46830 1.90035 0.035370 -0.94334 2.57886 C 0.92689 0.97629 1.91393 H 1.76840 1.04148 2.61989 H 1.76840 1.04148 2.61989 1.49871 0.54272 C 0.92689 0.97629 1.91393 H 0.10841 1.57028 2.3217 C 0.10841 1.57028 2.32217 C 4.66374 -0.68166 C 2.31601 0.51387 -0.08774 C 2.31601 0.51387 -0.08774 C 3.32760 0.88299 -0.97867 H 3.45423 1.93407 -1.22262 C C -0.68166 C C	Н	-2.67232	2.26555	-0.57624
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*] -1.44933 1.55180 1.35488 TS [4b/4:bH*] -1.31140 1.06682 O 1.18397 -1.31140 1.06682 C 0.48519 -0.46830 1.90035 O 0.33370 -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 0.5472 H 0.10841 1.57028 2.32217 C 2.31601 0.51387 -0.08774 C 2.31601 0.51387 -0.08774 C 3.32760 0.88299 -0.97867 H 4.66856 -2.16256 -1.65861 C 4.94994 0.24188 -2.23750 C <td>Н</td> <td>-4.26740</td> <td>2.29259</td> <td>0.20937</td>	Н	-4.26740	2.29259	0.20937
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*] -1.44933 1.55180 1.35488 TS [4b/4:bH*] -1.18397 -1.31140 1.06682 C 0.48519 -0.46830 1.90035 O -0.38370 -0.94334 2.57896 C 0.92689 0.90629 1.91939 H 1.76840 1.04148 2.61989 H 0.10841 1.57028 2.32217 C 1.36394 1.49871 0.54272 H 0.10841 1.57028 2.32217 C 1.36394 1.49871 0.54272 H 0.18647 2.46192 0.68166 C 2.31601 0.51387 -0.08774 C 3.32760 0.82899 -0.97867 H 4.86747 2.46192 0.68166 C 4.17105 -0.06726 -1.54867 H 4.94994 0.24188 -2.23750	Н	-3.97868	1.24970	-1.21215
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 -1.31140 1.06682 C 0.48519 -0.46830 1.90035 O -0.38370 -0.94334 2.57896 C 0.92688 0.97629 1.91939 H 1.76840 1.44871 0.54272 PI 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 -1.2294 H 4.66856 -2.16256 -1.65861 C 3.01691 -1.8651 -0.35414 H 4.66856 -2.16256 -1.65861 C 0.15395	Н	-1.94442	0.08456	2.21703
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 0.10841 1.57028 2.32217 C 1.366394 1.49871 0.54272 H 0.10841 1.57028 2.32217 C 3.31601 0.51387 -0.08774 R 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 3.01691 -1.80651 -0.3541 H 2.87400 -2.84625 -0.66343	Н	-2.90052	1.57949	2.39126
TS [4b/4:bH*]-916.7322648ImgFreq/IR inten: -860.8006/6016.3728O 1.18397 -1.31140 1.06682 C 0.48519 -0.46830 1.90035 O -0.38370 -0.93334 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 2.46192 0.68166 C 2.31601 0.51387 -0.08774 C 3.32760 0.8229 -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 -0.8229 0.21775 C 0.7344 -0.33508 O -1.48392 0.61103 -1.46171 O -0.87687 2.49441 0.19068 H -2.50880 0.03355 -1.10169 H -0.51826 -0.59118 C -3.09648 -1.72614 0.4128 C -4.45959 -0.85845 -1.6557 H -4.71666 0.04746 -2.24546	Н	-1.44933	1.55180	1.35488
-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 0.10841 1.57028 2.32217 C 1.36394 1.49871 0.54272 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 4.94994 0.24188 -2.2262 C 4.17105 -0.06726 -1.54867 H 4.96856 -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	TS [4b/4 ⁻ :bH ⁺]			
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 -1.2234 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<	-916.7322648	ImgFreq/IR inten: -860.8006/6016.3728		
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 0.51387 -0.0874 C 2.31601 0.51387 -0.0874 C 3.32760 0.88299 -0.97867 H 3.45423 1.93407 -1.22262 C 4.17105 -0.06726 -1.54867 H 3.45423 1.93407 -1.22262 C 4.17105 -0.06726 -1.54867 H 3.45423 1.93407 -1.22262 C 4.01350 -1.41482 -1.22394 H 2.87400 2.84651 -0.33541 H 2.87400 2.84625 -0.06343 C 2.17926 -0.84229 0.21775 C 0.15395 1.79229 -0.36791 N -0.87687<	0	1.18397	-1.31140	1.06682
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 <t< td=""><td>С</td><td>0.48519</td><td>-0.46830</td><td>1.90035</td></t<>	С	0.48519	-0.46830	1.90035
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 <td< td=""><td>0</td><td>-0.38370</td><td>-0.94334</td><td>2.57896</td></td<>	0	-0.38370	-0.94334	2.57896
H1.768401.041482.61989H0.108411.570282.32217C1.363941.498710.54272H1.867472.461920.68166C2.316010.51387-0.08774C3.327600.88299-0.97867H3.454231.93407-1.22262C4.17105-0.06726-1.54867H4.949940.24188-2.23750C4.01350-1.41482-1.22394H4.66856-2.16256-1.65861C3.01691-1.80651-0.33541H2.87400-2.84625-0.06343C2.17926-0.842290.21775C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	С	0.92689	0.97629	1.91939
H0.108411.570282.32217C1.363941.498710.54272H1.867472.461920.68166C2.316010.51387-0.08774C3.327600.88299-0.97867H3.454231.93407-1.22262C4.17105-0.06726-1.54867H4.949940.24188-2.23750C4.01350-1.41482-1.22394H4.66856-2.16256-1.65861C3.01691-1.80651-0.33541H2.87400-2.84625-0.06343C2.17926-0.842290.21775C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	Н	1.76840	1.04148	2.61989
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	Н	0.10841	1.57028	2.32217
H1.867472.461920.68166C2.316010.51387-0.08774C3.327600.88299-0.97867H3.454231.93407-1.22262C4.17105-0.06726-1.54867H4.949940.24188-2.23750C4.01350-1.41482-1.22394H4.66856-2.16256-1.65861C3.01691-1.80651-0.33541H2.87400-2.84625-0.06343C2.17926-0.842290.21775C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	С	1.36394	1.49871	0.54272
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 -3.09648 -1.72614 0.14128	Н	1.86747	2.46192	0.68166
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 <tr< td=""><td>С</td><td>2.31601</td><td>0.51387</td><td>-0.08774</td></tr<>	С	2.31601	0.51387	-0.08774
H3.454231.93407-1.22262C4.17105-0.06726-1.54867H4.949940.24188-2.23750C4.01350-1.41482-1.22394H4.66856-2.16256-1.65861C3.01691-1.80651-0.33541H2.87400-2.84625-0.06343C2.17926-0.842290.21775C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	С	3.32760	0.88299	-0.97867
C4.17105-0.06726-1.54867H4.949940.24188-2.23750C4.01350-1.41482-1.22394H4.66856-2.16256-1.65861C3.01691-1.80651-0.33541H2.87400-2.84625-0.06343C2.17926-0.842290.21775C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.716860.004746-2.24546	Н	3.45423	1.93407	-1.22262
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C4.01350-1.41482-1.22394H4.66856-2.16256-1.65861C3.01691-1.80651-0.33541H2.87400-2.84625-0.06343C2.17926-0.842290.21775C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	Н	4.94994	0.24188	-2.23750
H4.66856-2.16256-1.65861C3.01691-1.80651-0.33541H2.87400-2.84625-0.06343C2.17926-0.842290.21775C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	С	4.01350	-1.41482	-1.22394
C3.01691-1.80651-0.33541H2.87400-2.84625-0.06343C2.17926-0.842290.21775C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.140130.478720.32619C-4.140130.47867-2.24546	Н	4.66856	-2.16256	-1.65861
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C2.17926-0.842290.21775C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	Н	2.87400	-2.84625	-0.06343
C0.153951.79229-0.36791N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	С	2.17926	-0.84229	0.21775
N-0.865900.77344-0.33508O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	С	0.15395	1.79229	-0.36791
O-1.483920.61103-1.46171O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	Ν	-0.86590	0.77344	-0.33508
O-0.876872.494410.19068H-2.508800.03355-1.10169H0.453492.09137-1.38114N-3.54199-0.51826-0.59118C-3.09648-1.726140.14128C-4.140130.478720.32619C-4.45959-0.85845-1.69557H-4.716860.04746-2.24546	0	-1.48392	0.61103	-1.46171
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C -4.45959 -0.85845 -1.69557 H -4.71686 0.04746 -2.24546	С	-4.14013	0.47872	0.32619
Н -4.71686 0.04746 -2.24546	С	-4.45959	-0.85845	-1.69557
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С		-1.11754	0.06377	1.42054
Н		-1.28352	-0.23042	2.46290
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0 C O	-0.12819 1.05676 1.81981	-1.83583 -1.79696 -2.70914	0.25735 -0.43943 -0.32106
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0 C O C H	-0.12819 1.05676 1.81981 1.25744 0.86249	-1.83583 -1.79696 -2.70914 -0.63030 -0.95891	0.25735 -0.43943 -0.32106 -1.38393 -2.35248
0 C O C H H	-0.12819 1.05676 1.81981 1.25744 0.86249 2.33145	-1.83583 -1.79696 -2.70914 -0.63030 -0.95891 -0.49941	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264
0 C O C H H C	-0.12819 1.05676 1.81981 1.25744 0.86249 2.33145 0.54203	-1.83583 -1.79696 -2.70914 -0.63030 -0.95891 -0.49941 0.68189	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741
0 C O C H H C H	-0.12819 1.05676 1.81981 1.25744 0.86249 2.33145 0.54203 0.44453	-1.83583 -1.79696 -2.70914 -0.63030 -0.95891 -0.49941 0.68189 1.28860	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017
0 C 0 C H H C H C	-0.12819 1.05676 1.81981 1.25744 0.86249 2.33145 0.54203 0.44453 -0.84493	-1.83583 -1.79696 -2.70914 -0.63030 -0.95891 -0.49941 0.68189 1.28860 0.38349	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017 -0.46810
0 C 0 C H H C H C C C	-0.12819 1.05676 1.81981 1.25744 0.86249 2.33145 0.54203 0.44453 -0.84493 -1.88549	-1.83583 -1.79696 -2.70914 -0.63030 -0.95891 -0.49941 0.68189 1.28860 0.38349 1.31441	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017 -0.46810 -0.53609
0 C 0 C H H C H C H H	-0.12819 1.05676 1.81981 1.25744 0.86249 2.33145 0.54203 0.44453 -0.84493 -1.88549 -1.69463	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\end{array}$	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017 -0.46810 -0.53609 -0.98678
0 C 0 C H H C C H C H C H C H	-0.12819 1.05676 1.81981 1.25744 0.86249 2.33145 0.54203 0.44453 -0.84493 -1.88549 -1.69463 -3.14571	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\end{array}$	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017 -0.46810 -0.53609 -0.98678 -0.02870
0 C 0 C H H C H C H C H H C H H C H H C H H C H H C H H H C H H H C H H H H H H H H H H H H H	-0.12819 1.05676 1.81981 1.25744 0.86249 2.33145 0.54203 0.44453 -0.84493 -1.88549 -1.69463 -3.14571 -3.94169	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\end{array}$	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017 -0.46810 -0.53609 -0.98678 -0.02870 -0.08861
0 C 0 C H H C H C H C H C H C H C H C H C H C C H C C H C C H C C C C C C C C C C C C C	$\begin{array}{r} -0.12819\\ 1.05676\\ 1.81981\\ 1.25744\\ 0.86249\\ 2.33145\\ 0.54203\\ 0.44453\\ -0.84493\\ -1.88549\\ -1.69463\\ -3.14571\\ -3.94169\\ -3.37914\end{array}$	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\\ -0.23100\end{array}$	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017 -0.46810 -0.53609 -0.98678 -0.02870 -0.08861 0.55333
0 C 0 C H H C H C H C H C H C H H C H H C H H C H H C H H C H H H C H H H C H H H H H H H H H H H H H	$\begin{array}{r} -0.12819\\ 1.05676\\ 1.81981\\ 1.25744\\ 0.86249\\ 2.33145\\ 0.54203\\ 0.44453\\ -0.84493\\ -1.88549\\ -1.69463\\ -3.14571\\ -3.94169\\ -3.37914\\ -4.35974\end{array}$	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\\ -0.23100\\ -0.47426\end{array}$	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017 -0.46810 -0.53609 -0.98678 -0.02870 -0.08861 0.55333 0.94830
0 C 0 C H H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C C C C C C C C C	$\begin{array}{c} -0.12819\\ 1.05676\\ 1.81981\\ 1.25744\\ 0.86249\\ 2.33145\\ 0.54203\\ 0.44453\\ -0.84493\\ -1.88549\\ -1.69463\\ -3.14571\\ -3.94169\\ -3.37914\\ -4.35974\\ -2.35802\end{array}$	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\\ -0.23100\\ -0.47426\\ -1.17145\end{array}$	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017 -0.46810 -0.53609 -0.98678 -0.02870 -0.08861 0.55333 0.94830 0.62617
0 C 0 C H H C H C H C H C H C H C H C H H C H H C H H C H H C H H C H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H H H C H H H H H C H H H H H H H H H H H H H	$\begin{array}{c} -0.12819\\ 1.05676\\ 1.81981\\ 1.25744\\ 0.86249\\ 2.33145\\ 0.54203\\ 0.44453\\ -0.84493\\ -1.88549\\ -1.69463\\ -3.14571\\ -3.94169\\ -3.37914\\ -4.35974\\ -2.35802\\ -2.51389\end{array}$	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\\ -0.23100\\ -0.47426\\ -1.17145\\ -2.14879\end{array}$	0.25735 - 0.43943 - 0.32106 - 1.38393 - 2.35248 - 1.51264 - 1.00741 - 1.91017 - 0.46810 - 0.53609 - 0.98678 - 0.02870 - 0.08861 0.55333 0.94830 0.62617 1.06833
0 C 0 C H H C C H C C C H C C C H C C C C H C C C C C C C C C C C C C	$\begin{array}{c} -0.12819\\ 1.05676\\ 1.81981\\ 1.25744\\ 0.86249\\ 2.33145\\ 0.54203\\ 0.44453\\ -0.84493\\ -1.88549\\ -1.69463\\ -3.14571\\ -3.94169\\ -3.37914\\ -4.35974\\ -2.35802\\ -2.51389\\ -1.09904\end{array}$	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\\ -0.23100\\ -0.47426\\ -1.17145\\ -2.14879\\ -0.85574\end{array}$	0.25735 - 0.43943 - 0.32106 - 1.38393 - 2.35248 - 1.51264 - 1.00741 - 1.91017 - 0.46810 - 0.53609 - 0.98678 - 0.02870 - 0.08861 0.55333 0.94830 0.62617 1.06833 0.11969
0 C 0 C H H C C H C C H C C H C C H C C H C C H C C C C H C C C C C H C C C C C C C C C C C C C	$\begin{array}{c} -0.12819\\ 1.05676\\ 1.81981\\ 1.25744\\ 0.86249\\ 2.33145\\ 0.54203\\ 0.44453\\ -0.84493\\ -1.88549\\ -1.69463\\ -3.14571\\ -3.94169\\ -3.37914\\ -4.35974\\ -2.35802\\ -2.51389\\ -1.09904\\ 1.29765\end{array}$	$\begin{array}{r} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\\ -0.23100\\ -0.47426\\ -1.17145\\ -2.14879\\ -0.85574\\ 1.55358\end{array}$	0.25735 - 0.43943 - 0.32106 - 1.38393 - 2.35248 - 1.51264 - 1.00741 - 1.91017 - 0.46810 - 0.53609 - 0.98678 - 0.02870 - 0.08861 0.55333 0.94830 0.62617 1.06833 0.11969 - 0.03733
0 C 0 C H H C H C H C H C H C H C H C H C H C H C H C H C H C H C C H C C H C C H C C H C C C H C C C H C C C H C C C C H C C C C C C C C C C C C C	$\begin{array}{c} -0.12819\\ 1.05676\\ 1.81981\\ 1.25744\\ 0.86249\\ 2.33145\\ 0.54203\\ 0.44453\\ -0.84493\\ -1.88549\\ -1.69463\\ -3.14571\\ -3.94169\\ -3.37914\\ -4.35974\\ -2.35802\\ -2.51389\\ -1.09904\\ 1.29765\\ 1.40832\end{array}$	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\\ -0.23100\\ -0.47426\\ -1.17145\\ -2.14879\\ -0.85574\\ 1.55358\\ 2.83195\end{array}$	0.25735 - 0.43943 - 0.32106 - 1.38393 - 2.35248 - 1.51264 - 1.00741 - 1.91017 - 0.46810 - 0.53609 - 0.98678 - 0.02870 - 0.08861 0.55333 0.94830 0.62617 1.06833 0.11969 - 0.03733 - 0.17108
0 C 0 C H H C C H C C N N N N N N N N N N N N N	$\begin{array}{c} -0.12819\\ 1.05676\\ 1.81981\\ 1.25744\\ 0.86249\\ 2.33145\\ 0.54203\\ 0.44453\\ -0.84493\\ -1.88549\\ -1.69463\\ -3.14571\\ -3.94169\\ -3.37914\\ -4.35974\\ -2.35802\\ -2.51389\\ -1.09904\\ 1.29765\\ 1.40832\\ 1.92257\end{array}$	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\\ -0.23100\\ -0.47426\\ -1.17145\\ -2.14879\\ -0.85574\\ 1.55358\\ 2.83195\\ 1.26709\end{array}$	0.25735 -0.43943 -0.32106 -1.38393 -2.35248 -1.51264 -1.00741 -1.91017 -0.46810 -0.53609 -0.98678 -0.02870 -0.08861 0.55333 0.94830 0.62617 1.06833 0.11969 -0.03733 -0.17108 1.07929
0 C 0 C H H C C H C C C H C C C H C C C H C C C C C N C C C C C C C C C C C C C	$\begin{array}{c} -0.12819\\ 1.05676\\ 1.81981\\ 1.25744\\ 0.86249\\ 2.33145\\ 0.54203\\ 0.44453\\ -0.84493\\ -1.88549\\ -1.69463\\ -3.14571\\ -3.94169\\ -3.37914\\ -4.35974\\ -2.35802\\ -2.51389\\ -1.09904\\ 1.29765\\ 1.40832\\ 1.92257\\ 2.24011\end{array}$	$\begin{array}{c} -1.83583\\ -1.79696\\ -2.70914\\ -0.63030\\ -0.95891\\ -0.49941\\ 0.68189\\ 1.28860\\ 0.38349\\ 1.31441\\ 2.28342\\ 1.01614\\ 1.75011\\ -0.23100\\ -0.47426\\ -1.17145\\ -2.14879\\ -0.85574\\ 1.55358\\ 2.83195\\ 1.26709\\ -0.05191\end{array}$	0.25735 - 0.43943 - 0.32106 - 1.38393 - 2.35248 - 1.51264 - 1.00741 - 1.91017 - 0.46810 - 0.53609 - 0.98678 - 0.02870 - 0.08861 0.55333 0.94830 0.62617 1.06833 0.11969 - 0.03733 - 0.17108 1.07929 1.43425

Н	1.92282	-0.16138	2.34187
TS [6.1/6.2]w			
-818.6277658	ImgFreq/IR inten: -1607.8191/738.1699		
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С	1.00489	-2.10932	-0.01706
0	1.77664	-2.93073	0.38556
С	1.19975	-1.25564	-1.25135
Н	0.63631	-1.72099	-2.06874
Н	2.25402	-1.27360	-1.51368
С	0.67100	0.18514	-1.05687
Н	0.70638	0.68574	-2.02832
С	-0.76489	0.07350	-0.60191
С	-1.78192	0.92900	-1.03225
Н	-1.53290	1.75804	-1.68687
С	-3.09855	0.74325	-0.62041
Н	-3.87316	1.42251	-0.95972
С	-3.41726	-0.32270	0.22193
Н	-4.44058	-0.47390	0.54874
С	-2.42632	-1.20719	0.63429
Н	-2.64703	-2.05172	1.27676
С	-1.11675	-1.00596	0.21205
С	1.65049	0.95176	-0.12461
0	2.93870	0.85745	-0.64084
Ν	1.60611	1.05087	1.21370
0	0.46352	1.28364	1.77341
Н	3.55795	1.00147	0.09110
Н	1.03227	2.32781	-0.18048
Н	-0.08834	2.40681	0.92537
0	0.13864	3.05983	0.12535
Н	0.50355	3.87696	0.49282
TS [6.2/6.3]w			
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С	-0.51589	2.25439	0.28275
0	-0.34387	3.40888	0.02013
С	0.25164	1.49666	1.34413
Н	-0.30897	1.64930	2.27439
Н	1.21065	1.99747	1.47452
С	0.40406	-0.02295	1.12946
Н	0.54826	-0.48052	2.11007
С	-0.85634	-0.59849	0.51629
С	-1.16147	-1.96026	0.61622
Н	-0.46608	-2.61585	1.13214
С	-2.32992	-2.47907	0.06933
Н	-2.54662	-3.53804	0.15732
С	-3.22241	-1.62796	-0.58512

Н	-4.14011	-2.02014	-1.01051
С	-2.94129	-0.27120	-0.69173
Н	-3.61711	0.41245	-1.19287
С	-1.76157	0.23248	-0.14499
С	1.66267	-0.43662	0.37246
0	2.50533	-1.18167	1.00490
Ν	1.94228	-0.09643	-0.86479
0	1.08016	0.84969	-1.44761
Н	3.47864	-1.33604	0.22825
Н	0.78689	0.45506	-2.28042
Н	3.16646	-0.51171	-1.16774
0	4.08394	-1.18486	-0.80379
Н	4.91311	-0.70410	-0.70410
TS [6.2/7] ⁺ w			
-819.0805505	ImgFreq/IR inten: -164.8451/83.6549		
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С	-1.24055	-0.12272	0.77942
0	-2.48773	-0.42659	1.00717
С	-0.47822	0.64732	1.83680
Н	-0.09265	-0.04521	2.58759
Н	-1.14299	1.36581	2.31375
С	0.65632	1.30580	1.03219
Н	1.23802	2.04202	1.58430
С	1.51139	0.18696	0.45112
С	2.89674	0.25362	0.30298
Н	3.42661	1.14291	0.62819
С	3.59618	-0.81662	-0.24855
Н	4.67369	-0.76099	-0.35004
С	2.91208	-1.95868	-0.66600
Н	3.45651	-2.79180	-1.09544
С	1.52806	-2.04165	-0.53388
Н	0.97993	-2.92094	-0.85134
С	0.84932	-0.96883	0.02257
С	-0.05796	1.90068	-0.15266
0	0.49542	2.80552	-0.91622
Ν	-1.19049	1.30788	-0.35300
0	-1.76824	1.49263	-1.59681
Н	-0.04448	2.98320	-1.70746
Н	-2.72628	1.53329	-1.44991
0	-3.66463	-2.21265	-0.52750
Н	-2.84883	-1.14925	0.41683
Н	-3.25017	-2.94789	-0.99255
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TS [7/8] ⁺ w			
-819.0097791	ImgFreq/IR inten:		
	-1840.9797/1056.4662		
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0	0.95958	2.81888	-0.14980
С	0.09893	1.29243	1.69782
Н	-0.83302	1.80879	1.91870
Н	0.83403	1.51569	2.47333
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Н	-0.13298	-0.83102	2.37007
С	-1.30317	-0.44144	0.57109
С	-2.24073	-1.45062	0.78941
Н	-2.08869	-2.15675	1.59918
С	-3.37769	-1.54176	-0.01169
Н	-4.10456	-2.32357	0.17463
С	-3.58543	-0.62694	-1.04275
Н	-4.47252	-0.69772	-1.66160
С	-2.65686	0.38362	-1.29437
Н	-2.79600	1.09188	-2.10289
С	-1.53877	0.45311	-0.48394
С	1.17662	-0.56177	0.66673
0	1.64525	-1.74037	0.54088
Ν	1.61161	0.54699	0.11159
0	2.54083	0.59816	-0.89119
Н	2.45033	-1.87402	-0.07498
Н	2.69841	1.55530	-1.02112
Н	-0.18799	2.53398	-0.87487
0	3.66270	-2.24535	-0.93414
Н	4.07266	-1.66461	-1.58366
Н	4.07208	-3.11634	-0.97852
TS [7/8] ⁺ 2w			
-819.0457766	ImgFreq/IR inten: -392.6944/79.8358		
0	0.36530	1.16578	-0.10171
C	1.56486	0.18478	0.59102
0	2.63578	0.81430	0.57014
C	0.82979	-0.43639	1.77256
H	0.38480	0.31984	2.41605
Н	1.53924	-1.03252	2.35050
С	-0.22730	-1.31856	1.06351
H	-0.61779	-2.13372	1.67122
C G	-1.32993	-0.44444	0.48424
C .	-2.67339	-0.82390	0.47852
Н	-2.96074	-1.77592	0.91352
U H	-3.64112	0.01334	-0.06676
Н	-4.68327	-0.28314	-0.05600

С	-3.26291	1.23432	-0.62582
Н	-4.01185	1.88910	-1.05707
С	-1.92664	1.62462	-0.64112
Н	-1.63084	2.56685	-1.09045
С	-0.96386	0.78695	-0.08353
С	0.55259	-1.83613	-0.12316
0	0.22547	-2.89280	-0.80726
Ν	1.51991	-1.01459	-0.38205
0	2.26922	-1.07937	-1.51738
Н	0.77776	-3.02099	-1.59910
Н	3.09376	-0.60279	-1.29803
Н	2.50841	2.40621	0.12971
Н	0.97212	2.41909	-0.25917
0	1.84158	3.06489	-0.24887
Н	1.75771	3.86004	0.29705
TS [8+2w/8:H ₃ O+]			
-819.0948271	ImgFreq/IR inten: -565.7872/3670.1894		
0	-0.58889	-0.26831	1.67487
С	1.74675	-1.76937	-0.06437
0	2.57743	-2.50008	0.39216
С	0.37404	-1.97313	-0.64597
Н	-0.25903	-2.44515	0.10617
Н	0.43487	-2.65413	-1.49722
С	-0.13575	-0.55352	-1.04088
Н	-0.16889	-0.46308	-2.13145
С	-1.49526	-0.16365	-0.49862
С	-2.57603	0.06144	-1.35249
Н	-2.43303	-0.01821	-2.42587
С	-3.83302	0.38226	-0.84624
Н	-4.66327	0.55052	-1.52184
С	-4.01342	0.48437	0.53098
Н	-4.98776	0.73255	0.93673
С	-2.94541	0.27031	1.39999
Н	-3.08738	0.35302	2.47408
С	-1.69463	-0.05023	0.88299
С	0.97830	0.37561	-0.59009
0	0.96132	1.62113	-0.67983
Ν	1.98944	-0.36407	-0.12788
0	3.15433	0.17124	0.36554
Н	1.94193	2.34136	-0.25947
Н	3.65266	-0.60919	0.68697
Н	-0.81049	-0.18153	2.61029
0	2.82185	2.99373	0.14086
Н	3.65066	2.52692	0.30803
Н	2.96195	3.88924	-0.19189

TS [2.1/2.2]	ImgErag/ID inten: 2165 4786/564 3004		
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C C	-0.42107	-0.72609	1.70817
	-0.13107	-1.51689	2 40225
C C	0.18679	-1.06641	0.06061
н	0.68866	-2 03723	0.08643
C C	-1 05275	-1 26946	-0.82409
C 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
Н	1.12367	2.23938	-2.20539
С	-0.06778	3.61979	-1.06222
Н	0.01930	4.41859	-1.79051
С	-0.81033	3.80958	0.10423
Н	-1.30043	4.75932	0.29018
С	-0.93173	2.78143	1.03337
Н	-1.50358	2.90221	1.94621
С	-0.29774	1.56726	0.78713
С	2.48885	0.00142	0.07696
0	3.32780	-1.87752	-1.15614
Ν	3.35353	-1.08627	-0.25725
0	4.21098	-1.16000	0.74978
Н	3.05898	0.92106	-0.06310
Н	3.37219	-0.36356	1.23960
0	-0.98673	-1.39563	-2.02068
0	-2.18164	-1.31384	-0.11122
С	-3.41651	-1.54908	-0.84518
С	-4.54999	-1.54834	0.15652
Н	-3.32322	-2.50293	-1.36792
Н	-3.52159	-0.76276	-1.59515
Н	-4.41663	-2.33194	0.90521
Н	-5.49616	-1.72808	-0.36108
H	-4.62159	-0.58845	0.67244
TS [2.1/2.2]w			
-1085.8869486	ImgFreq/IR inten: -1383.00/4/101.//90	0.58570	1 70505
0	-0.42203	0.58579	1.70505
	-0.23935	-0./3014	1.36795
0 C	-0.1/390	-1.54802	2.24295
с u	-0.09089	-1.03103	-0.110/4 0.10/12
II C	0.57005	-2.01008	-0.19412
C C	-1.44409	-1.13304	-0.04237
с ц	0.79055	0.05139	-U.0U40J 1 88107
11	0.74455	-0.101/0	-1.00107

Ethyl ester of 3-coumarin-carboxylic acid

С		0.19344	1.38862	-0.50412
С		0.20452	2.45348	-1.40686
Н		0.65211	2.30921	-2.38565
С		-0.35879	3.68214	-1.07074
Н		-0.34450	4.49817	-1.78500
С		-0.95014	3.85501	0.18148
Н		-1.39467	4.80804	0.44795
С		-0.97946	2.80446	1.09375
Н		-1.43472	2.91098	2.07180
С		-0.40702	1.58635	0.74029
С		2.23181	-0.01107	-0.32654
0		2.56637	-1.99594	-1.44658
Ν		3.01750	-1.06761	-0.79276
0		4.26854	-1.08684	-0.41006
Н		2.78517	0.92174	-0.40496
Н		2.75985	-0.17251	1.22208
0		-1.55177	-1.13969	-2.04221
0		-2.46228	-1.30882	0.01223
С		-3.78355	-1.49508	-0.56648
С		-4.76244	-1.66286	0.57484
Н		-3.74946	-2.37109	-1.21710
Н		-4.01080	-0.62514	-1.18588
Н		-5.76961	-1.81028	0.17552
Н		-4.77696	-0.77963	1.21713
Н		-4.50850	-2.52958	1.18858
Н		4.19916	-0.73043	0.92429
0		3.64422	-0.43116	1.83634
H		4.01142	0.35637	2.25743
TS [2.2 ⁺ 2w/3.1 ⁺] -1086.2166867	ImgFreq/IR inten:			
0	-1423./933/11/0.4/11	1 02035	1 47000	1 70118
C C		0.21885	-0.95961	1.70110
0		0.90205	-1 24335	2 74835
C		0.70014	0.04697	0 76247
C C		1 94231	-0.39556	-0.01995
Н		1.09104	0.85976	1 38479
C		-0.36576	0.61524	-0.23255
Н		0.07365	0.69310	-1 22961
C C		-1 60530	-0 24874	-0 32985
C 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
С		-3.87062	-1.89069	-0.52266
H		-4.74498	-2.52765	-0.59257
==				0.07201

С	-2.98516	-2.05524	0.53455
Н	-3.13941	-2.81087	1.29575
С	-1.86137	-1.23765	0.61817
С	-0.66486	2.03199	0.21703
Ν	0.39426	3.08719	-0.03732
0	1.30890	2.81340	-1.02466
0	1.00880	3.38051	1.19393
Н	-0.98753	2.13078	1.25158
Н	1.86542	2.01421	-0.78551
0	-1.62608	2.76447	-0.66048
Н	-2.52392	2.88809	-0.30867
Н	-0.82157	3.61732	-0.61217
Н	1.47856	4.22095	1.05697
0	2.56443	0.43805	-0.66264
0	2.22417	-1.66438	0.07067
С	3.43700	-2.18262	-0.59839
Н	3.74320	-2.99760	0.05396
Н	4.18761	-1.39446	-0.58117
С	3.11447	-2.65235	-2.00030
Н	4.00909	-3.10345	-2.43736
Н	2.81210	-1.82467	-2.64487
Н	2.32806	-3.40965	-1.99442
TS [2.2 ⁺ w/3.2 ⁺]			
-1086.2448778	ImgFreq/IR inten: -820.6690/2136.9112		
-1086.2448778 O	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009	0.16650	1.78406
-1086.2448778 O C	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870	0.16650 -0.78281	1.78406 1.26769
-1086.2448778 O C O	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023	0.16650 -0.78281 -1.29170	1.78406 1.26769 1.96435
-1086.2448778 O C O C	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783	0.16650 -0.78281 -1.29170 -1.02623	1.78406 1.26769 1.96435 -0.20531
-1086.2448778 O C O C C	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990	0.16650 -0.78281 -1.29170 -1.02623 -1.37231	1.78406 1.26769 1.96435 -0.20531 -0.78435
-1086.2448778 O C O C C H	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581	0.16650 -0.78281 -1.29170 -1.02623 -1.37231 -1.87135	1.78406 1.26769 1.96435 -0.20531 -0.78435 -0.45885
-1086.2448778 O C O C C H C	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635	0.16650 -0.78281 -1.29170 -1.02623 -1.37231 -1.87135 0.29667	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\end{array}$
-1086.2448778 O C O C C H C H	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067	0.16650 -0.78281 -1.29170 -1.02623 -1.37231 -1.87135 0.29667 0.22345	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\end{array}$
-1086.2448778 O C O C C H C H C	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067 -0.18939	0.16650 -0.78281 -1.29170 -1.02623 -1.37231 -1.87135 0.29667 0.22345 1.36460	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\\ -0.33448\end{array}$
-1086.2448778 O C O C C H C H C C C	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067 -0.18939 -0.55722	$\begin{array}{c} 0.16650\\ -0.78281\\ -1.29170\\ -1.02623\\ -1.37231\\ -1.87135\\ 0.29667\\ 0.22345\\ 1.36460\\ 2.45995\end{array}$	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\end{array}$
-1086.2448778 O C O C C H C C H C C H	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067 -0.18939 -0.55722 -0.08661	$\begin{array}{c} 0.16650\\ -0.78281\\ -1.29170\\ -1.02623\\ -1.37231\\ -1.87135\\ 0.29667\\ 0.22345\\ 1.36460\\ 2.45995\\ 2.60701 \end{array}$	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\end{array}$
-1086.2448778 O C O C C H C C H C C H C C	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067 -0.18939 -0.55722 -0.08661 -1.54213	$\begin{array}{c} 0.16650\\ -0.78281\\ -1.29170\\ -1.02623\\ -1.37231\\ -1.87135\\ 0.29667\\ 0.22345\\ 1.36460\\ 2.45995\\ 2.60701\\ 3.34529\end{array}$	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\end{array}$
-1086.2448778 O C O C C H C C H C C H C H	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067 -0.18939 -0.55722 -0.08661 -1.54213 -1.81845	0.16650 -0.78281 -1.29170 -1.02623 -1.37231 -1.87135 0.29667 0.22345 1.36460 2.45995 2.60701 3.34529 4.18982	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\\ -1.29266\end{array}$
-1086.2448778 O C O C C H C C H C C H C C H C C H C C	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067 -0.18939 -0.55722 -0.08661 -1.54213 -1.81845 -2.18166	$\begin{array}{c} 0.16650\\ -0.78281\\ -1.29170\\ -1.02623\\ -1.37231\\ -1.87135\\ 0.29667\\ 0.22345\\ 1.36460\\ 2.45995\\ 2.60701\\ 3.34529\\ 4.18982\\ 3.14134 \end{array}$	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\\ -1.29266\\ 0.54897\end{array}$
-1086.2448778 O C O C C H C H C H C H C H C H	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067 -0.18939 -0.55722 -0.08661 -1.54213 -1.81845 -2.18166 -2.94966	0.16650 - 0.78281 - 1.29170 - 1.02623 - 1.37231 - 1.87135 0.29667 0.22345 1.36460 2.45995 2.60701 3.34529 4.18982 3.14134 3.82837	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\\ -1.29266\\ 0.54897\\ 0.88455\end{array}$
-1086.2448778 O C O C C H C C H C C H C C H C C H C C H C C	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067 -0.18939 -0.55722 -0.08661 -1.54213 -1.81845 -2.18166 -2.94966 -1.83747	0.16650 -0.78281 -1.29170 -1.02623 -1.37231 -1.87135 0.29667 0.22345 1.36460 2.45995 2.60701 3.34529 4.18982 3.14134 3.82837 2.05283	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\\ -1.29266\\ 0.54897\\ 0.88455\\ 1.35122\end{array}$
-1086.2448778 O C O C C H C H C H C H C H C H	ImgFreq/IR inten: -820.6690/2136.9112 -0.42009 0.29870 1.22023 0.23783 -1.14990 0.87581 0.80635 0.87067 -0.18939 -0.55722 -0.08661 -1.54213 -1.81845 -2.18166 -2.94966 -1.83747 -2.30558	0.16650 - 0.78281 - 1.29170 - 1.02623 - 1.37231 - 1.87135 0.29667 0.22345 1.36460 2.45995 2.60701 3.34529 4.18982 3.14134 3.82837 2.05283 1.87764	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\\ -1.29266\\ 0.54897\\ 0.88455\\ 1.35122\\ 2.31252\end{array}$
-1086.2448778 O C O C C H C C H C C H C C H C C H C C H C C H C	$\begin{tabular}{lllllllllllllllllllllllllllllllllll$	0.16650 - 0.78281 - 1.29170 - 1.02623 - 1.37231 - 1.87135 0.29667 0.22345 1.36460 2.45995 2.60701 3.34529 4.18982 3.14134 3.82837 2.05283 1.87764 1.19843	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\\ -1.29266\\ 0.54897\\ 0.88455\\ 1.35122\\ 2.31252\\ 0.88760\end{array}$
-1086.2448778 O C O C C H C C H C C H C C H C C H C C H C C H C C H C	$\begin{array}{r} \mbox{ImgFreq/IR inten: -820.6690/2136.9112} \\ -0.42009 \\ 0.29870 \\ 1.22023 \\ 0.23783 \\ -1.14990 \\ 0.87581 \\ 0.80635 \\ 0.87067 \\ -0.18939 \\ -0.55722 \\ -0.08661 \\ -1.54213 \\ -1.81845 \\ -2.18166 \\ -2.94966 \\ -1.83747 \\ -2.30558 \\ -0.85714 \\ 2.23713 \end{array}$	0.16650 -0.78281 -1.29170 -1.02623 -1.37231 -1.87135 0.29667 0.22345 1.36460 2.45995 2.60701 3.34529 4.18982 3.14134 3.82837 2.05283 1.87764 1.19843 0.57909	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\\ -1.29266\\ 0.54897\\ 0.88455\\ 1.35122\\ 2.31252\\ 0.88760\\ -0.20331\end{array}$
-1086.2448778 O C O C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C C C H C	$\begin{array}{r} \mbox{ImgFreq/IR inten: -820.6690/2136.9112} \\ -0.42009 \\ 0.29870 \\ 1.22023 \\ 0.23783 \\ -1.14990 \\ 0.87581 \\ 0.80635 \\ 0.87067 \\ -0.18939 \\ -0.55722 \\ -0.08661 \\ -1.54213 \\ -1.81845 \\ -2.18166 \\ -2.94966 \\ -1.83747 \\ -2.30558 \\ -0.85714 \\ 2.23713 \\ 2.94768 \end{array}$	0.16650 -0.78281 -1.29170 -1.02623 -1.37231 -1.87135 0.29667 0.22345 1.36460 2.45995 2.60701 3.34529 4.18982 3.14134 3.82837 2.05283 1.87764 1.19843 0.57909 -0.70762	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\\ -1.29266\\ 0.54897\\ 0.88455\\ 1.35122\\ 2.31252\\ 0.88760\\ -0.20331\\ 0.19969\end{array}$
-1086.2448778 O C O C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C N O O C C N O C C N O C C N O C C N O C O C	$\begin{array}{r} \mbox{ImgFreq/IR inten: -820.6690/2136.9112} \\ -0.42009 \\ 0.29870 \\ 1.22023 \\ 0.23783 \\ -1.14990 \\ 0.87581 \\ 0.80635 \\ 0.87067 \\ -0.18939 \\ -0.55722 \\ -0.08661 \\ -1.54213 \\ -1.54213 \\ -1.81845 \\ -2.18166 \\ -2.94966 \\ -1.83747 \\ -2.30558 \\ -0.85714 \\ 2.23713 \\ 2.94768 \\ 4.20356 \end{array}$	0.16650 -0.78281 -1.29170 -1.02623 -1.37231 -1.87135 0.29667 0.22345 1.36460 2.45995 2.60701 3.34529 4.18982 3.14134 3.82837 2.05283 1.87764 1.19843 0.57909 -0.70762 -0.40195	$\begin{array}{c} 1.78406\\ 1.26769\\ 1.96435\\ -0.20531\\ -0.78435\\ -0.45885\\ -0.76530\\ -1.85134\\ -0.33448\\ -1.11339\\ -2.07967\\ -0.67210\\ -1.29266\\ 0.54897\\ 0.88455\\ 1.35122\\ 2.31252\\ 0.88760\\ -0.20331\\ 0.19969\\ 0.70880\end{array}$

Н		2.17772	1.11030	0.75055
Н		4.66897	0.08910	0.00179
0		3.02739	1.27073	-1.11542
Н		3.25521	2.14954	-0.78879
Н		2.11500	-1.30005	1.26417
Н		3.53137	-2.29950	-0.69783
0		-1.43624	-1.15388	-1.92789
0		-1.88127	-2.00299	0.12858
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Н		-3.34545	-3.37303	0.39062
Н		-3.10117	-2.89457	-1.30557
С		-4.27913	-1.48325	-0.14230
Н		-5.24406	-1.93431	-0.38819
Н		-4.12075	-0.64615	-0.82433
Н		-4.33891	-1.10828	0.88170
TS [3.1 ⁺ /3.2 ⁺]				
-1086.2410391	ImgFreq/IR inten:			
	-1144.7969/2716.0642			
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С		-0.13567	-0.88543	1.48553
0		0.54777	-1.51476	2.31787
C		-0.00186	-1.17710	0.01752
C		-1.31743	-1.30236	-0.77931
Н		0.50326	-2.13655	-0.10214
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Н		0.99958	-0.12225	-1.55883
С		0.06858	1.25801	-0.18529
С		0.07398	2.38302	-1.00904
Н		0.72153	2.40149	-1.87927
С		-0.75993	3.46665	-0.73522
Н		-0.74414	4.33256	-1.38674
С		-1.62186	3.43395	0.35964
Н		-2.27405	4.27458	0.56605
С		-1.65101	2.32187	1.20043
Н		-2.29821	2.27617	2.06818
С		-0.80835	1.26642	0.90762
С		2.27032	-0.01313	0.18969
Ν		3.32132	0.19854	-0.75012
0		3.31078	-0.72795	-1.79633
0		4.52494	0.06146	-0.01394
Н		2.37477	0.73925	0.96842
Н		3.53697	-1.60510	-1.43245
Н		5.15648	0.66931	-0.42699
0		2.50974	-1.36178	0.90911
Н		3.38726	-1.32814	1.32795
Н		1.62903	-1.63744	1.68815

0	-1.37527	-1.07759	-1.95633
0	-2.28336	-1.76342	0.00594
С	-3.59102	-2.06162	-0.60815
Н	-3.99125	-2.84618	0.03117
Н	-3.40605	-2.46081	-1.60449
С	-4.47604	-0.83360	-0.63448
Н	-5.45664	-1.11006	-1.03071
Н	-4.06480	-0.05498	-1.27927
Н	-4.62430	-0.42927	0.36912
TS [2.2/4']			
-1009.3845499	ImgFreq/IR inten: -774.9873/21.7264		
0	-1.18943	-2.29431	-0.24983
С	0.09088	-2.11347	0.17343
0	0.87363	-3.01367	0.09284
С	0.41016	-0.75205	0.79101
Н	0.00767	-0.77917	1.80995
С	1.92320	-0.58410	0.93097
С	-0.28183	0.40602	0.01047
Н	0.18228	0.51059	-0.97222
С	-1.76164	0.07290	-0.12385
С	-2.76576	1.04570	-0.17483
Н	-2.48585	2.09361	-0.10717
С	-4.10030	0.67321	-0.31347
Н	-4.86833	1.43762	-0.35264
С	-4.44552	-0.67493	-0.40310
Н	-5.48433	-0.96783	-0.51095
С	-3.45814	-1.65437	-0.36112
Н	-3.69469	-2.70912	-0.44005
С	-2.13008	-1.26904	-0.22331
С	-0.10399	1.67134	0.78109
Ν	0.46270	2.79085	0.35313
0	1.00197	2.69072	-0.95071
0	-0.73573	3.56609	0.44742
Н	1.50628	3.51102	-1.04834
Н	-0.43303	1.72062	1.81217
0	2.49016	-0.54793	1.99335
0	2.50540	-0.46075	-0.26304
С	3.95482	-0.33885	-0.27780
Н	4.37120	-1.21424	0.22378
Н	4.22870	0.54564	0.30077
С	4.39039	-0.24166	-1.72307
Н	5.47862	-0.14855	-1.77252
Н	3.95149	0.63161	-2.21071
Н	4.09991	-1.13311	-2.28286

TS [2.2/4'']			
-1009.3866489	ImgFreq/IR inten: -897.0411/42.6806		
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С	-0.32071	-0.77258	1.27250
0	-0.67531	-1.57055	2.08358
С	-0.31564	-0.99247	-0.23453
Н	-0.24140	-2.07485	-0.37962
С	-1.61565	-0.53837	-0.91319
С	0.87775	-0.32134	-0.92439
Н	0.70271	-0.33872	-2.00576
С	0.99118	1.12512	-0.46264
С	1.46726	2.15706	-1.27570
Н	1.76770	1.93378	-2.29515
С	1.54118	3.46108	-0.79827
Н	1.90743	4.25378	-1.44098
С	1.13175	3.74444	0.50661
Н	1.18457	4.75973	0.88477
С	0.64722	2.73255	1.32759
Н	0.31885	2.92870	2.34170
С	0.58539	1.42954	0.83885
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Ν	2.36864	-2.00054	0.12613
0	3.73346	-2.23184	0.41881
0	1.76925	-2.95827	-0.73874
Н	3.71173	-2.77134	1.22229
Н	3.09054	-0.47134	-1.08102
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0	-2.64529	-0.52909	-0.06620
С	-3.95142	-0.19790	-0.61650
Н	-4.16938	-0.90278	-1.42102
Н	-3.89491	0.80230	-1.05066
С	-4.95465	-0.28264	0.51255
Н	-5.95221	-0.04215	0.13502
Н	-4.71324	0.42263	1.31065
Н	-4.98386	-1.28707	0.93955
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0	-0.74195	-1.59036	2.26275
С	-0.34948	-1.24175	-0.08829
С	-1.64319	-0.92246	-0.84874
Н	-0.24827	-2.32896	-0.11370
С	0.85550	-0.60347	-0.82359
Н	0.67244	-0.74156	-1.89308
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Н	1.77491	1.50101	-2.36017
С	1.42830	3.17725	-1.05907
Н	1.82015	3.90380	-1.76250
С	0.94224	3.59163	0.18325
Н	0.95737	4.64257	0.45191
С	0.43343	2.66130	1.08115
Н	0.05082	2.95494	2.05178
С	0.41960	1.31301	0.73057
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Н	2.50184	-3.05935	-1.34674
Н	3.71933	-1.28859	-0.76648
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Н	-3.73486	0.56314	-1.45156
С	-4.81934	0.32731	0.42239
Н	-5.79940	0.55538	-0.00542
Н	-4.42855	1.23747	0.88231
Н	-4.95435	-0.42234	1.20475
H TS [6.2/6.3]	-4.95435	-0.42234	1.20475
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H TS [6.2/6.3] -1009.4706740 O	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427	-0.42234 0.29626	1.20475 1.74619
H TS [6.2/6.3] -1009.4706740 O C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341	-0.42234 0.29626 -0.95570	1.20475 1.74619 1.26302
H TS [6.2/6.3] -1009.4706740 O C O	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556	-0.42234 0.29626 -0.95570 -1.83733	1.20475 1.74619 1.26302 2.03035
H TS [6.2/6.3] -1009.4706740 O C O C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444	-0.42234 0.29626 -0.95570 -1.83733 -1.12764	1.20475 1.74619 1.26302 2.03035 -0.24575
H TS [6.2/6.3] -1009.4706740 O C O C C C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602
H TS [6.2/6.3] -1009.4706740 O C O C C C H	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966
H TS [6.2/6.3] -1009.4706740 O C C C C H C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309
H TS [6.2/6.3] -1009.4706740 O C C C C H C H	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573
H TS [6.2/6.3] -1009.4706740 O C O C C H C H C H C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394
H TS [6.2/6.3] -1009.4706740 O C O C C H C H C H C C C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566 1.42352	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020 2.13817	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394 -1.09241
H TS [6.2/6.3] -1009.4706740 O C O C C H C C H C C H C C H	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566 1.42352 1.87598	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020 2.13817 1.94810	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394 -1.09241 -2.05977
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H TS [6.2/6.3] -1009.4706740 O C O C C H C C H C C H C C H C C H H C H	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566 1.42352 1.87598 1.31141 1.67420	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020 2.13817 1.94810 3.44036 4.26814	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394 -1.09241 -2.05977 -0.61587 -1.21507
H TS [6.2/6.3] -1009.4706740 O C O C C H C C H C C H C C H C C H C C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566 1.42352 1.87598 1.31141 1.67420 0.73250	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020 2.13817 1.94810 3.44036 4.26814 3.67708	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394 -1.09241 -2.05977 -0.61587 -1.21507 0.63193
H TS [6.2/6.3] -1009.4706740 O C O C O C H C H C H C H C H C H H C H H C H H	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566 1.42352 1.87598 1.31141 1.67420 0.73250 0.64234	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020 2.13817 1.94810 3.44036 4.26814 3.67708 4.69059	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394 -1.09241 -2.05977 -0.61587 -1.21507 0.63193 1.00799
H TS [6.2/6.3] -1009.4706740 O C O C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566 1.42352 1.87598 1.31141 1.67420 0.73250 0.64234 0.26630	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020 2.13817 1.94810 3.44036 4.26814 3.67708 4.69059 2.61619	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394 -1.09241 -2.05977 -0.61587 -1.21507 0.63193 1.00799 1.40105
H TS [6.2/6.3] -1009.4706740 O C O C C C H C C H C C H C C H C C H C H	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566 1.42352 1.87598 1.31141 1.67420 0.73250 0.64234 0.26630 -0.18339	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020 2.13817 1.94810 3.44036 4.26814 3.67708 4.69059 2.61619 2.77059	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394 -1.09241 -2.05977 -0.61587 -1.21507 0.63193 1.00799 1.40105 2.37508
H TS [6.2/6.3] -1009.4706740 O C O C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566 1.42352 1.87598 1.31141 1.67420 0.73250 0.64234 0.26630 -0.18339 0.39039	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020 2.13817 1.94810 3.44036 4.26814 3.67708 4.69059 2.61619 2.77059 1.32084	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394 -1.09241 -2.05977 -0.61587 -1.21507 0.63193 1.00799 1.40105 2.37508 0.90956
H TS [6.2/6.3] -1009.4706740 O C O C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C	-4.95435 ImgFreq/IR inten: -1882.8793/388.3928 -0.04427 -0.30341 -0.56556 -0.19444 -1.45031 -0.10378 1.03357 0.96782 0.96566 1.42352 1.87598 1.31141 1.67420 0.73250 0.64234 0.26630 -0.18339 0.39039 2.36007	-0.42234 0.29626 -0.95570 -1.83733 -1.12764 -0.67914 -2.20011 -0.38098 -0.40479 1.06020 2.13817 1.94810 3.44036 4.26814 3.67708 4.69059 2.61619 2.77059 1.32084 -1.00300	1.20475 1.74619 1.26302 2.03035 -0.24575 -1.00602 -0.41966 -0.80309 -1.89573 -0.33394 -1.09241 -2.05977 -0.61587 -1.21507 0.63193 1.00799 1.40105 2.37508 0.90956 -0.44631

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Н	1.77208	-3.50534	1.08586
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Н	-4.03172	-0.95854	-1.52956
Н	-3.62290	0.75311	-1.37582
С	-4.79252	-0.02979	0.28651
Н	-5.76159	0.23513	-0.14486
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Н	-4.90972	-0.96312	0.84102
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С	-0.57786	-1.26624	-0.15893
С	-1.77683	-0.74951	-0.96300
Н	-0.56897	-2.34902	-0.29058
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Н	0.67039	-0.75294	-1.81816
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С	0.62748	3.48006	0.46122
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С	0.15411	2.48370	1.30822
Н	-0.26008	2.71248	2.28330
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Ν	2.68769	-1.36692	0.83592
0	3.09798	-0.17379	1.11440
Н	2.20499	-3.41614	0.03587
Н	3.02713	-0.89176	-1.06058
Н	3.58101	0.33022	-0.23184
0	3.74171	0.04715	-1.23589
Н	4.65591	-0.25590	-1.32731
0	-1.78679	-0.70227	-2.16793
0	-2.79972	-0.39882	-0.17791
С	-4.01476	0.04980	-0.83973
Н	-4.35050	-0.74484	-1.50887

Н	-3.76905	0.92166	-1.44926
С	-5.03065	0.36457	0.23620
Н	-5.96236	0.70125	-0.22660
Н	-4.67380	1.15651	0.89815
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C	-1.62110	-1.39657	-0.55656
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C	0.65933	-0.34555	-0.67394
Н	0.42496	-0.59128	-1.71061
C	0.37587	1.12462	-0.44512
С	0.71167	2.08984	-1.40047
Н	1.20738	1.77242	-2.31300
С	0.41769	3.43411	-1.19964
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Н	-0.47426	4.87695	0.13291
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H	-1.08883	3.16941	1.84571
C	-0.27246	1.54641	0.71688
C	2.13871	-0.70278	-0.55949
0	2.70051	-1.18898	-1.61302
N	2.87538	-0.54246	0.51659
0	2.18091	-0.18466	1.68508
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H	2.02403	0.60684	2.01981
H	4.0/106	-1.07996	0.31145
U U	4.80309	-1.54519	-0.51103
П	5.09005	-2.44579	-0.52577
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0 C	-2.07072	-1.28244	0.23100
U U	-5.99702	-1.49820	-0.52309
п u	-4.39398	-1.63493	0.32424
II C	-3.92042	-2.30044	-1.03700
ч	-4.55051 5 57140	-0.22274	-0.93120
н	-5.57140 2 05221	0.37039	-1.20203 -1.78/57
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TS [6 2/7]+w	-4.58002	0.30234	-0.17570
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Н	-1.26239	-1.13239	-2.23281
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С	-1.66032	-2.57548	0.08031
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С	-1.65224	-3.21604	1.31659
Н	-2.06406	-4.21417	1.40893
С	-1.11225	-2.57594	2.43256
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С	-0.57520	-1.29562	2.32226
Н	-0.15042	-0.78329	3.17743
С	-0.58685	-0.67592	1.08233
С	-2.14059	0.55690	-1.18791
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Н	-3.96109	1.07937	-1.14114
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Н	1.51759	4.45788	2.10538
0	1.44703	-1.66450	-2.03015
0	2.43361	-0.20890	-0.61217
С	3.67240	-0.99818	-0.60942
Н	4.01838	-1.07314	-1.64100
Н	3.42650	-2.00099	-0.25767
С	4.66298	-0.29212	0.28629
Н	5.59822	-0.85693	0.30584
Н	4.29326	-0.21935	1.31138
Н	4.88454	0.71269	-0.07898
TS [7/8]+w			
-1086.2689347	ImgFreq/IR inten: -1839.7895/970.5662		
0	0.08406	-0.18210	-1.35989
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Н	-0.05454	-1.78843	1.69948
С	-0.69001	0.25114	1.25670
Н	-0.77698	0.53895	2.30229
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С	-0.19270	1.40713	0.38806
С	-0.11509	2.72247	0.84643
Н	-0.44738	2.95874	1.85166
С	0.40878	3.72345	0.02974
Н	0.47286	4.73992	0.40083
С	0.85841	3.41860	-1.25372
Н	1.26763	4.20001	-1.88631
С	0.78350	2.11384	-1.74295
Н	1.11288	1.86521	-2.74687
С	0.26119	1.14065	-0.91179
С	-2.01762	-0.24462	0.70225
0	-3.14873	0.26095	1.01149
Ν	-1.76152	-1.20566	-0.15642
0	-2.66400	-1.72984	-1.03926
Н	-3.97845	-0.10447	0.54178
Н	-2.16188	-2.44549	-1.48395
Н	0.54867	-1.17193	-1.84882
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Н	-5.43594	-1.19739	-0.74801
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0	2.07253	-0.17786	2.26541
0	2.47453	-1.10819	0.24462
С	3.92581	-0.95481	0.42198
Н	4.20092	-1.47367	1.34082
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С	4.60070	-1.53612	-0.79811
Н	5.68416	-1.44880	-0.68617
Н	4.31530	-1.00308	-1.70785
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TS [7/8] ⁺ 2w			
-1086.3192152	ImgFreq/IR inten: -241.5133/103.9918		
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0	1.32662	-2.52020	0.52634
С	-0.18667	-1.01586	-0.77318
С	-1.53165	-1.02251	-0.06197
Н	-0.25155	-1.76060	-1.57295
С	0.24861	0.35502	-1.36575
Н	-0.31872	0.67145	-2.23613
С	0.27109	1.39336	-0.25631
С	-0.10878	2.72419	-0.44094
Н	-0.45332	3.04948	-1.41684
С	-0.05195	3.62649	0.61636
Н	-0.35786	4.65561	0.46734
С	0.39782	3.20050	1.86537
Н	0.44650	3.90037	2.69119

С	0.79580	1.88177	2.06552
Н	1.16621	1.54967	3.02949
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С	1.69573	0.07247	-1.71632
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Ν	2.14074	-0.84886	-0.93741
0	3.42832	-1.26955	-0.88320
Н	3.29221	0.50633	-2.67057
Н	3.37496	-2.11070	-0.38158
Н	0.53154	-2.80744	2.42565
Н	0.60697	-1.26384	2.51646
0	0.04590	-2.05032	2.80338
Н	-0.77994	-1.92991	2.20961
0	-1.74127	-1.45660	1.06538
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Н	-3.86647	0.06146	0.58754
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С	-4.74169	0.04068	-1.40812
Н	-5.77578	0.05853	-1.05556
Н	-4.70723	-0.56446	-2.31592
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TS [8 ⁺ 2w/8:H ₃ O ⁺]			
-1086.3464809	ImgFreq/IR inten: -104.2035/161.0798		
-1086.3464809 O	ImgFreq/IR inten: -104.2035/161.0798 0.84579	0.90551	1.45784
-1086.3464809 O C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635	0.90551 -1.93547	1.45784 0.02528
-1086.3464809 O C O	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568	0.90551 -1.93547 -2.90840	1.45784 0.02528 0.70111
-1086.3464809 O C O C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253	0.90551 -1.93547 -2.90840 -1.32698	1.45784 0.02528 0.70111 -0.62093
-1086.3464809 O C O C C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129	0.90551 -1.93547 -2.90840 -1.32698 -1.30988	1.45784 0.02528 0.70111 -0.62093 0.31559
-1086.3464809 O C O C C H	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054	1.45784 0.02528 0.70111 -0.62093 0.31559 -1.47510
-1086.3464809 O C O C C H C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689	1.45784 0.02528 0.70111 -0.62093 0.31559 -1.47510 -1.14785
-1086.3464809 O C O C C H C H	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211	1.45784 0.02528 0.70111 -0.62093 0.31559 -1.47510 -1.14785 -2.23224
-1086.3464809 O C O C C H C H C C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120	1.45784 0.02528 0.70111 -0.62093 0.31559 -1.47510 -1.14785 -2.23224 -0.54810
-1086.3464809 O C O C C H C H C C H C C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020	1.45784 0.02528 0.70111 -0.62093 0.31559 -1.47510 -1.14785 -2.23224 -0.54810 -1.28600
-1086.3464809 O C O C C H C H C C H C C H	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683	1.45784 0.02528 0.70111 -0.62093 0.31559 -1.47510 -1.14785 -2.23224 -0.54810 -1.28600 -2.32216
-1086.3464809 O C O C C H C H C C H C C H C C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004 -1.98545	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456	1.45784 0.02528 0.70111 -0.62093 0.31559 -1.47510 -1.14785 -2.23224 -0.54810 -1.28600 -2.32216 -0.69726
-1086.3464809 O C O C C H C C H C C H C H H C H	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004 -1.98545 -2.71679	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456 3.61806	$\begin{array}{c} 1.45784\\ 0.02528\\ 0.70111\\ -0.62093\\ 0.31559\\ -1.47510\\ -1.14785\\ -2.23224\\ -0.54810\\ -1.28600\\ -2.32216\\ -0.69726\\ -1.27582\end{array}$
-1086.3464809 O C O C C H C C H C C H C C H C C H C C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004 -1.98545 -2.71679 -1.74970	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456 3.61806 3.39308	$\begin{array}{c} 1.45784\\ 0.02528\\ 0.70111\\ -0.62093\\ 0.31559\\ -1.47510\\ -1.14785\\ -2.23224\\ -0.54810\\ -1.28600\\ -2.32216\\ -0.69726\\ -1.27582\\ 0.63755\end{array}$
-1086.3464809 O C O C C H C H C H C H C H H C H	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004 -1.98545 -2.71679 -1.74970 -2.29492	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456 3.61806 3.39308 4.20712	$\begin{array}{c} 1.45784\\ 0.02528\\ 0.70111\\ -0.62093\\ 0.31559\\ -1.47510\\ -1.14785\\ -2.23224\\ -0.54810\\ -1.28600\\ -2.32216\\ -0.69726\\ -1.27582\\ 0.63755\\ 1.10234 \end{array}$
-1086.3464809 O C O C C H C H C C H C H C C H C C H C C H C C H C C H C C H C C H C C C H C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004 -1.98545 -2.71679 -1.74970 -2.29492 -0.80710	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456 3.61806 3.39308 4.20712 2.68763	$\begin{array}{c} 1.45784\\ 0.02528\\ 0.70111\\ -0.62093\\ 0.31559\\ -1.47510\\ -1.14785\\ -2.23224\\ -0.54810\\ -1.28600\\ -2.32216\\ -0.69726\\ -1.27582\\ 0.63755\\ 1.10234\\ 1.38199\end{array}$
-1086.3464809 O C O C C H C H C C H C H C H C H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004 -1.98545 -2.71679 -1.74970 -2.29492 -0.80710 -0.60850	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456 3.61806 3.39308 4.20712 2.68763 2.95155	$\begin{array}{c} 1.45784\\ 0.02528\\ 0.70111\\ -0.62093\\ 0.31559\\ -1.47510\\ -1.14785\\ -2.23224\\ -0.54810\\ -1.28600\\ -2.32216\\ -0.69726\\ -1.27582\\ 0.63755\\ 1.10234\\ 1.38199\\ 2.41636\end{array}$
-1086.3464809 O C O C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004 -1.98545 -2.71679 -1.74970 -2.29492 -0.80710 -0.60850 -0.11116	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456 3.61806 3.39308 4.20712 2.68763 2.95155 1.64000	$\begin{array}{c} 1.45784\\ 0.02528\\ 0.70111\\ -0.62093\\ 0.31559\\ -1.47510\\ -1.14785\\ -2.23224\\ -0.54810\\ -1.28600\\ -2.32216\\ -0.69726\\ -1.27582\\ 0.63755\\ 1.10234\\ 1.38199\\ 2.41636\\ 0.78741\end{array}$
-1086.3464809 O C O C C C H C C H C C H C C H C C H C C H C C H C C H C C H C	$\begin{array}{l} \mbox{ImgFreq/IR inten: -104.2035/161.0798} \\ 0.84579 \\ 1.09635 \\ 1.28568 \\ -0.12253 \\ -0.12253 \\ -1.34129 \\ -0.37555 \\ 0.36048 \\ 0.22617 \\ -0.34045 \\ -1.27778 \\ -1.47004 \\ -1.98545 \\ -2.71679 \\ -1.74970 \\ -2.29492 \\ -0.80710 \\ -0.60850 \\ -0.11116 \\ 1.86881 \end{array}$	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456 3.61806 3.39308 4.20712 2.68763 2.95155 1.64000 0.08940	$\begin{array}{c} 1.45784\\ 0.02528\\ 0.70111\\ -0.62093\\ 0.31559\\ -1.47510\\ -1.14785\\ -2.23224\\ -0.54810\\ -1.28600\\ -2.32216\\ -0.69726\\ -1.27582\\ 0.63755\\ 1.10234\\ 1.38199\\ 2.41636\\ 0.78741\\ -0.88648\end{array}$
-1086.3464809 O C O C C H C H C H C H C H C H C H C H	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004 -1.98545 -2.71679 -1.74970 -2.29492 -0.80710 -0.60850 -0.11116 1.86881 2.67072	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456 3.61806 3.39308 4.20712 2.68763 2.95155 1.64000 0.08940 0.99953	$\begin{array}{c} 1.45784\\ 0.02528\\ 0.70111\\ -0.62093\\ 0.31559\\ -1.47510\\ -1.14785\\ -2.23224\\ -0.54810\\ -1.28600\\ -2.32216\\ -0.69726\\ -1.27582\\ 0.63755\\ 1.10234\\ 1.38199\\ 2.41636\\ 0.78741\\ -0.88648\\ -1.12165\end{array}$
-1086.3464809 O C O C C H C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C N C N	ImgFreq/IR inten: -104.2035/161.0798 0.84579 1.09635 1.28568 -0.12253 -1.34129 -0.37555 0.36048 0.22617 -0.34045 -1.27778 -1.47004 -1.98545 -2.71679 -1.74970 -2.29492 -0.80710 -0.60850 -0.11116 1.86881 2.67072 2.18315	0.90551 -1.93547 -2.90840 -1.32698 -1.30988 -1.96054 0.08689 0.12211 1.29120 2.02020 1.75683 3.06456 3.61806 3.39308 4.20712 2.68763 2.95155 1.64000 0.08940 0.99953 -1.11810	$\begin{array}{c} 1.45784\\ 0.02528\\ 0.70111\\ -0.62093\\ 0.31559\\ -1.47510\\ -1.14785\\ -2.23224\\ -0.54810\\ -1.28600\\ -2.32216\\ -0.69726\\ -1.27582\\ 0.63755\\ 1.10234\\ 1.38199\\ 2.41636\\ 0.78741\\ -0.88648\\ -1.12165\\ -0.35624\end{array}$

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Н	3.27435	-2.27699	0.63278
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