

Supporting Information

**Correlations between ECD spectra and absolute configuration of bridged-ring
lactones: Revisiting Beecham's rule**

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Table S1. Source and experimental data of compounds **5-51**.

Entry	Name	Source*	AC assignment method	Experimental data	
				ECD ($\Delta\epsilon/\lambda(\text{nm})$)	$[\alpha]_D$
1	1,5-Quinide (5a)	Synthesis	ECD	-2.70 (222)*	-29.7 (1, MeOH)
2	Quinic acid 1,5-lactone triacetate (5b)	Synthesis	ECD	-3.85 (217)*	/
3	3,4-O-Isopropyliden-1,5- γ -quinide (6a)	Synthesis	ECD	-2.40 (222)*	-30.3 (1, MeOH)
4	3,4-O-Isopropyliden-1,5- γ -quinide 2-acetate (6b)	Synthesis	ECD	-4.40 (218)*	/
5	3,4-O-Isopropyliden-1,5- γ -quinide 2-sulfate (6c)	Synthesis	ECD	-3.43 (218)*	/
6	Jhanilactone (7)	NP (<i>Eupatorium jhanii</i> Robinson)	X-ray diffraction	-1.43 (214)	-5 (CHCl ₃)
7	Epicaltholide (8)	NP (<i>Caltha palustris</i>)	ECD	+2.32 (217)	/
8	Rosololactone (9)	NP (<i>Holarrhena floribunda</i>)	Modified Horeau's method	+1.04 (224)*	-3 (1.4, CHCl ₃)
9	Heteroscyphin C (10)	NP (<i>Heteroscyphus tener</i>)	ECD	+1.53 (228)	+21 (0.1, MeOH)
10	Rubesanolide D (11a)	NP (<i>Isodon rubescens</i>)	X-ray diffraction	-6.27 (216)	-62 (1.93, MeOH)
11	Rubesanolide C (11b)	NP (<i>Isodon rubescens</i>)	X-ray diffraction	-3.05 (217)	-48.9
12	Norflickinflimiod B (12a)	NP (<i>Flickingeria fimbriata</i>)	X-ray diffraction	-0.12 (220)	-2.7 (0.3 CHCl ₃)
13	Norflickinflimiod C (12b)	NP (<i>Flickingeria fimbriata</i>)	ECD	-0.31 (221)	-13.3 (0.1 CHCl ₃)
14	Corialactone A (13)	NP (<i>Coriaria nepalensis</i>)	ECD	+0.88 (224.5)	+13.7 (0.07, MeOH)
15	Corialactone C (14)	NP (<i>Coriaria nepalensis</i>)	X-ray diffraction	+1.25 (229.5)	+109.6 (0.1, MeOH)
16	Corialactone D (15)	NP (<i>Coriaria nepalensis</i>)	ECD	+3.12 (207.5)	+20.6 (0.07, MeOH)
17	Dendrobine (16a)	NP (<i>Dendrobium nobile</i> Lindl)	Total synthesis	3.6 (225) ^a	-52.6 (1.6, CHCl ₃)
18	Dendramine (16b)	NP (<i>Dendrobium hildebrandii</i> Rolfe)	Comparison with analogues	3.2 (225) ^a	-25 (0.1, CHCl ₃)
19	Methyl tetrahydro-gibberellate (17)	NP (plant hormone)	ORD	/	+59 (1, MeOH); +50 (600), +100 (400), +550

					(290)
20	Gibberellin C (18)	NP (plant hormone)	X-ray diffraction	-2.05 (290)	+48 (1, MeOH)
21	(3 <i>S</i>)-4-Oxatricyclo[4.3.1.0 ^{3,7}]decan-5-one (19)	Synthesis	ECD	+0.88 (222.5)*	+8.1 (0.5, MeOH)
22	(1 <i>S</i>)-1,4-Dimethyl-6- <i>endo</i> -hydroxy-5- <i>exo</i> -iodo-bicyclo-[2.2.1]heptane-2- <i>endo</i> -carboxylic acid lactone (20a)	Synthesis	ECD	+0.15 (264), -0.5 (229), +0.1 (210)	/
23	(1 <i>R</i>)-6- <i>endo</i> -Hydroxy-5- <i>exo</i> -iodo-bicyclo [2.2.1] heptane-2- <i>endo</i> -carboxylic acid lactone (21a)	Synthesis	ECD and OR	>0 (260) ^a <0 (220) ^a	Enantiomer: -240 (2.0, C ₆ H ₆)
24	(1 <i>R</i>)-6- <i>endo</i> -Hydroxy-5- <i>exo</i> -iodo-1-methylbicyclo[2.2.1]-heptane-2- <i>endo</i> -carboxylic acid lactone (22a)	Synthesis	ECD	+0.44 (257), -1.06 (225)	+75.8 (2.01, CCl ₄)
25	(1 <i>R</i>)-1,5-Dimethyl-6- <i>endo</i> -hydroxy-6- <i>exo</i> -iodo-bicyclo-[2.2.1]heptane-2- <i>endo</i> -carboxylic acid lactone (23a)	Synthesis	ECD	+0.44 (274) -0.07 (233) >0 (220)	101.5 (1, CCl ₄)
26	Diospyrolide (24)	NP (<i>Diospyros maritima</i>)	X-ray diffraction	-3.6 (216)	+30.8 (0.25, CHCl ₃)
27	Cleistocalyxolide A (25)	NP (<i>Cleistocalyx operculatus</i>)	ECD	>0 (220) ^a	+16.4 (0.18, MeOH)
28	14β-Hydroxy-(5β,14β)-androstane-17β,carboxylic acid lactone (26)	Synthesis	ECD	>0 (227) ^a	/
29	5-Hydroxyl-A-nor-5α-cholestan-1α-yl carboxylic acid lactone (27)	Synthesis	ECD	+0.87 (220)*	+38.3 (0.98, MeOH)
30	(+)-3,11,12-Trihydroxypicr-otoxane-2(15)-lactone (28)	NP (<i>Dendrobium nobile</i>)	X-ray diffraction	+1.56 (221)	+9.1 (0.21, MeOH)
31	(-)-3,11,13-Trihydroxypicr-otoxane-2(15)-lactone (29)	NP (<i>Dendrobium nobile</i>)	ECD	-1.16 (217)	-4.7 (0.23, MeOH)
32	Portentol (30)	NP (<i>Roccella Portentosa</i>)	ECD	-1.93 (234)	+21 (1.02, MeOH)
33	Dihydroketopicrotoxinic acid (31)	Synthesis	ECD	-4.5 (228)	-80 (0.45, MeOH)

34	δ -Nobilonine (32)	Synthesis	ECD	-0.75 (225)	-76 (0.45, MeOH)
35	α -Bromocampholide (33a)	Synthesis	ORD	/	+16 (589), +64 (365), +480 (254)
36	Dibromocampholide (33b)	Synthesis	ORD	/	+59 (EtOH); +191 (589), +680 (365), +3360 (254)
37	Kudinchalactone A (34a)	NP (<i>Ilex kudincha</i>)	ECD	-29.8 (232)	-23.1 (0.2, MeOH)
38	3 β ,21 α -Dihydroxytaraxast- 28,20 β -olide (34b)	NP (<i>Cleistocalyx operculatus</i>)	ECD	-2.5 (220)	-1.1 (0.17, MeOH)
39	(1 <i>S</i> ,5 <i>R</i>)-9-Oxabicyclo[3.3.2]decane-4, 10 -Dione (35a)	Synthesis	ECD	-0.82 (293), +0.79 (220)	-85 (0.013, EtOH)
40	Ethyl (1 <i>S</i> ,2 <i>R</i> ,5 <i>R</i>)-4,10-dioxo-9-oxabicyclo[3.3.2]- decane-2-carboxylate (35b)	Synthesis	ECD	-2.16 (300), +1.93 (225)	-54 (0.11, EtOH)
41	(1 <i>R</i> ,5 <i>R</i> ,7 <i>S</i>)-7-Methyl-9-oxa-bicyclo[3.3.2]decane- 4, 10 -Dione (35c)	Synthesis	ECD	+1.7 (293), -1.39 (220)	+145 (0.069, EtOH)
42	1 <i>R</i> ,9 <i>R</i> -9-Bromo-2-oxa-homoadamantane-3,7-dione (36a)	Synthesis	ECD	+1.83 (302), 0 (260), +1.16 (234) <0 (200-220)	/
43	1 <i>R</i> ,9 <i>R</i> -9-Iodo-2-oxa-homoadamantane-3,7-dione (36b)	Synthesis	ECD	-0.87 (299), -0.57 (275), -0.59 (260), - 0.42 (240)	/
44	1 <i>R</i> ,9 <i>R</i> -9-Chloro-2-oxa-homoadamantane-3,7-dione (36d)	Synthesis	ECD	-1.45(298), 0 (260), +0.96 (230), 0 (210)	/
45	Illihenlactone B (37)	NP (<i>Illicium henryi</i>)	ECD	+0.88 (220)	-32.6 (0.52, MeOH)
46	Aduncin (38)	NP (<i>Dendrobium aduncum</i>)	ECD	-2.8 (228)	-5.8 (0.4, Me ₂ CO)
47	Cephanolide E (39)	NP (<i>Cephalotaxus sinensis</i>)	X-ray diffraction	-16.46 (236), +15.47 (206)	-103 (0.5, MeOH)

48	Cephanolide F (40)	NP (<i>Cephalotaxus sinensis</i>)	X-ray diffraction	+8.2 (207)	-4 (0.3, MeOH)
49	Cephanolide G (41)	NP (<i>Cephalotaxus sinensis</i>)	ECD	+22.5 (203)	+95 (0.1, MeOH)
50	Cephanolide H (42)	NP (<i>Cephalotaxus sinensis</i>)	ECD	+1.16 (222), -0.48 (206)	-7 (0.1, MeOH)
51	Cephanolide I (43)	NP (<i>Cephalotaxus sinensis</i>)	ECD	+2 (210), +2.5 (198)	-10 (0.1, MeOH)
52	Fortalpinoid L (44)	NP (<i>Cephalotaxus fortunei</i>)	ECD	+13.16 (222)	-102 (0.1, MeOH)
53	Marsupellin A (45)	NP (<i>Marsupella alpine</i>)	X-ray diffraction	<0 (220) ^a	+208 (0.7, MeOH)
54	Corialactone E (46)	NP (<i>Coriaria nepalensis</i>)	ECD	>0 (208) ^a	+9.1 (0.21, MeOH)
55	Cephanolides A (47)	NP (<i>Cephalotaxus sinensis</i>)	X-ray diffraction	+2.39 (238), +1.72 (224), -3.35 (209)	-10 (0.1, MeOH)
56	Cephanolides B (48)	NP (<i>Cephalotaxus sinensis</i>)	ECD	+2.67 (227), -6.08 (204)	-13 (0.1, MeOH)
57	12-Deoxypicrosalvin (49)	NP (<i>Podocarpus imbricatus</i> / Blume)		+3.1 (243), +1.9 (234), +3.1 (220), -16.12 (204)	-23 (0.1, MeOH)
58	(+)-Cochlactone A (50)	NP (<i>Ganoderma cochlear</i>)	X-ray diffraction	>0 (260) ^a >0 (220) ^a	-4.3 (0.36, MeOH)
59	Annotinolide B (51)	NP (<i>Lycopodium annotinum</i>)	X-ray diffraction	/	/

NP: Natural product. * : ECD data were converted from molar ellipticity ($[\theta]=3300\Delta\epsilon$). ^a : ECD data was observed from experiment spectrum.

Table S2. Cartesian coordinates of conformers of **1a-5l** (Cartesian coordinates of simplified structures can be provided if necessary).

Molecule	solvent	Conformers ^a	Entry
1a	/	1aC1	1
1a-A	/	1a-AC1	2
1b	/	1bC1-1bC2	3-4
1c	/	1cC1-1cC6	5-10
1d	/	1dC1-1dC2	11-12
1e	/	1eC1-1eC2	13-14
1f	/	1fC1-1fC3	15-17
1g	/	1gC1-1gC3	18-20
1h	/	1hC1	21
1i	/	1iC1	22
1j	/	1jC1	23
1k	/	1kC1	24
1l	/	1lC1	25
2a	/	2aC1	26
2a-A	/	2a-AC1	27
2b	/	2bC1-2bC2	28-29
2c	/	2cC1-2cC6	30-35
2d	/	2dC1-2dC2	36-37
2e	/	2eC1-2eC2	38-39
2f	/	2fC1-2fC2	40-41
2g	/	2gC1	42
2h	/	2hC1	43
2i	/	2iC1	44
2j	/	2jC1	45
2k	/	2kC1	46
2l	/	2lC1	47
3a	/	3aC1	48
3b	/	3bC1	49
3c	/	3cC1	50
3d	/	3dC1	51
3e	/	3eC1	52
4a	/	4aC1	53
4b	/	4bC1	54
4c	/	4cC1	55
4d	/	4dC1	56
5a	CH ₃ OH	5aC1-5aC8	57-64

5b	CH ₃ OH	5bC1-5bC8	65-72
5c	CH ₃ OH	5cC1	73
6a	CH ₃ OH	6aC1-6aC4	74-77
6b	CH ₃ OH	6bC1-6bC4	78-81
6c	CH ₃ OH	6bC1-6bC8	82-89
7	CH ₃ OH	7C1-7C2	90-91
8	CH ₃ OH	8C1-8C6	92-97
9	CH ₃ OH	9C1-9C3	98-100
10	CH ₃ OH	10C1-10C3	101-103
11a	CH ₃ OH	11aC1-11aC6	104-109
11b	CH ₃ OH	11bC1-11bC8	110-117
12a	CH ₃ CN	12aC1-12aC8	118-125
12b	CH ₃ CN	12bC1-12bC9	126-134
13	CH ₃ OH	13C1	135
16a	CH ₃ OH	16aC1-16aC2	136-137
16b	CH ₃ OH	16bC1-16bC3	138-140
17	CH ₃ OH	17C1-17C10	141-150
18	1,4-dioxane	18C1-18C4	151-154
19	CH ₃ CN	19C1	155
20a	CH ₃ CN	20aC1	156
20b	CH ₃ CN	20bC1	157
21a	CH ₃ CN	21aC1	158
21b	CH ₃ CN	21bC1	159
22a	CH ₃ CN	22aC1	160
22b	CH ₃ CN	22bC1	161
23a	CH ₃ CN	23aC1	162
23b	CH ₃ CN	23bC1	163
24	CH ₃ OH	24C1-24C2	164-165
25	CH ₃ OH	25C1-25C6	166-171
26	CH ₃ OH	26C1	172
27	iso-octane	27C1-27C3	173-175
28	CH ₃ CN	28C1-28C4	176-179
29	CH ₃ CN	29C1-29C6	180-185
30	1,4-dioxane	30C1-30C2	186-187
31	CH ₃ OH	31C1-31C10	188-197
32	CH ₃ OH	32C1-32C6	198-203
33a	CHCl ₃	33aC1	204
33b	CHCl ₃	33bC1	205

33c	CHCl ₃	33cC1	206
34a	CH ₃ OH	34aC1-34aC4	207-210
34b	CH ₃ OH	34bC1-34bC6	211-216
35a	C ₂ H ₅ OH	35aC1-35aC2	217-218
35b	C ₂ H ₅ OH	35bC1-35bC6	219-224
35c	C ₂ H ₅ OH	35cC1	225
36a	CHCl ₃	36aC1	226
36b	CHCl ₃	36bC1	227
36c	CHCl ₃	36cC1	228
36d	CHCl ₃	36dC1	229
37	CH ₃ OH	37C1-37C4	230-233
38	CH ₃ OH	38C1-38C2	234-235
39	CH ₃ OH	39C1-39C4	236-239
40	CH ₃ OH	40C1	240
41	CH ₃ OH	41C1-41C6	241-246
42	CH ₃ OH	42C1-42C3	247-249
43	CH ₃ OH	43C1-43C4	250-253
44	CH ₃ OH	44C1-44C7	254-260
45	CH ₃ OH	45C1-45C4	261-264
46	CH ₃ OH	46C1-46C5	265-269
47	CH ₃ OH	47C1-47C2	270-271
48	CH ₃ OH	48C1-48C2	272-273
49	CH ₃ OH	49C1-49C4	274-277
50	CH ₃ OH	50C1-50C4	278-281
51	CH ₃ OH	51C1	282

a: Ten lowest-energy conformers are given if the amount is over ten, and the conformers over 2% content are listed.

1) Conformer **1aC1**

O	0.60196900	0.04438700	1.16300800
C	-0.53864400	0.85965400	0.78684000
H	-1.01999000	1.24385800	1.68236900
C	-1.22987500	0.00383200	-0.29280200
H	-2.03289500	0.57603300	-0.76421600
C	0.11813900	0.31750700	-1.02186700
H	0.29677600	0.15314700	-2.08018600
C	1.07400500	-0.34665100	-0.05744300
C	0.03682200	1.71511800	-0.34450700
H	-0.69855900	2.36528700	-0.81761800
H	0.96798300	2.24556000	-0.14323100
O	2.01956500	-1.05122300	-0.21829700
C	-1.65516400	-1.41376200	-0.00791300
H	-0.87596900	-1.97576300	0.51054600
H	-1.88985400	-1.93987400	-0.93624400
H	-2.55145500	-1.42774900	0.61704900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -383.480142

2) Conformer **1a-AC1**

O	2.14656300	-0.54912700	0.30950000
C	0.96811900	-1.09279500	0.96985100
H	1.23170400	-2.02977200	1.45626300
C	-0.12001800	-0.92335000	-0.11728300
C	0.20478200	0.59245500	0.19395500
C	1.65104500	0.60272300	-0.23434100
C	0.43409000	0.15027600	1.67634800
H	-0.48375400	0.00873700	2.23863400
H	1.15890000	0.71813300	2.26115700
O	2.28894300	1.36330700	-0.89352400
C	0.18999200	-1.46720800	-1.49967900
H	0.10880300	-2.55790500	-1.49365000
H	1.19167700	-1.20977700	-1.84389300
H	-0.52382600	-1.09094100	-2.23601900
C	-1.57162000	-1.22708800	0.25570700
H	-1.83713700	-2.21989100	-0.12001900
H	-1.71591300	-1.26776500	1.33805000
C	-2.51624900	-0.17591500	-0.33342700
H	-2.47644100	-0.21694000	-1.42804700
H	-3.54563900	-0.42185500	-0.05798000
C	-2.18385700	1.24163800	0.12606600
H	-2.89408100	1.94864900	-0.31089500
H	-2.31575500	1.30924900	1.21260500

C	-0.75805500	1.65235100	-0.24108900
H	-0.50069800	2.61735700	0.20518500
H	-0.67125500	1.78075000	-1.32585000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -539.308063

3) Conformer **1bC1**

O	1.18457000	0.18460900	-1.07375200
C	0.73788900	-1.13491600	-0.66364100
H	0.86502200	-1.83215800	-1.48762600
C	-0.59546800	-0.83988700	0.04907400
H	-0.96833100	-1.74450600	0.53850400
C	0.39427700	-0.10747200	1.01761800
H	0.13986800	0.24242700	2.01318100
C	0.95566100	0.91523400	0.05655500
C	1.37848600	-1.27395400	0.71931400
H	1.10443300	-2.19277500	1.23699400
H	2.44842500	-1.07707900	0.79452800
O	1.17297800	2.08113800	0.15910600
C	-1.71251400	-0.09891200	-0.64672000
H	-1.30676400	0.75448200	-1.19808400
H	-2.15330900	-0.76493400	-1.39676200
C	-2.78881900	0.37279300	0.31900700
H	-3.22703000	-0.46536800	0.86817800
H	-3.59701800	0.88130200	-0.21014600
H	-2.38273900	1.07532300	1.05115000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -422.731547

4) Conformer **1bC2**

O	0.78006300	-0.21683600	1.19104500
C	0.09141200	0.98569700	0.75830300
H	-0.36255100	1.47175600	1.61746400
C	-0.66288400	0.51358100	-0.50246500
H	-1.11665300	1.37153700	-1.00741900
C	0.81094900	0.34293300	-0.99387700
H	1.09962500	0.18500500	-2.02856600
C	1.28319100	-0.68429100	0.01031200
C	1.12085400	1.62815000	-0.17481900
H	0.76097800	2.53203200	-0.66551100
H	2.13077100	1.76020500	0.21471800
O	1.92778300	-1.67883900	-0.09855800
C	-1.61832400	-0.65474100	-0.45275300
H	-1.81582900	-0.98545900	-1.47808900

H	-1.14753600	-1.50064100	0.05692500
C	-2.92675200	-0.30314600	0.23779800
H	-2.75928200	-0.01134000	1.27782700
H	-3.61097300	-1.15380800	0.24172700
H	-3.43199300	0.52701700	-0.26396300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -422.731703

5) Conformer 1cC1

O	-1.51401300	0.37994300	1.10332600
C	-1.33188000	-1.01069700	0.72561000
H	-1.52906400	-1.64705200	1.58425300
C	-0.01342100	-0.98146300	-0.07080000
H	0.16276100	-1.95343700	-0.54072600
C	-0.91622500	-0.11529000	-1.01393600
H	-0.66541800	0.15192900	-2.03563800
C	-1.22829000	1.02133400	-0.06751200
C	-2.06998400	-1.07787300	-0.61342900
H	-1.99365400	-2.04707600	-1.10554700
H	-3.09119900	-0.69632700	-0.63863200
O	-1.24161800	2.20353400	-0.20695500
C	1.25571300	-0.42987300	0.53263600
H	1.04342800	0.50147300	1.06812100
H	1.61920000	-1.13848300	1.28679500
C	2.34783100	-0.18672100	-0.50026700
H	2.55091100	-1.11847500	-1.04129000
H	1.98489700	0.52747200	-1.24750700
C	3.63333200	0.33622200	0.11732100
H	4.03715400	-0.37110000	0.84719800
H	3.46280200	1.28374200	0.63528500
H	4.40077700	0.50568800	-0.64101600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.983634

6) Conformer 1cC2

O	-1.13165500	0.34408800	1.18890400
C	-0.73691100	-0.99338400	0.78513700
H	-0.37632100	-1.54114900	1.65140300
C	0.06656400	-0.73808700	-0.50752100
H	0.30497900	-1.68998300	-0.99107300
C	-1.34740300	-0.26151200	-0.97317300
H	-1.62368400	-0.07531700	-2.00655400
C	-1.55330400	0.87480300	0.00303000
C	-1.90877500	-1.42099400	-0.10198900

H	-1.77053600	-2.39650500	-0.56736000
H	-2.91148100	-1.31510800	0.31334000
O	-1.96643600	1.98327800	-0.12787600
C	1.25529300	0.19212300	-0.52196600
H	1.49117200	0.44306800	-1.56298100
H	1.00002500	1.13683100	-0.03036600
C	2.48418200	-0.40921700	0.14589700
H	2.24676700	-0.65070700	1.18804200
H	2.73242700	-1.36088400	-0.33874000
C	3.68857900	0.51550600	0.10200800
H	3.47684300	1.46110200	0.60814500
H	3.96863000	0.74928200	-0.92890900
H	4.55656200	0.06501000	0.58829100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.983755

7) Conformer **1cC3**

O	-1.73623900	0.16029700	0.94344300
C	-1.10904500	-1.12869200	0.71069500
H	-1.28583500	-1.77619500	1.56542700
C	0.27951400	-0.74453900	0.16309200
H	0.79625500	-1.63977100	-0.19078600
C	-0.62674200	-0.19030600	-0.98847500
H	-0.26734500	0.11523700	-1.96618800
C	-1.41689200	0.83094800	-0.20230600
C	-1.52694600	-1.43183100	-0.72996900
H	-1.09428400	-2.35011300	-1.12607300
H	-2.58871400	-1.35599200	-0.96668700
O	-1.72888700	1.95664000	-0.43144000
C	1.20043100	0.16223400	0.94592400
H	0.61657800	0.96395100	1.40778500
H	1.63471100	-0.41586800	1.77074900
C	2.32201000	0.77366900	0.11102200
H	1.88503900	1.37336400	-0.69514200
H	2.87297800	1.47880500	0.74079600
C	3.29368600	-0.24062400	-0.47115900
H	3.74139800	-0.85455300	0.31608900
H	4.10686600	0.25611900	-1.00485700
H	2.80725400	-0.91563200	-1.18007400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.982174

8) Conformer **1cC4**

O	1.27195500	-0.22153900	1.16562600
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C	0.44713700	0.92237000	0.82038400
H	-0.00883300	1.32401100	1.72115000
C	-0.31880900	0.43013900	-0.42591900
H	-0.87137200	1.25955700	-0.87332300
C	1.13963800	0.42914800	-0.98984200
H	1.39129000	0.34446500	-2.04262900
C	1.76016100	-0.58600700	-0.05664200
C	1.36149200	1.70349500	-0.12680900
H	0.89122600	2.58658000	-0.55842300
H	2.37134800	1.91974800	0.22337700
O	2.49427700	-1.50472200	-0.24031400
C	-1.14195100	-0.83627700	-0.38863900
H	-1.38240900	-1.12479700	-1.41892500
H	-0.54150500	-1.65152600	0.02580200
C	-2.43186100	-0.71040600	0.41711200
H	-2.89113900	-1.70131300	0.48455100
H	-2.18767000	-0.42513300	1.44663400
C	-3.44319600	0.26702100	-0.16153900
H	-3.06791500	1.29345200	-0.16967800
H	-4.36694800	0.26646900	0.42121900
H	-3.70159300	0.00168800	-1.19088900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.982298

9) Conformer **1cC5**

O	1.64204800	0.07571500	-1.00646900
C	1.29804100	-1.18056100	-0.36211400
H	1.62370400	-2.00772400	-0.98756800
C	-0.15158100	-0.94359100	0.10075100
H	-0.48210300	-1.77521700	0.73069200
C	0.59555100	0.11153900	0.99005000
H	0.16292200	0.62284900	1.84354000
C	1.16612600	0.98309900	-0.10536500
C	1.74215000	-0.93328000	1.08097100
H	1.50539800	-1.75453400	1.75690900
H	2.75923700	-0.57077200	1.23360600
O	1.22610300	2.16402800	-0.24401600
C	-1.21821500	-0.56821000	-0.90505600
H	-0.92941500	0.34370900	-1.43812900
H	-1.24917800	-1.36101000	-1.66156400
C	-2.61706800	-0.39901000	-0.32057500
H	-3.31630600	-0.25833900	-1.15086000
H	-2.91867500	-1.33182000	0.17068300
C	-2.76292900	0.76045900	0.65256700

H	-2.18489500	0.60201600	1.56554900
H	-3.80593300	0.89219200	0.94897700
H	-2.42241600	1.69803400	0.20466800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.981303

10) Conformer **1cC6**

O	1.00381800	-0.04476300	1.23084600
C	0.33827000	1.05927800	0.56435500
H	-0.22721800	1.63135500	1.29402400
C	-0.24771400	0.39353800	-0.70206600
H	-0.65811800	1.15657900	-1.37064300
C	1.28004200	0.22838400	-0.99014200
H	1.69365500	-0.04940500	-1.95498400
C	1.65768500	-0.63917200	0.18915400
C	1.45296000	1.62063800	-0.32024300
H	1.12851500	2.43638400	-0.96577400
H	2.40491400	1.84657200	0.16132400
O	2.33844500	-1.61022600	0.28897700
C	-1.14859500	-0.81984000	-0.63875200
H	-1.00284000	-1.39421900	-1.56047800
H	-0.82964800	-1.47351600	0.18023100
C	-2.63217800	-0.49902900	-0.49088300
H	-2.95622300	0.11253900	-1.34136600
H	-3.19309400	-1.43595200	-0.56469700
C	-3.00039000	0.20017200	0.80841500
H	-4.08280300	0.31556000	0.89823500
H	-2.56284300	1.19933900	0.87150700
H	-2.65287800	-0.36912600	1.67500200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.981481

11) Conformer **1dC1**

O	0.58169500	0.13732600	1.16717500
C	-0.67442800	0.74195500	0.79508400
H	-1.21124600	1.06045900	1.68447800
C	-1.21699400	-0.23113700	-0.27974400
H	-2.13370900	0.15402100	-0.74043800
C	0.03860800	0.27258400	-1.02353200
H	0.22844000	0.11069100	-2.07936300
C	1.10208500	-0.20141800	-0.05052500
C	-0.27551800	1.65112700	-0.37134700
H	-1.11218300	2.16513500	-0.84394000
H	0.55923400	2.32834700	-0.19672800

O	2.15965200	-0.71685300	-0.21218800
O	-1.26034200	-1.59661000	-0.04785600
H	-2.02109100	-1.80821800	0.49932100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -419.397244

12) Conformer **1dC2**

O	0.58838100	0.14070500	1.15879800
C	-0.67548900	0.73701700	0.78837800
H	-1.21466200	1.04595900	1.67886700
C	-1.21833000	-0.23122700	-0.26808700
H	-2.13157000	0.15722100	-0.73280100
C	0.04909500	0.27659900	-1.02847900
H	0.24186100	0.12261900	-2.08574400
C	1.10798900	-0.19766300	-0.05609200
C	-0.27751400	1.65022900	-0.37719000
H	-1.11702800	2.15962100	-0.84985000
H	0.55159600	2.33312700	-0.19806800
O	2.16006000	-0.72696600	-0.21834300
O	-1.33130600	-1.55589700	0.11890400
H	-1.58179300	-2.09101400	-0.63845900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -419.397295

13) Conformer **1eC1**

O	0.74385100	-0.24024000	1.18804600
C	0.06413500	0.97188300	0.79846900
H	-0.36956200	1.45232000	1.67048800
C	-0.70637900	0.53199800	-0.47403000
H	-1.21438800	1.38344000	-0.94678900
C	0.73558700	0.35454600	-0.99455600
H	0.99482200	0.20915600	-2.03790400
C	1.21569300	-0.69662800	-0.01141000
C	1.06560600	1.62535600	-0.15880800
H	0.70511800	2.54408500	-0.62084000
H	2.08527200	1.73826400	0.20685600
O	1.86477700	-1.68162500	-0.14911900
O	-1.48555200	-0.60449700	-0.47158100
C	-2.71554000	-0.43669500	0.19076600
H	-2.57222900	-0.22789600	1.25754700
H	-3.26756300	-1.36949600	0.08509000
H	-3.30069000	0.37826400	-0.25580300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -458.636083

14) Conformer **1eC2**

O	1.13046800	0.15625500	-1.08645600
C	0.60590200	-1.13476700	-0.69903800
H	0.65414700	-1.82100700	-1.53906800
C	-0.67413600	-0.77396500	0.06066100
H	-1.13374100	-1.65268500	0.53292400
C	0.37627300	-0.12005200	1.02354200
H	0.17336800	0.22255700	2.03287300
C	0.97735200	0.87981000	0.05963700
C	1.25538900	-1.35322300	0.67190700
H	0.93390700	-2.26457700	1.17557600
H	2.33641700	-1.23129600	0.72223200
O	1.28047800	2.02311900	0.18251800
O	-1.59591300	-0.00301300	-0.61009300
C	-2.65188100	0.44176700	0.20817700
H	-3.19125400	-0.40297600	0.65673400
H	-3.33530600	1.00330800	-0.42707100
H	-2.29118900	1.09836900	1.00872500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -458.635773

15) Conformer **1fC1**

O	0.60111000	0.12829500	1.16463100
C	-0.61147600	0.80956500	0.77952200
H	-1.12686100	1.17312000	1.66445900
C	-1.23156800	-0.13352100	-0.27534100
H	-2.09816500	0.35387000	-0.74258800
C	0.06691400	0.27573600	-1.02368200
H	0.25022000	0.09296700	-2.07833800
C	1.08868300	-0.27132200	-0.04467800
C	-0.14241300	1.68068200	-0.39092900
H	-0.94033100	2.24650200	-0.87101800
H	0.73739100	2.29999000	-0.22002300
O	2.10114800	-0.87379500	-0.20251700
N	-1.39322800	-1.51693200	0.05615100
H	-1.51874600	-2.08299900	-0.77298800
H	-2.18982300	-1.66776700	0.66118200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -399.521708

16) Conformer **1fC2**

O	0.57492900	0.07742500	1.15806800
C	-0.66290100	0.74835500	0.79549000

H	-1.19573900	1.03863900	1.69678100
C	-1.22390900	-0.17352700	-0.29377100
H	-2.09885700	0.27116500	-0.77242100
C	0.08689800	0.34584800	-1.02531600
H	0.28904300	0.23532300	-2.08622000
C	1.10677200	-0.21150200	-0.06922100
C	-0.20734200	1.69371800	-0.31651600
H	-1.02506900	2.24524700	-0.78010100
H	0.63575100	2.34679800	-0.09293500
O	2.12789800	-0.80211900	-0.23082300
N	-1.48539800	-1.52923200	0.04287300
H	-0.71395300	-1.95978800	0.53730600
H	-1.71310600	-2.09256300	-0.76447200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -399.525695

17) Conformer **1fC3**

O	0.58481800	0.08312100	1.16451600
C	-0.63601600	0.77819500	0.80297500
H	-1.15015200	1.10329600	1.70365700
C	-1.22547300	-0.15430900	-0.29174000
H	-2.10094500	0.30073900	-0.75879100
C	0.07077300	0.31924000	-1.02151700
H	0.25863800	0.17786200	-2.08084900
C	1.09821900	-0.23744900	-0.06371400
C	-0.17222700	1.69098700	-0.33097600
H	-0.97849900	2.25791700	-0.79602800
H	0.69470200	2.32100700	-0.13390700
O	2.11689200	-0.82993400	-0.22720800
N	-1.44182400	-1.54960600	-0.11070300
H	-2.33720700	-1.73984300	0.31774900
H	-0.71910400	-1.97921700	0.45445300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -399.525234

18) Conformer **1gC1**

O	0.78413400	-0.20454500	1.19694900
C	0.10333100	0.99401000	0.77002300
H	-0.32780600	1.50047300	1.62878000
C	-0.68821500	0.52545200	-0.47645700
H	-1.15897900	1.39529100	-0.96300700
C	0.75806100	0.32491400	-0.99875000
H	1.01578800	0.14809500	-2.03881900
C	1.23106300	-0.70584100	0.01017000

C	1.10854800	1.61535300	-0.20540000
H	0.75053100	2.52147300	-0.69316500
H	2.13096200	1.73281500	0.15216000
O	1.86419500	-1.70510500	-0.10931200
N	-1.52364300	-0.62432000	-0.37316600
H	-1.61658600	-1.07635400	-1.27299500
C	-2.81674400	-0.36375800	0.21917900
H	-2.68906700	-0.07226500	1.26481500
H	-3.41488500	-1.27576300	0.20662200
H	-3.38734800	0.43289300	-0.28591400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -438.764811

19) Conformer **1gC2**

O	1.11617500	0.19830000	-1.08755100
C	0.64626900	-1.12370900	-0.70522600
H	0.70867500	-1.79133100	-1.56010100
C	-0.64104000	-0.80376500	0.06075800
H	-1.04928300	-1.69334100	0.54807500
C	0.43201400	-0.13492500	1.03514000
H	0.24031400	0.18360700	2.05455700
C	0.97493100	0.89546000	0.08275800
C	1.33239400	-1.33551600	0.64429000
H	1.03980600	-2.26149000	1.13897800
H	2.41231400	-1.19290900	0.67523000
O	1.22117800	2.05449900	0.19988400
N	-1.67050300	-0.09542400	-0.60437500
H	-1.29202500	0.65013500	-1.17498200
C	-2.73622800	0.37962900	0.25294400
H	-3.22596400	-0.47241800	0.73248900
H	-3.48648800	0.89270100	-0.35024900
H	-2.40269000	1.06758300	1.04397600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -438.768018

20) Conformer **1gC3**

O	-0.57710000	0.46473500	1.13603600
C	-0.47215400	-0.96055400	0.88965000
H	-0.34116600	-1.48433800	1.83292700
C	0.47648800	-1.05110300	-0.34451000
H	0.45699500	-2.07603300	-0.72178000
C	-0.72504200	-0.28016600	-0.98745000
H	-0.85495200	-0.14017600	-2.05591000
C	-0.76377500	0.95743900	-0.12351800

C	-1.62174100	-1.18925600	-0.09429300
H	-1.69867500	-2.20950900	-0.46849600
H	-2.59466500	-0.79823600	0.20209300
O	-0.92794700	2.11042200	-0.37505800
N	1.81639200	-0.59026400	-0.43777000
H	2.45833800	-1.34420700	-0.24549900
C	2.23895400	0.63437800	0.21459500
H	1.70927400	1.49288600	-0.20028700
H	3.29983800	0.78054400	0.00438500
H	2.09426500	0.64524400	1.30228800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -438.760867

21) Conformer **1hC1**

O	1.16735800	-0.23874600	-1.17585200
C	0.64164200	-1.29558600	-0.34310900
H	0.46173100	-2.18352900	-0.94230800
C	-0.42045800	-0.57185700	0.51220900
H	-0.81641600	-1.25289300	1.28662600
C	0.85982200	0.14642400	1.02882100
H	0.90521300	0.76633100	1.91840800
C	1.31009700	0.77673200	-0.27497300
C	1.55673400	-1.23466000	0.88358700
H	1.28217300	-1.93176000	1.67464200
H	2.62973600	-1.24714100	0.69534200
O	1.72452600	1.85987800	-0.53638500
N	-1.42462700	0.20830000	-0.13456700
C	-2.34793500	-0.60835300	-0.88649000
H	-3.05768000	0.03410500	-1.41102000
H	-2.92365000	-1.30555700	-0.25100200
H	-1.80874800	-1.19082700	-1.63590200
C	-2.09907400	1.09568500	0.78501700
H	-2.80055100	1.72516300	0.23424200
H	-1.37587300	1.75159400	1.27298400
H	-2.66359000	0.55705300	1.56748400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -478.009889

22) Conformer **1iC1**

O	0.56948400	0.15100000	1.16318000
C	-0.72343300	0.67887200	0.80016800
H	-1.28188400	0.95299400	1.68954000
C	-1.20314800	-0.30035200	-0.27534800
H	-2.15415700	-0.01774400	-0.73093500

C	0.02096200	0.26173900	-1.02712000
H	0.21483500	0.11755500	-2.08436400
C	1.11300100	-0.14267000	-0.05583600
C	-0.38492700	1.61533100	-0.36744000
H	-1.25167100	2.08002500	-0.83664200
H	0.40734500	2.34035900	-0.18934800
O	2.19988000	-0.58993100	-0.22087300
F	-1.22490100	-1.62658500	0.01852700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -443.424866

23) Conformer **1jC1**

O	-0.80350700	0.22025000	1.16584000
C	-0.26417300	-1.06520500	0.80347800
H	-0.02916700	-1.64061400	1.69305100
C	0.74334800	-0.73337100	-0.30587100
H	1.17727700	-1.62163800	-0.76023700
C	-0.54511200	-0.27292900	-1.02479600
H	-0.60215800	-0.04740300	-2.08397000
C	-1.01399100	0.79672000	-0.05656400
C	-1.20032300	-1.50676000	-0.33131600
H	-0.92818100	-2.45363300	-0.79618700
H	-2.26831300	-1.45632600	-0.12256000
O	-1.48151900	1.87411900	-0.22454500
Cl	2.03601500	0.42081900	0.00176200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -803.701773

24) Conformer **1kC1**

O	-1.24425600	0.29545500	1.16638600
C	-0.91054300	-1.05783300	0.80460100
H	-0.75895600	-1.66074300	1.69389400
C	0.12282900	-0.89160900	-0.31527900
H	0.41608500	-1.83462300	-0.76959300
C	-1.08126800	-0.23579100	-1.02480400
H	-1.11135800	-0.00676300	-2.08421100
C	-1.37464500	0.89474000	-0.05653000
C	-1.91460300	-1.35210300	-0.32127400
H	-1.79720500	-2.33048000	-0.78538100
H	-2.96014400	-1.13535000	-0.10308600
O	-1.67655600	2.02955100	-0.22474900
Br	1.72935600	0.12067100	-0.00014300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -2917.498230

25) Conformer **1IC1**

O	-1.61512000	0.32218300	1.16670100
C	-1.35396500	-1.04763200	0.80447900
H	-1.22654600	-1.65533100	1.69434500
C	-0.32317900	-0.93835100	-0.32462500
H	-0.08817000	-1.89657500	-0.78107300
C	-1.50011300	-0.22096500	-1.02412200
H	-1.52956200	0.00755900	-2.08368100
C	-1.72819800	0.92459500	-0.05681200
C	-2.38434000	-1.29081400	-0.31014300
H	-2.32179000	-2.27420800	-0.77398400
H	-3.41573400	-1.02018900	-0.08178700
O	-1.97510100	2.07286800	-0.22460700
I	1.52910100	0.05881800	-0.00081600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -641.360358

26) Conformer **2aC1**

O	-1.00287500	0.80790500	-0.77174800
C	0.38507000	1.02355600	-0.40483500
H	0.77673600	1.88056800	-0.94730500
C	0.95279800	-0.40717400	-0.47997200
H	0.65087000	-0.93857500	-1.38719500
C	-0.03658900	-0.56889000	0.72682200
H	-0.03939600	-1.41238600	1.41089500
C	-1.32244700	-0.28286700	-0.01225500
C	0.33552700	0.88999700	1.11948200
H	1.30408500	0.96968900	1.60734100
H	-0.41213400	1.48602800	1.64389400
O	-2.38815400	-0.81230100	-0.01183600
C	2.42248600	-0.63026200	-0.21377200
H	2.77699600	-0.14519000	0.69670800
H	3.02049000	-0.25221600	-1.04712700
H	2.62950800	-1.69891000	-0.12135600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -383.476562

27) Conformer **2a-AC1**

O	-1.82929700	-0.32792500	-0.93976600
H	0.62940700	-1.58302900	2.06751400
H	1.30762600	0.04414800	2.13465500
H	2.87104700	-1.38138500	0.87845500

H	1.56517200	-2.02785600	-0.09433000
H	2.77405100	0.76840200	-0.23608600
H	2.85257100	-0.48785900	-1.44237200
H	0.46598200	-0.26092600	-1.96299600
H	1.22383200	1.32219900	-2.04598500
H	1.52910800	2.20308200	0.70806000
H	-0.10020500	2.71676100	1.11836400
H	0.55275200	3.06287400	-0.47508500
H	-2.43299800	0.04100500	1.49045500
H	-1.38783400	1.45229300	1.82713600
H	-2.16585400	1.72266200	-0.83098100
C	0.89532200	-0.71358400	1.46020500
C	1.92744100	-1.11874800	0.39217600
C	2.20127100	-0.05303100	-0.67896100
C	0.94357200	0.51684000	-1.35999400
C	0.51598100	2.31030600	0.31802800
O	-0.93680400	-2.30951300	-0.33033300
C	-1.57408100	0.62253900	1.15217500
C	-0.99898200	-1.12502700	-0.21343300
C	-0.28774000	-0.15718300	0.72910500
C	-0.00025100	1.00589600	-0.27235000
C	-1.54851000	0.96318000	-0.35628800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -539.299202

28) Conformer **2bC1**

O	-1.60428900	0.54691900	-0.80363100
C	-0.37266700	1.22377800	-0.43776000
H	-0.27810700	2.14331000	-1.01024200
C	0.63915000	0.06272800	-0.45617200
H	0.54683000	-0.57236000	-1.34346500
C	-0.26197900	-0.37814900	0.75218300
H	-0.00247500	-1.15077400	1.46962400
C	-1.55594800	-0.56174300	-0.00563500
C	-0.40304300	1.13371600	1.09013200
H	0.47530200	1.54810800	1.57939700
H	-1.31590300	1.46439500	1.58693000
O	-2.38434600	-1.41599100	0.00856300
C	2.10122900	0.34693800	-0.18586200
H	2.49461100	0.92932000	-1.02684100
H	2.22790400	0.97329200	0.70123800
C	2.91610800	-0.92795800	-0.02867900
H	2.56998600	-1.51994800	0.82222500
H	3.97215400	-0.70253600	0.13256900

H	2.84167400	-1.55608700	-0.92014100
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No imaginary frequency.
Gibbs Free Energies (a.u.) = -422.727957

29) Conformer **2bC2**

O	-1.27344300	0.46257700	-1.07995900
C	0.00900800	0.90492500	-0.56143500
H	0.47889900	1.57108900	-1.28033400
C	0.60770600	-0.42038300	-0.04596800
H	0.50327400	-1.24083600	-0.76364700
C	-0.59848700	-0.26225800	0.94303600
H	-0.72062000	-0.83348300	1.85864100
C	-1.71636100	-0.34419800	-0.06931300
C	-0.34144000	1.27112000	0.88256100
H	0.50858300	1.58750700	1.48252200
H	-1.19054900	1.93939000	1.03058500
O	-2.74984600	-0.93403000	-0.08446200
C	2.00256100	-0.43460800	0.54225800
H	2.12391200	0.34588100	1.29814700
H	2.13521600	-1.38589900	1.06846700
C	3.08071600	-0.28992100	-0.52166300
H	2.99970700	-1.07761900	-1.27524900
H	4.07795700	-0.35256500	-0.08158700
H	3.00771900	0.67009800	-1.03903400

No imaginary frequency.
Gibbs Free Energies (a.u.) = -422.727915

30) Conformer **2cC1**

O	2.14112800	-0.47675200	-0.77639800
C	0.95066500	-1.23043400	-0.42431300
H	0.92899600	-2.16114200	-0.98602000
C	-0.13643100	-0.14061800	-0.47733700
H	-0.06876600	0.48752400	-1.37164500
C	0.70966900	0.37476500	0.74141900
H	0.38507100	1.13687200	1.44343600
C	2.00293700	0.63573800	0.00551100
C	0.94536800	-1.11989500	1.10247600
H	0.08733100	-1.58647800	1.58063000
H	1.86853200	-1.38220100	1.62061600
O	2.77182200	1.54391200	0.02374300
C	-1.58033400	-0.52083100	-0.23138100
H	-1.91665200	-1.14827400	-1.06625700
H	-1.68696600	-1.13432700	0.66863200

C	-2.49631500	0.69106800	-0.12114200
H	-2.16371100	1.32407500	0.70872300
H	-2.39566500	1.30101800	-1.02577400
C	-3.95286000	0.31015500	0.08005300
H	-4.08717300	-0.27167500	0.99628200
H	-4.32092500	-0.29645100	-0.75210200
H	-4.58986300	1.19408800	0.15300400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.980054

31) Conformer **2cC2**

O	-1.79944000	0.50102700	-1.04258800
C	-0.52777800	0.96078100	-0.51224700
H	-0.09460300	1.68858100	-1.19336600
C	0.12951700	-0.36925100	-0.08810800
H	0.04603200	-1.14698800	-0.85421800
C	-1.06826500	-0.32097800	0.92273800
H	-1.15509100	-0.95254400	1.80197500
C	-2.19628000	-0.38403300	-0.07953600
C	-0.87157000	1.22201700	0.95592600
H	-0.02568000	1.53321300	1.56442200
H	-1.74361000	1.84579200	1.15577400
O	-3.20612500	-1.01248600	-0.11969600
C	1.53083500	-0.36506600	0.48324300
H	1.63560000	0.37222700	1.28520000
H	1.71002900	-1.34146300	0.94867100
C	2.59910900	-0.11466400	-0.57359000
H	2.48783400	-0.84938300	-1.37882600
H	2.43522800	0.86570300	-1.03456600
C	4.00831900	-0.18234700	-0.01050100
H	4.15698100	0.56375200	0.77513000
H	4.75677300	-0.00162200	-0.78487800
H	4.21172100	-1.16434700	0.42540600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.979961

32) Conformer **2cC3**

O	1.95320100	-0.08080300	-0.96069000
C	0.94456100	-1.09772500	-0.71876800
H	0.98380200	-1.84475000	-1.50781400
C	-0.28760500	-0.23922100	-0.37422700
H	-0.42630800	0.59406300	-1.06834800
C	0.63163000	0.09146800	0.85649100

H	0.29838800	0.58102400	1.76657300
C	1.76010400	0.75543100	0.10289700
C	1.13100800	-1.37928800	0.77430100
H	0.42500600	-2.09641800	1.18610200
H	2.14476900	-1.59524100	1.11358500
O	2.38136400	1.75217700	0.29545100
C	-1.61050000	-0.92668900	-0.10970700
H	-1.98686800	-1.31304900	-1.06519000
H	-1.47612800	-1.79812300	0.53661500
C	-2.66785200	-0.01448700	0.50827500
H	-3.54510200	-0.62389800	0.74710300
H	-2.30024200	0.36966000	1.46631700
C	-3.09455800	1.14548800	-0.37737600
H	-2.27555000	1.84305700	-0.56642200
H	-3.90228100	1.71436100	0.08800000
H	-3.45672500	0.78845700	-1.34592700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.978581

33) Conformer **2cC4**

O	1.51627400	-0.58107100	1.07586300
C	0.39169400	0.33738900	1.03482200
H	-0.09909300	0.35049700	2.00452100
C	-0.27552900	-0.05149500	-0.30141800
H	-0.37365400	-1.13333300	-0.42572200
C	1.07956500	0.53511100	-0.83117400
H	1.27202700	0.79572400	-1.86777500
C	2.00985100	-0.46975900	-0.19398200
C	1.00183800	1.55639500	0.33969100
H	0.29802000	2.36525200	0.15786400
H	1.93734200	1.94108600	0.74755200
O	2.95014100	-1.07289100	-0.60443900
C	-1.54885200	0.64527300	-0.73416200
H	-1.41885500	1.73086000	-0.73479800
H	-1.74533300	0.36547300	-1.77595800
C	-2.76834300	0.29204000	0.11471700
H	-2.59110300	0.59640200	1.15253500
H	-3.61184500	0.89647200	-0.23348700
C	-3.15780100	-1.17728500	0.07415900
H	-3.33033800	-1.50993100	-0.95356000
H	-4.07695300	-1.35324500	0.63705500
H	-2.38607400	-1.81957100	0.50447300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.978448

34) Conformer **2cC5**

O	2.04064300	-0.42964500	-0.74108800
C	0.97328700	-1.29836500	-0.27918200
H	1.08095300	-2.28174900	-0.73077400
C	-0.26264500	-0.39235400	-0.43272600
H	-0.29256500	0.12398800	-1.39824200
C	0.50826400	0.37954800	0.69927400
H	0.08068100	1.16176400	1.31818100
C	1.74670500	0.73502900	-0.08925500
C	0.95646100	-1.01430700	1.22408600
H	0.17212000	-1.53951200	1.76487500
H	1.90755400	-1.08195600	1.75362100
O	2.37542600	1.74028300	-0.19274800
C	-1.62901100	-0.97275200	-0.11712300
H	-1.74161000	-1.90535300	-0.68261800
H	-1.70696200	-1.24619400	0.94000600
C	-2.78635900	-0.04740400	-0.48168700
H	-2.74707300	0.16499600	-1.55610200
H	-3.72325600	-0.58864500	-0.31570700
C	-2.81790400	1.26047800	0.29228800
H	-2.83940500	1.08176400	1.37145900
H	-3.70507500	1.84390200	0.03688100
H	-1.94669600	1.88264600	0.07506700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.977677

35) Conformer **2cC6**

O	-1.47543600	1.22333800	-0.17578200
C	-0.27704500	0.84525300	0.55311600
H	0.29079700	1.73754000	0.80047800
C	0.23725200	-0.34307100	-0.28977900
H	0.22701600	-0.14193100	-1.36643200
C	-1.09850200	-0.95202600	0.26331500
H	-1.35044600	-2.00778900	0.22268800
C	-2.06158800	0.00806400	-0.39223100
C	-0.82628000	-0.15684700	1.57127700
H	-0.06755500	-0.61604100	2.20046900
H	-1.68311900	0.16258500	2.16567900
O	-3.08512800	-0.14965500	-0.97884600
C	1.52404700	-1.05448100	0.08471900
H	1.66411900	-1.07716300	1.16995800
H	1.43128000	-2.09961500	-0.23064600
C	2.76978300	-0.46420000	-0.57004200

H	3.61990100	-1.11044800	-0.32939800
H	2.65562300	-0.50957000	-1.65899300
C	3.09161100	0.96212600	-0.15367000
H	3.17919800	1.04757300	0.93367100
H	2.32350400	1.66506900	-0.48386700
H	4.03853400	1.29142600	-0.58681700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -461.977640

36) Conformer **2dC1**

O	-0.94897300	0.87550700	-0.71431600
C	0.44099100	1.03095900	-0.34793500
H	0.86230100	1.90368300	-0.84086300
C	0.95001800	-0.42157100	-0.51643100
H	0.67427000	-0.90978900	-1.45836500
C	-0.01935200	-0.62606600	0.68430600
H	-0.03042400	-1.51962400	1.29987600
C	-1.30139000	-0.24882200	-0.01736100
C	0.42957900	0.78643500	1.16330900
H	1.42386000	0.77460700	1.60296900
H	-0.27113400	1.37292800	1.75796200
O	-2.38536300	-0.73691400	-0.03741700
O	2.27237300	-0.66992000	-0.15398500
H	2.83775000	-0.49680300	-0.91115800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -419.394303

37) Conformer **2dC2**

O	-0.94821600	0.86433100	-0.72090700
C	0.44482100	1.01721000	-0.36449700
H	0.87508300	1.87302900	-0.87688700
C	0.94939500	-0.42544800	-0.51822400
H	0.66932000	-0.92817200	-1.45054600
C	-0.02603100	-0.61618500	0.70181600
H	-0.04863100	-1.49556100	1.33856000
C	-1.30448600	-0.24685200	-0.00555400
C	0.43712200	0.79958700	1.15122800
H	1.43487300	0.78878300	1.58333800
H	-0.25509000	1.40318000	1.73847500
O	-2.38810000	-0.73709300	-0.02588900
O	2.30768900	-0.54438100	-0.23637600
H	2.54854600	-1.47398800	-0.25616900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -419.394731

38) Conformer **2eC1**

O	-1.26158700	0.40535700	-1.08864600
C	0.02484800	0.88951900	-0.63878900
H	0.47210500	1.51708500	-1.40478700
C	0.63764300	-0.41672300	-0.06569200
H	0.57275000	-1.29154000	-0.72706700
C	-0.52365500	-0.20889300	0.94944200
H	-0.59863500	-0.74251400	1.89120900
C	-1.67224500	-0.34551900	-0.02022400
C	-0.25241800	1.31708300	0.80449300
H	0.64269100	1.62667100	1.33880300
H	-1.08276000	2.00401800	0.97016400
O	-2.70394200	-0.93463700	0.02708800
O	1.87938200	-0.32179800	0.54055400
C	2.94626400	-0.40517600	-0.37557700
H	2.91038000	-1.34517000	-0.94034200
H	3.86848600	-0.37278600	0.20320300
H	2.94154000	0.43111300	-1.08507300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -458.632429

39) Conformer **2eC2**

O	-1.53272500	0.59751800	-0.79670100
C	-0.27035800	1.20571100	-0.43878600
H	-0.10881900	2.11077400	-1.01735400
C	0.66250700	-0.01410400	-0.46417700
H	0.58940800	-0.65989300	-1.34923100
C	-0.25209900	-0.40452000	0.76158200
H	-0.03337700	-1.19319200	1.47446800
C	-1.55233700	-0.51023800	0.00700200
C	-0.26808000	1.11587400	1.08944400
H	0.66642900	1.45328300	1.53160900
H	-1.13507900	1.51757700	1.61440000
O	-2.42766800	-1.31571100	0.01494900
O	1.97571400	0.30584100	-0.16939000
C	2.80903900	-0.82377000	-0.05207100
H	2.51222700	-1.46078600	0.78942100
H	3.82117900	-0.45922200	0.11858300
H	2.79343300	-1.42343400	-0.97072500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -458.632954

40) Conformer **2fC1**

O	-0.97239500	0.87442100	-0.70663000
C	0.41651600	1.03918800	-0.32923500
H	0.82795500	1.92229400	-0.81180200
C	0.95251600	-0.39543700	-0.52043800
H	0.64418900	-0.85968900	-1.46687700
C	-0.02660400	-0.62788000	0.67800300
H	-0.03763400	-1.52563700	1.28918900
C	-1.31078700	-0.26242800	-0.02693700
C	0.39126600	0.78498700	1.17896600
H	1.38131400	0.78269600	1.62578500
H	-0.32951600	1.35395000	1.76645600
O	-2.38754300	-0.76754600	-0.05663700
N	2.33779500	-0.56960900	-0.17345700
H	2.93657500	-0.22087400	-0.91210000
H	2.55461100	-1.55106400	-0.05246700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -399.520466

41) Conformer **2fC2**

O	-0.97442400	0.80772700	-0.77940900
C	0.41290800	1.01640400	-0.42464900
H	0.81473600	1.86088000	-0.97974400
C	0.95684000	-0.43999800	-0.47828400
H	0.65090000	-0.98345400	-1.37614000
C	-0.02485700	-0.55955200	0.73760200
H	-0.02776300	-1.39685400	1.42842400
C	-1.30759200	-0.26691700	0.00000100
C	0.38185600	0.89779300	1.10150600
H	1.35862200	0.97169800	1.57763700
H	-0.34304300	1.51543200	1.63307700
O	-2.38028300	-0.78116400	0.00819600
N	2.32286000	-0.75005800	-0.19265700
H	2.69104800	-0.25299500	0.60642300
H	2.91820200	-0.56318400	-0.98842000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -399.518485

42) Conformer **2gC1**

O	-1.26718900	0.57929700	-1.01410000
C	0.01883300	0.97041700	-0.47279300
H	0.48125800	1.70807800	-1.12284900
C	0.62562100	-0.40850000	-0.12025300
H	0.52410400	-1.15100400	-0.92828700
C	-0.55377600	-0.36136500	0.90274600

H	-0.65409000	-1.03773500	1.74686400
C	-1.69164900	-0.33338600	-0.09005400
C	-0.28424900	1.16751000	1.01306000
H	0.60292100	1.38449200	1.60134700
H	-1.12131200	1.81808800	1.26757600
O	-2.72638600	-0.91776700	-0.14732900
N	1.92496000	-0.37795900	0.48340700
H	2.05025500	-1.20148100	1.05802600
C	3.00133900	-0.27816700	-0.48317100
H	2.97503600	-1.06050900	-1.25775400
H	3.96060100	-0.33553200	0.03324900
H	2.95838900	0.69001300	-0.98779100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -438.762869

43) Conformer **2hC1**

O	1.16737000	-0.23874800	-1.17585300
C	0.64164200	-1.29558700	-0.34311600
H	0.46173300	-2.18352800	-0.94231800
C	-0.42046100	-0.57185900	0.51220100
H	-0.81642300	-1.25289600	1.28661600
C	0.85981700	0.14642000	1.02882000
H	0.90520300	0.76632500	1.91840900
C	1.31010700	0.77672700	-0.27497000
C	1.55672200	-1.23466900	0.88359100
H	1.28214900	-1.93176700	1.67464300
H	2.62972600	-1.24715600	0.69535700
O	1.72453000	1.85987600	-0.53638000
N	-1.42462800	0.20830100	-0.13457600
C	-2.09905300	1.09570900	0.78500300
H	-2.80053800	1.72517600	0.23422700
H	-1.37583900	1.75162700	1.27294000
H	-2.66355600	0.55709700	1.56749300
C	-2.34795700	-0.60835800	-0.88646700
H	-1.80878800	-1.19086000	-1.63587000
H	-3.05769900	0.03409500	-1.41100500
H	-2.92367500	-1.30553800	-0.25095300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -478.009889

44) Conformer **2iC1**

O	-0.92717100	0.90913300	-0.67620200
C	0.46932200	1.02507900	-0.32484200

H	0.90951000	1.89832200	-0.79713600
C	0.93455000	-0.42223500	-0.55191500
H	0.70258700	-0.89382400	-1.50911000
C	-0.01259100	-0.66230300	0.65751300
H	-0.03664400	-1.57847100	1.23809000
C	-1.29645700	-0.23142700	-0.01261000
C	0.47496200	0.72384200	1.17819600
H	1.47496800	0.67970400	1.60423700
H	-0.20379300	1.30237400	1.80463900
O	-2.38942500	-0.69530400	-0.03489700
F	2.25193600	-0.63516400	-0.25888800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -443.421144

45) Conformer **2jC1**

O	-1.37766000	0.77497100	-0.77404500
C	-0.01983800	1.09813400	-0.39073400
H	0.32938000	1.97174200	-0.93268300
C	0.62907400	-0.29394300	-0.47603000
H	0.45688900	-0.86254400	-1.38849100
C	-0.32443800	-0.53732800	0.72991700
H	-0.25542900	-1.39213000	1.39408600
C	-1.62745100	-0.33819600	-0.01605100
C	-0.05459800	0.94206500	1.13325600
H	0.91393400	1.07607300	1.60881000
H	-0.84119900	1.47658200	1.66521500
O	-2.65115500	-0.93958000	-0.02188700
Cl	2.35355600	-0.36336700	-0.10950700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -803.699183

46) Conformer **2kC1**

O	-1.97461900	0.72192500	-0.79792500
C	-0.64199000	1.13501900	-0.40541800
H	-0.34123700	2.01719000	-0.96211700
C	0.08645600	-0.21657500	-0.45432400
H	-0.03221000	-0.81381800	-1.35599700
C	-0.86068600	-0.49189500	0.74648300
H	-0.75066100	-1.32643300	1.43046700
C	-2.16530300	-0.38831800	-0.01897200
C	-0.69072600	1.00953800	1.12092900
H	0.25959200	1.21416500	1.60823700
H	-1.51799100	1.50467600	1.62875600
O	-3.15094100	-1.04988300	-0.02008400

Br	1.97201400	-0.17882100	-0.04964200
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No imaginary frequency.
Gibbs Free Energies (a.u.) = -2917.495936

47) Conformer **2IC1**

O	-2.43753000	0.69735800	-0.80511500
C	-1.11393500	1.14442200	-0.41144000
H	-0.83785200	2.03229200	-0.97162200
C	-0.35166700	-0.18869000	-0.45063400
H	-0.45900600	-0.79251900	-1.34949700
C	-1.29540400	-0.47976600	0.74964200
H	-1.17105900	-1.30601900	1.44117500
C	-2.60077200	-0.41320800	-0.02147200
C	-1.16860600	1.02720100	1.11530600
H	-0.22724600	1.26090600	1.60795300
H	-2.01155200	1.50364800	1.61544600
O	-3.56871400	-1.10067100	-0.02090200
I	1.73469800	-0.11342600	-0.03063600

No imaginary frequency.
Gibbs Free Energies (a.u.) = -641.358474

48) Conformer **3aC1**

O	-0.35750600	-1.53084100	0.18450700
C	-1.06382100	-0.51326600	0.94246300
H	-1.94480100	-0.95245700	1.40273400
C	-1.07444600	0.68522200	-0.02115400
H	-1.45723700	1.57321900	0.48994400
C	0.47024400	0.58054100	0.24195500
C	0.69216000	-0.81597600	-0.30814000
C	0.07520200	0.17414300	1.69576000
H	-0.24625800	1.03136800	2.28815300
H	0.75842900	-0.46456700	2.25750800
O	1.54475000	-1.26289700	-1.00992600
C	-1.64168000	0.56321500	-1.41256400
H	-2.73403800	0.55020500	-1.38390300
H	-1.30895500	-0.35050100	-1.90907700
H	-1.33864300	1.41272400	-2.02958000
C	1.47077200	1.63332100	-0.11682400
H	2.47045200	1.34654000	0.21703000
H	1.21516100	2.59114900	0.34130800
H	1.51735200	1.76901700	-1.19973500

No imaginary frequency.
Gibbs Free Energies (a.u.) = -422.739518

49) Conformer **3bC1**

O	0.17719900	-1.34583400	0.75116200
C	-0.79279700	-0.35205700	1.18552500
H	-1.47784300	-0.79422000	1.90052700
C	-1.22630800	0.32104100	-0.13507900
H	-1.85250500	1.18958100	0.08405900
C	0.26442400	0.74327000	-0.05743300
C	0.93187900	-0.62360500	-0.11979700
C	0.08854800	0.87121900	1.47049700
H	0.96037500	0.72451400	2.10707800
H	-0.48009400	1.75751000	1.74980400
O	1.85922100	-1.03066700	-0.73820800
C	-1.75645900	-0.48213600	-1.29359400
H	-1.73928700	0.11317600	-2.20908700
H	-2.79043600	-0.78331600	-1.11134400
H	-1.16796000	-1.38516600	-1.46632900
F	0.80007500	1.70261400	-0.82878400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -482.680425

50) Conformer **3cC1**

O	1.51435000	1.00707900	0.09226600
C	1.45707600	-0.20611700	0.88859000
H	2.43682200	-0.41817600	1.30508200
C	0.65899800	-1.17528700	-0.00747200
H	0.41930000	-2.08452800	0.54851800
C	-0.42930700	-0.10378100	0.29862800
C	0.22851900	1.11531900	-0.33996400
C	0.18438100	0.00404700	1.71569700
H	0.07870200	0.94942300	2.24691000
H	-0.07742800	-0.84804500	2.34116500
O	-0.19160600	1.97364200	-1.04161000
C	1.07556000	-1.47298100	-1.42233200
H	1.91078900	-2.17667200	-1.43601700
H	1.38400800	-0.57191600	-1.95570700
H	0.24796300	-1.92641600	-1.97255000
Cl	-2.11961600	-0.33744900	-0.01656000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -842.958427

51) Conformer **3dC1**

O	2.07960000	0.87214300	0.06716000
C	1.91208800	-0.32376700	0.87300600
H	2.87218900	-0.63289200	1.27549200

C	1.00461800	-1.21246400	-0.00274500
H	0.68390600	-2.08930900	0.56409700
C	0.03798200	-0.03252800	0.31242700
C	0.80441700	1.10965100	-0.34585000
C	0.68135900	0.01951900	1.71900800
H	0.68070800	0.97387900	2.24458200
H	0.34535900	-0.79753900	2.35545200
O	0.46565900	2.00336400	-1.04731300
C	1.36504500	-1.55954600	-1.42147800
H	1.75421400	-0.69792800	-1.96706100
H	0.48638000	-1.93002800	-1.95447700
H	2.12415700	-2.34455700	-1.44292800
Br	-1.83263000	-0.09973900	-0.00114700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -2956.754648

52) Conformer **3eC1**

O	2.48597100	0.84366400	0.04825100
C	2.30721900	-0.34550800	0.86100000
H	3.26796100	-0.67028800	1.25118900
C	1.37226200	-1.22029300	0.00113600
H	1.04377900	-2.08967000	0.57483300
C	0.42800600	-0.02024800	0.32251400
C	1.20960300	1.10340400	-0.34900400
C	1.09499600	0.02378900	1.72117100
H	1.11930900	0.98000000	2.24298900
H	0.75318900	-0.78342300	2.36695400
O	0.88256000	2.00241300	-1.05016300
C	1.70932500	-1.57979900	-1.42001200
H	0.81811300	-1.93888800	-1.94017000
H	2.45535600	-2.37715900	-1.44674600
H	2.10546800	-0.72730100	-1.97481300
I	-1.64603600	-0.05528200	0.00226800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -680.617021

53) Conformer **4aC1**

O	-0.22177000	0.98206800	1.16162200
C	0.50202600	-0.25747900	1.04467200
H	0.63950100	-0.70993700	2.02260800
C	1.63176900	0.13187600	0.06440500
H	2.08272200	1.09073400	0.33109700
C	0.39130400	0.27225600	-0.89270900
H	0.44371400	0.35135900	-1.97376200

C	-0.31551700	1.38323700	-0.14398400
C	-0.17660700	-0.95062100	-0.14125700
H	0.29745600	-1.88442500	-0.42437200
O	-0.81947600	2.39584700	-0.50363300
C	2.70836800	-0.86621900	-0.29308300
H	3.37383900	-1.02237000	0.55965800
H	3.31556900	-0.48085000	-1.11511600
H	2.32482200	-1.84084200	-0.59696700
Cl	-1.91739500	-1.22384100	-0.11149000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -842.953627

54) Conformer **4bC1**

O	0.32278500	0.53687100	1.17604200
C	0.23381400	-0.85622300	0.82400500
H	0.17737800	-1.46800000	1.71934500
C	1.28806200	-0.99663400	-0.29672000
H	1.23803200	-1.98770100	-0.75369300
C	0.27921900	-0.03226500	-1.01053900
H	0.27767700	0.19137200	-2.07219300
C	0.36359500	1.13848200	-0.05167200
C	-0.80673700	-0.87082500	-0.30200900
H	-0.93572600	-1.85334700	-0.75005700
O	0.47255200	2.30749900	-0.22654900
C	2.71657100	-0.57729000	-0.05655800
H	3.23096400	-1.31722100	0.56085100
H	2.78042800	0.38714100	0.44977300
H	3.25621200	-0.49982200	-1.00295200
Cl	-2.40204800	-0.17875600	-0.02270900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -842.956922

55) Conformer **4cC1**

O	-1.16138300	-0.49014500	1.14629900
C	0.06282500	0.27668900	1.06160000
H	0.36368600	0.61785800	2.04816900
C	-0.17069600	1.17551500	-0.16783500
H	0.74649700	1.70452300	-0.42618000
C	-0.17565300	-0.22435100	-0.86644500
H	-0.08833900	-0.39020500	-1.93535600
C	-1.36566800	-0.83981800	-0.16233200
C	0.90029300	-0.65430300	0.17080900
H	0.93371000	-1.70259700	0.46206800
O	-2.28858000	-1.47994500	-0.54894800

C	-1.37187300	2.08217800	-0.24148500
H	-2.29143700	1.57628200	0.05903400
H	-1.50810200	2.45348000	-1.25976200
H	-1.23601100	2.94826500	0.41049700
Cl	2.55319600	-0.13778500	-0.17077300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -842.954761

56) Conformer **4dC1**

O	-1.52666900	-0.14963500	1.10350600
C	-0.12132200	0.20475200	1.11772100
H	0.23112100	0.31801900	2.13948900
C	-0.07738100	1.28872200	0.01975600
H	-0.92198000	1.97670800	0.12003800
C	-0.42335700	0.03162900	-0.85725600
H	-0.34605400	-0.02363200	-1.93839800
C	-1.77487600	-0.26406200	-0.24185900
C	0.40248200	-0.84888600	0.12591500
H	0.03417500	-1.85918700	0.29745300
O	-2.83371300	-0.53475500	-0.70622400
C	1.16837600	2.09641600	-0.26061700
H	1.02036200	2.68646800	-1.16840400
H	2.06591000	1.49870000	-0.38827100
H	1.33807900	2.79974300	0.55912500
Cl	2.14223000	-0.99841900	-0.13066200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -842.946064

57) Conformer **5aC1**

O	-2.06850200	0.95526100	1.35651700
H	1.91415400	-1.19244500	-1.20548300
C	1.14331900	0.72513700	-0.62809800
C	1.46955800	-0.73823400	-0.31016800
C	-1.03648400	0.36270200	0.62765300
C	-1.52491100	-0.21998500	-0.69623800
O	-0.77485200	-1.28727500	-1.00730600
O	-2.42147700	0.18114900	-1.38346100
C	0.12370200	1.32927900	0.33818800
C	0.19517400	-1.49449700	0.05542900
H	2.23258200	2.34550200	-0.74346700
C	-0.47907000	-0.89025900	1.27479900
H	-1.28690100	-1.53413500	1.62787600
H	-2.59579300	1.48587800	0.74622400
H	0.72904300	0.75419700	-1.64355600

H	-0.27121500	2.26037900	-0.07887900
H	2.99067500	-0.13096700	0.68485700
H	0.60484700	1.56168500	1.29173800
O	2.38257200	1.40564700	-0.60523600
H	0.37435200	-2.56553400	0.12346500
O	2.34987600	-0.84692700	0.78233600
H	0.21960400	-0.69227200	2.08504400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -648.312299

58) Conformer **5aC2**

O	-2.08440000	0.92069400	1.36908000
H	1.95604900	-1.14354100	-1.19269400
C	1.12607000	0.76138100	-0.64347100
C	1.48083100	-0.69487500	-0.31536800
C	-1.04599000	0.35205500	0.62924000
C	-1.53055300	-0.24129600	-0.69124600
O	-0.75916700	-1.29324300	-1.00556800
O	-2.43589600	0.14089000	-1.37765900
C	0.09102700	1.34078700	0.32754200
C	0.22045500	-1.48095600	0.05319300
H	2.84576100	1.25109200	0.03513200
C	-0.45898200	-0.88772900	1.27511700
H	-1.24993800	-1.54749200	1.63695200
H	-2.59843900	1.48338600	0.77690300
H	0.70306900	0.77496600	-1.65178200
H	-0.31902600	2.26213400	-0.09401100
H	3.00772700	-1.40239600	0.68360600
H	0.56945000	1.59074600	1.27857200
O	2.29186300	1.54604600	-0.70036500
H	0.41763000	-2.54931200	0.12020700
O	2.37893700	-0.68232800	0.77900000
H	0.23988000	-0.67225500	2.08117700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -648.312596

59) Conformer **5aC3**

O	-2.07039800	0.97769400	1.33880500
H	1.90355500	-1.21738900	-1.18668000
C	1.14831800	0.72184100	-0.62672000
C	1.46343500	-0.74824600	-0.29559000
C	-1.03943700	0.37262900	0.61878700
C	-1.52593300	-0.22646400	-0.69850300
O	-0.77703000	-1.29940600	-0.99279100

O	-2.41758300	0.16816900	-1.39587500
C	0.11990400	1.33472800	0.31726900
C	0.18745400	-1.49675400	0.07808000
H	2.82771200	1.40069100	-1.36045600
C	-0.48815800	-0.87216400	1.28581500
H	-1.29926100	-1.50743800	1.64694900
H	-2.57917800	1.52442400	0.72720800
H	0.75999200	0.75972900	-1.64979800
H	0.59484000	1.58662700	1.26909400
H	2.94562800	-0.08259800	0.70895900
H	-0.26740600	2.25832800	-0.11985500
O	2.33483400	1.49278800	-0.53878200
H	0.35980800	-2.56798000	0.16115800
O	2.34909500	-0.83966500	0.79289000
H	0.20946400	-0.66446200	2.09462100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -648.312461

60) Conformer **5aC4**

O	-2.01517500	1.12733800	1.28168900
H	1.90474600	-1.24148700	-1.16598300
C	1.14580500	0.69708000	-0.64730500
C	1.46140600	-0.75810000	-0.28545100
C	-1.03687000	0.39795900	0.60771700
C	-1.52788600	-0.22081300	-0.70758300
O	-0.78463400	-1.30967400	-0.97226100
O	-2.41455700	0.14677100	-1.42348700
C	0.13124400	1.33840900	0.29878300
C	0.17997100	-1.49319500	0.09751300
H	2.24609800	2.30446200	-0.82230400
C	-0.49106700	-0.84705200	1.29434600
H	-1.29978900	-1.48105200	1.66644200
H	-2.76102700	0.55106200	1.48092400
H	0.73381000	0.69928900	-1.66391400
H	-0.25668800	2.26047900	-0.14217200
H	2.98755800	-0.13570600	0.69319300
H	0.61457700	1.59000600	1.24639400
O	2.38844300	1.37084600	-0.64041100
H	0.35145800	-2.56326900	0.19645400
O	2.33837000	-0.84068500	0.81212000
H	0.20405500	-0.62628100	2.10165300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -648.310835

61) Conformer **5aC5**

O	-2.03465900	1.09899800	1.28957500
H	1.94692100	-1.19427100	-1.15354500
C	1.12956600	0.73231900	-0.66527900
C	1.47355200	-0.71522900	-0.29142000
C	-1.04627200	0.38854400	0.60920800
C	-1.53391600	-0.24366700	-0.69992500
O	-0.76883800	-1.31663900	-0.96792000
O	-2.43191400	0.10395200	-1.41187200
C	0.09916800	1.35083300	0.28476700
C	0.20615600	-1.47942100	0.09748400
H	2.85208600	1.22809500	0.00108500
C	-0.46981100	-0.84234900	1.29651500
H	0.22600200	-0.60292600	2.09835700
H	-2.76679800	0.50771800	1.49551200
H	0.70896900	0.71814000	-1.67447100
H	-0.30517100	2.26147200	-0.16220100
H	2.99280100	-1.40286400	0.73266600
H	0.57964700	1.62261100	1.22882100
O	2.30021500	1.50751600	-0.74202200
H	0.39538700	-2.54692800	0.19647500
O	2.37030400	-0.67455200	0.80346900
H	-1.26136600	-1.49143500	1.67936800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -648.310825

62) Conformer **5aC6**

O	-2.01718300	1.15201300	1.25756900
H	1.89388700	-1.26867600	-1.14389400
C	1.15136100	0.69243800	-0.64743400
C	1.45539000	-0.76833200	-0.26916600
C	-1.03957700	0.40896900	0.59751100
C	-1.52875100	-0.22904100	-0.70884200
O	-0.78690400	-1.32299000	-0.95460000
O	-2.41124500	0.13046800	-1.43413900
C	0.12769200	1.34431600	0.27399300
C	0.17242800	-1.49432000	0.12338100
H	2.83307300	1.34406000	-1.39970900
C	-0.49944600	-0.82553300	1.30657700
H	0.19489800	-0.59327700	2.11142800
H	-2.76230400	0.57957500	1.46988400
H	0.76610300	0.70123500	-1.67218500
H	-0.25323400	2.25653200	-0.18950200
H	2.94187300	-0.08334000	0.71604800

H	0.60450700	1.61847700	1.21878500
O	2.34248700	1.45800200	-0.57953700
H	0.33670300	-2.56392900	0.23950300
O	2.33798800	-0.83145200	0.82388100
H	-1.31124200	-1.44995700	1.68812400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -648.310734

63) Conformer **5aC7**

O	-2.08440200	0.92072000	1.36906300
H	1.95604400	-1.14355400	-1.19268700
C	1.12607300	0.76137700	-0.64348100
C	1.48083300	-0.69487800	-0.31536400
C	-1.04599100	0.35206500	0.62923400
C	-1.53056000	-0.24130600	-0.69123700
O	-0.75916500	-1.29325500	-1.00555000
O	-2.43591100	0.14086000	-1.37764800
C	0.09102200	1.34079500	0.32751600
C	0.22045700	-1.48095200	0.05321000
H	2.84579100	1.25103000	0.03509400
C	-0.45897700	-0.88770800	1.27513000
H	0.23989000	-0.67221900	2.08118200
H	-2.59850500	1.48331100	0.77684600
H	0.70308200	0.77494800	-1.65179600
H	-0.31903500	2.26213100	-0.09405500
H	3.00774700	-1.40237900	0.68359600
H	0.56944300	1.59077500	1.27854100
O	2.29187000	1.54604300	-0.70036400
H	0.41763400	-2.54930700	0.12024200
O	2.37894500	-0.68232200	0.77899900
H	-1.24992900	-1.54746700	1.63697800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -648.312596

64) Conformer **5aC8**

O	-2.03467900	1.09904200	1.28952000
H	1.94688900	-1.19430600	-1.15352900
C	1.12956300	0.73230900	-0.66530600
C	1.47355200	-0.71523300	-0.29140500
C	-1.04628400	0.38857100	0.60919000
C	-1.53392100	-0.24371400	-0.69991100
O	-0.76882900	-1.31668000	-0.96786100
O	-2.43192700	0.10386500	-1.41187100
C	0.09913700	1.35085500	0.28469300

C	0.20616300	-1.47940700	0.09755400
H	2.85216700	1.22788600	0.00096500
C	-0.46979800	-0.84227900	1.29655500
H	-1.26134000	-1.49135200	1.67945700
H	-2.76677800	0.50774400	1.49555100
H	0.70899300	0.71808900	-1.67450800
H	0.57960800	1.62270300	1.22872900
H	2.99279000	-1.40288000	0.73268800
H	-0.30521700	2.26145500	-0.16234000
O	2.30021400	1.50751200	-0.74200800
H	0.39539600	-2.54690900	0.19659200
O	2.37034500	-0.67451800	0.80344600
H	0.22602900	-0.60280700	2.09836800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -648.310823

65) Conformer **5bC1**

H	-0.24304000	-0.54764100	-1.84826100
H	3.70997900	2.10586300	-1.92407600
C	2.59063800	2.17942700	-0.11989400
H	3.85937700	3.63081000	-1.00938700
H	-1.95838100	1.99498300	0.12549200
H	-5.98115500	0.16375700	-1.15872000
H	-0.80963900	-1.98496300	-0.98366700
C	0.76764200	-0.92960700	0.02317300
H	3.39265100	-3.32593500	-1.70351900
H	4.63817100	-3.13450300	-0.43893200
H	-5.12921100	-1.35930300	-1.53058600
H	0.61387100	-1.56855900	0.89576400
H	-0.65884900	1.69105400	-1.05761700
O	-2.76190700	-0.38061800	-1.00763000
O	-0.87569000	0.28482800	1.92192700
H	4.28447300	-1.81343700	-1.58468200
H	-4.82494600	0.06713900	-2.51615600
O	1.71377000	1.22213100	-0.48071800
H	1.80618000	0.37831500	1.39494100
O	-4.04739800	0.79405200	0.40869200
H	2.38180000	3.26035900	-1.94001800
C	-5.04654900	-0.27117400	-1.50253300
O	2.84424900	-2.18867800	1.13500200
C	-1.14165000	1.33163800	-0.15094200
O	-2.36991000	-1.36566500	1.72755300
C	2.82503800	-2.09404800	-0.06525600
O	1.84006100	-1.47289700	-0.73884000

C	3.85657000	-2.63092800	-1.00148500
H	0.04695800	2.08394100	1.54885000
C	3.17786900	2.84365800	-1.32058900
C	-1.60015800	-0.11353700	-0.25149300
C	-0.17580400	1.16623000	1.00964900
C	-0.47333000	-0.95409000	-0.86100500
O	2.84609100	2.43841000	1.02706200
C	1.10932700	0.46254800	0.56119500
C	-3.93951000	0.12235000	-0.58332800
C	-1.72381300	-0.49486500	1.22687000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1105.865805

66) Conformer **5bC2**

H	-0.22887000	-0.09170500	-1.83265200
H	4.34512900	3.02939500	-0.86480200
C	2.87687600	1.75064400	-0.01717300
H	2.70840400	3.73883800	-0.76230000
H	-2.14392400	1.97824200	0.47997500
H	-6.01833100	0.21003600	-1.26593900
H	-0.74679800	-1.68419800	-1.25833800
C	0.73791300	-0.75247600	-0.01578500
H	4.58797900	-2.88930800	-0.82000100
H	4.52310200	-1.16835900	-1.26291800
H	-5.07090800	-1.17725700	-1.86765400
H	0.59396100	-1.54685700	0.71957000
H	-0.79464800	1.95178300	-0.68650500
O	-2.78079600	-0.19781900	-1.07946600
O	-1.02508000	0.03920500	1.99392000
H	3.58393500	-2.33371700	-2.19368500
H	-4.81599700	0.41662300	-2.56987800
O	1.54503900	1.54910800	-0.06613200
H	1.66674400	0.34058200	1.59691500
O	-4.17281700	0.64917700	0.46449200
H	3.05522300	2.52188800	-1.98573900
C	-5.05037100	-0.10926100	-1.64274500
O	2.71402200	-2.33647600	0.85357700
C	-1.28381100	1.41524000	0.12373300
O	-2.41934100	-1.62375100	1.46025000
C	2.80722400	-1.88033800	-0.25585900
O	1.87171300	-1.08334900	-0.80956200
C	3.94763500	-2.09469100	-1.19423400
H	-0.19000900	1.91884400	1.97052000
C	3.28100400	2.83222800	-0.96341600

C	-1.65925500	-0.01086000	-0.24274900
C	-0.34540600	1.09712900	1.27511500
C	-0.46954800	-0.67702700	-0.94242200
O	3.61692600	1.12937800	0.69924300
C	0.98645100	0.54098600	0.76922300
C	-3.99674800	0.16741500	-0.62356200
C	-1.80735000	-0.64875900	1.14201600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1105.865511

67) Conformer **5bC3**

H	-0.74680800	-1.68426900	-1.25817400
H	2.70856900	3.73875900	-0.76258100
C	2.87693800	1.75061400	-0.01730900
H	3.05528500	2.52170000	-1.98594000
H	-0.79458500	1.95177400	-0.68672900
H	-6.01810700	0.21125200	-1.26656500
H	-0.22883800	-0.09184900	-1.83265100
C	0.73791000	-0.75244800	-0.01570300
H	3.58360100	-2.33544100	-2.19316000
H	4.58844500	-2.88883400	-0.81920300
H	-5.07210400	-1.17812000	-1.86554900
H	0.59393200	-1.54674900	0.71973400
H	-2.14387500	1.97838700	0.47973000
O	-2.78077500	-0.19782800	-1.07948500
O	-1.02509300	0.03948500	1.99389700
H	4.52231500	-1.16840000	-1.26408300
H	-4.81523100	0.41417600	-2.57065200
O	1.54509600	1.54910700	-0.06627600
H	1.66674000	0.34075200	1.59689900
O	-4.17279200	0.64937800	0.46436100
H	4.34524800	3.02921400	-0.86506800
C	-5.05040400	-0.10971900	-1.64261300
O	2.71396800	-2.33643500	0.85382200
C	-1.28376900	1.41532700	0.12356000
O	-2.41939200	-1.62349000	1.46038500
C	2.80717900	-1.88042200	-0.25566400
O	1.87171300	-1.08342200	-0.80943100
C	3.94749100	-2.09502600	-1.19410200
H	-0.18998000	1.91910400	1.97030700
C	3.28111000	2.83210000	-0.96364500
C	-1.65924000	-0.01080300	-0.24277500
C	-0.34538500	1.09731800	1.27498700
C	-0.46953900	-0.67707100	-0.94236100

O	3.61695800	1.12940300	0.69918500
C	0.98646500	0.54108900	0.76917500
C	-3.99673300	0.16741500	-0.62360500
C	-1.80736700	-0.64854900	1.14205700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1105.865516

68) Conformer **5bC4**

H	-0.22884800	-0.09182300	-1.83265400
H	2.70855100	3.73876200	-0.76254900
C	2.87693000	1.75061500	-0.01728100
H	3.05529400	2.52170900	-1.98590700
H	-2.14388000	1.97836600	0.47977100
H	-4.81535500	0.41459000	-2.57052300
H	-0.74681400	-1.68425600	-1.25820700
C	0.73790700	-0.75245700	-0.01572300
H	3.58366900	-2.33518500	-2.19323500
H	4.58840100	-2.88886400	-0.81930900
H	-6.01814600	0.21106400	-1.26646400
H	0.59393200	-1.54677400	0.71969800
H	-0.79459400	1.95177500	-0.68669400
O	-2.78078300	-0.19782400	-1.07947900
O	-1.02508800	0.03943900	1.99390000
H	4.52242300	-1.16835900	-1.26391900
H	-5.07191500	-1.17796800	-1.86589900
O	1.54509000	1.54910100	-0.06625600
H	1.66674200	0.34071700	1.59689700
O	-4.17280300	0.64934100	0.46438800
H	4.34523700	3.02923100	-0.86501800
C	-5.05040200	-0.10963500	-1.64263500
O	2.71397500	-2.33644100	0.85377700
C	-1.28377400	1.41531400	0.12358800
O	-2.41938300	-1.62353300	1.46036400
C	2.80718700	-1.88040300	-0.25569900
O	1.87170900	-1.08341300	-0.80945900
C	3.94752300	-2.09495300	-1.19412000
H	-0.18997900	1.91905900	1.97034000
C	3.28110300	2.83210900	-0.96360900
C	-1.65924500	-0.01081100	-0.24277000
C	-0.34538500	1.09728600	1.27500600
C	-0.46954500	-0.67706300	-0.94237500
O	3.61694900	1.12939900	0.69921100
C	0.98646300	0.54106700	0.76918000
C	-3.99674000	0.16741500	-0.62359400

C	-1.80736400	-0.64858300	1.14205000
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No imaginary frequency.
Gibbs Free Energies (a.u.) = -1105.865515

69) Conformer **5bC5**

H	-1.10050100	-1.84584200	-0.83619000
H	1.92996800	3.51435400	-1.53123100
C	2.45920300	2.16393500	0.02389500
H	3.20397300	2.37674900	-1.95485300
H	-1.97863700	1.88078400	1.10768900
H	-5.52540900	0.34964800	-0.61226300
H	-0.65496400	-0.28521400	-1.54817800
C	0.64526300	-0.95085300	0.03941100
H	2.89419300	-3.04381000	-2.44552300
H	4.33950300	-3.03551300	-1.39740000
H	-5.07165200	-1.06458300	-1.55571000
H	0.63103900	-1.71309300	0.82153900
H	-0.92389800	1.82948800	-0.32676400
O	-3.06191100	-0.27665300	-0.09492100
O	-0.60712500	-0.06867700	2.35637700
H	3.82279000	-1.56070700	-2.25808500
H	-5.26592200	0.51070300	-2.37141900
O	1.51206600	1.26351600	-0.30377100
H	1.93993100	0.14980800	1.37416900
O	-2.78478700	0.99018200	-1.93130300
H	3.56976000	3.74084100	-0.86350200
C	-4.93185700	0.01411400	-1.46437000
O	2.85978200	-2.34240600	0.58198100
C	-1.22707700	1.29869600	0.57079600
O	-2.21632400	-1.60844000	2.20249100
C	2.63678600	-2.07295100	-0.57039000
O	1.56213600	-1.36788800	-0.96682500
C	3.48383800	-2.45850300	-1.73783500
H	0.26666400	1.77725400	2.12161200
C	2.82003200	3.00906400	-1.15218000
C	-1.71550600	-0.11569800	0.30702400
C	-0.06705700	0.95741200	1.48983000
C	-0.72700000	-0.84427200	-0.61486800
O	2.93176600	2.24891300	1.12727800
C	1.10139000	0.34870900	0.70698100
C	-3.48896200	0.31571400	-1.22713100
C	-1.59599700	-0.71357300	1.71311300

No imaginary frequency.
Gibbs Free Energies (a.u.) = -1105.865029

70) Conformer **5bC6**

H	1.00758000	-1.30120500	1.44787200
H	-3.95269000	3.33709600	0.01792300
C	-2.67593200	1.71686400	-0.48555200
H	-2.33323600	3.81716500	-0.56475400
H	1.06966500	1.86236700	-0.49803200
H	4.96202300	-0.41490900	2.10612800
H	0.60966900	0.42566500	1.43800900
C	-0.63060000	-0.78816200	0.15565600
H	-4.35421600	-2.17667200	2.21580400
H	-4.20536300	-0.42713900	1.93789000
H	5.20766900	1.34842800	2.22279900
H	-0.61923700	-1.80490300	-0.24240500
H	2.20793400	1.30217200	-1.74864100
O	3.09482100	-0.22225400	0.29195400
O	0.80318900	-0.94167900	-2.21951700
H	-3.15371800	-1.20399100	3.12014700
H	5.55551600	0.47147300	0.70665100
O	-1.35982100	1.43147900	-0.54362000
H	-1.78341800	-0.28554300	-1.59800600
O	2.78575100	1.68217300	1.44593900
H	-2.51570500	3.16305300	1.05885100
C	4.89512500	0.53536500	1.57304600
O	-2.75168300	-2.42339100	0.21624900
C	1.39440400	1.00729900	-1.08293500
O	2.31352200	-2.33483300	-1.34645700
C	-2.66433200	-1.58446500	1.07455400
O	-1.63676100	-0.71696000	1.16029600
C	-3.65645000	-1.34482400	2.16337200
H	0.02426400	0.86955900	-2.80427500
C	-2.89263200	3.09857300	0.03607800
C	1.78533400	-0.19637400	-0.24208000
C	0.27202400	0.35989600	-1.87588100
C	0.70461900	-0.46447700	0.81545600
O	-3.53823300	0.94557800	-0.81494700
C	-0.97144400	0.14496100	-1.01191000
C	3.48894600	0.76090400	1.12437700
C	1.71543700	-1.30281500	-1.30003800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1105.864414

71) Conformer **5bC7**

H	1.00758300	-1.30117200	1.44790300
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H	-2.51574900	3.16303800	1.05879000
C	-2.67594400	1.71682500	-0.48559300
H	-3.95271700	3.33705800	0.01783700
H	1.06966800	1.86235600	-0.49807100
H	5.55552200	0.47152900	0.70663100
H	0.60967200	0.42569700	1.43800000
C	-0.63059500	-0.78816000	0.15567200
H	-3.15370900	-1.20395400	3.12018200
H	-4.35425400	-2.17655800	2.21582300
H	4.96204800	-0.41487200	2.10610300
H	-0.61923600	-1.80491200	-0.24236100
H	2.20793900	1.30213700	-1.74866700
O	3.09482500	-0.22224500	0.29196400
O	0.80320100	-0.94172500	-2.21949900
H	-4.20531500	-0.42702500	1.93794200
H	5.20767000	1.34846900	2.22278500
O	-1.35983000	1.43145400	-0.54365800
H	-1.78341000	-0.28559400	-1.59800400
O	2.78575700	1.68220500	1.44591200
H	-2.33325600	3.81712800	-0.56482100
C	4.89513300	0.53540500	1.57302900
O	-2.75171000	-2.42335200	0.21629100
C	1.39440900	1.00727600	-1.08295500
O	2.31353500	-2.33485700	-1.34640800
C	-2.66434100	-1.58441500	1.07458300
O	-1.63675600	-0.71692400	1.16031100
C	-3.65644800	-1.34474300	2.16340500
H	0.02426900	0.86949900	-2.80429300
C	-2.89265800	3.09854100	0.03601200
C	1.78533900	-0.19637800	-0.24207400
C	0.27203000	0.35985500	-1.87588900
C	0.70462200	-0.46445900	0.81546800
O	-3.53823900	0.94551900	-0.81495900
C	-0.97144000	0.14493000	-1.01191700
C	3.48895000	0.76092900	1.12436600
C	1.71544400	-1.30284300	-1.30000800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1105.864414

72) Conformer **5bC8**

H	0.60967600	0.42571100	1.43799900
H	-3.95271800	3.33703700	0.01788600
C	-2.67594200	1.71682000	-0.48559400
H	-2.33330800	3.81712800	-0.56488600

H	2.20792800	1.30213200	-1.74868700
H	5.20766800	1.34845700	2.22279800
H	1.00759500	-1.30115400	1.44791400
C	-0.63059300	-0.78816400	0.15568500
H	-4.35412500	-2.17664500	2.21596900
H	-4.20546900	-0.42714200	1.93780700
H	5.55552100	0.47154200	0.70663100
H	-0.61922300	-1.80491800	-0.24234600
H	1.06966300	1.86236300	-0.49809300
O	3.09483100	-0.22222900	0.29194100
O	0.80319200	-0.94173500	-2.21949800
H	-3.15371200	-1.20371100	3.12015600
H	4.96204300	-0.41488000	2.10608800
O	-1.35982900	1.43144600	-0.54365200
H	-1.78341900	-0.28560500	-1.59799200
O	2.78574900	1.68220300	1.44592100
H	-2.51567700	3.16307200	1.05875200
C	4.89513000	0.53540500	1.57302900
O	-2.75170600	-2.42334400	0.21629700
C	1.39440000	1.00727600	-1.08296900
O	2.31353100	-2.33486200	-1.34640200
C	-2.66433300	-1.58441500	1.07459600
O	-1.63674100	-0.71692700	1.16032400
C	-3.65644400	-1.34473200	2.16341000
H	0.02424900	0.86948100	-2.80429800
C	-2.89265300	3.09854100	0.03600100
C	1.78534000	-0.19637200	-0.24207900
C	0.27202100	0.35984300	-1.87589400
C	0.70463000	-0.46444900	0.81547000
O	-3.53823600	0.94551600	-0.81496800
C	-0.97144400	0.14491900	-1.01191200
C	3.48894800	0.76093600	1.12436500
C	1.71543900	-1.30284700	-1.30000800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1105.864411

73) Conformer **5c1**

C	0.49275000	1.55899700	0.41393100
H	1.18907700	1.81591300	1.21782100
H	-0.03279600	2.47613900	0.13738500
C	-0.49909300	0.52755000	0.97883400
H	-1.15194500	0.96687200	1.73129500
C	0.26715700	-0.71159500	1.42134800
H	1.15209900	-0.48485600	2.01622600

H	-0.36828800	-1.40389500	1.97781000
C	0.60831000	-1.27004400	0.04907100
H	0.82813900	-2.33649400	0.03592500
C	1.69604600	-0.44472500	-0.61861800
H	2.58832700	-0.50440700	0.01224700
H	1.95996300	-0.87838200	-1.58629900
C	1.24667900	1.00743000	-0.79848400
H	2.10618700	1.64130400	-1.02626700
H	0.59204000	1.06282900	-1.67414700
C	-1.30381000	-0.04269700	-0.17019900
O	-0.64068800	-1.09652700	-0.68130300
O	-2.34819100	0.33346200	-0.63086000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -422.787079

74) Conformer **6aC1**

C	0.54649200	-0.99700000	0.15710000
C	0.39125000	-0.00549800	-1.00228600
C	-0.60728600	1.13444800	-0.74145900
H	-1.00913700	1.49785300	-1.69056100
H	-0.08794700	1.96686400	-0.26235700
C	-1.76331900	0.73969500	0.18800200
C	-1.19196200	0.23593000	1.49963500
H	-1.98039800	0.11671100	2.24517600
H	-0.39642400	0.86175700	1.90073900
C	-0.69135700	-1.11615300	1.02844200
H	-0.56065000	-1.85333400	1.81801200
O	1.61436900	-0.45392100	0.89446900
C	2.51323600	0.11557700	-0.04505300
O	1.70703800	0.49187600	-1.16511300
O	-1.75439400	-1.59786400	0.16160500
C	-2.40884200	-0.53883000	-0.33731000
O	-3.34472700	-0.63129800	-1.08033100
O	-2.69409300	1.76812600	0.34797200
H	-3.24739300	1.79366500	-0.44284800
C	3.13991000	1.34207200	0.57447600
H	2.36410600	2.04410100	0.88164600
H	3.79540100	1.82884300	-0.14883700
H	3.73385800	1.06148400	1.44569400
C	3.54501200	-0.90209800	-0.49477300
H	4.17692000	-0.47008800	-1.27230300
H	3.05907900	-1.79086900	-0.90058800
H	4.17609000	-1.19525100	0.34590000
H	0.11093200	-0.53585300	-1.91583000

H	0.80120900	-1.99008800	-0.23330600
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No imaginary frequency.
Gibbs Free Energies (a.u.) = -764.882116

75) Conformer **6aC2**

C	0.54649200	-0.99700300	0.15710300
C	0.39124800	-0.00550600	-1.00228600
C	-0.60727800	1.13444700	-0.74145400
H	-1.00912500	1.49786100	-1.69055400
H	-0.08793400	1.96685600	-0.26234500
C	-1.76331600	0.73969500	0.18800300
C	-1.19196300	0.23592700	1.49963700
H	-1.98040200	0.11670800	2.24517600
H	-0.39642600	0.86175200	1.90074500
C	-0.69135900	-1.11615500	1.02844300
H	-0.56065600	-1.85333800	1.81801200
O	1.61436600	-0.45391600	0.89447000
C	2.51323300	0.11557800	-0.04505400
O	1.70703900	0.49185400	-1.16512500
O	-1.75439600	-1.59786300	0.16160300
C	-2.40883900	-0.53882800	-0.33731200
O	-3.34472300	-0.63129100	-1.08033600
O	-2.69408800	1.76812800	0.34797100
H	-3.24739600	1.79365600	-0.44284400
C	3.54502100	-0.90209200	-0.49475800
H	4.17691800	-0.47008700	-1.27230100
H	3.05909700	-1.79087800	-0.90055300
H	4.17610800	-1.19522000	0.34591700
C	3.13989300	1.34208400	0.57446800
H	2.36408200	2.04412200	0.88160100
H	3.79540900	1.82883900	-0.14883300
H	3.73381300	1.06150900	1.44570900
H	0.11092000	-0.53586200	-1.91582600
H	0.80121300	-1.99009100	-0.23330000

No imaginary frequency.
Gibbs Free Energies (a.u.) = 764.882116

76) Conformer **6aC3**

C	0.53095600	-1.05868500	-0.21014100
C	0.50204400	0.25654000	-1.02517200
C	-0.79385000	1.06878100	-0.98280800
H	-1.33047500	0.97818800	-1.93023400
H	-0.51817300	2.11941700	-0.87118700
C	-1.74277900	0.72983900	0.18085000

C	-0.95420900	0.22030400	1.37404300
H	-1.59880100	0.13418800	2.25058300
H	-0.08193800	0.82499600	1.61667200
C	-0.58149000	-1.14772100	0.82651000
H	-0.33851200	-1.89342400	1.58092600
O	1.76611200	-1.02891100	0.47205200
C	2.51649300	0.09836300	0.02490100
O	1.53927600	1.01392300	-0.41967800
O	-1.78855500	-1.59977500	0.15385400
C	-2.50623200	-0.53080900	-0.19748200
O	-3.57746600	-0.59112500	-0.73461700
O	-2.61627000	1.78104100	0.47039500
H	-3.38549600	1.68596700	-0.10677100
C	3.25131800	0.69815600	1.19745500
H	3.80188300	1.58444900	0.87946900
H	3.96208700	-0.02450200	1.59998800
H	2.54362800	0.97678300	1.97876900
C	3.45329000	-0.31116800	-1.09966000
H	4.16491000	-1.05375800	-0.73585400
H	4.00731000	0.55704200	-1.46037500
H	2.90196500	-0.74644200	-1.93467500
H	0.76029500	0.04707600	-2.06769200
H	0.47329800	-1.93280100	-0.86664800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -764.882713

77) Conformer **6aC4**

C	0.53095700	-1.05868600	-0.21013500
C	0.50204400	0.25653700	-1.02517200
C	-0.79384900	1.06877800	-0.98280900
H	-1.33047500	0.97818500	-1.93023500
H	-0.51817200	2.11941500	-0.87119000
C	-1.74278000	0.72984000	0.18084900
C	-0.95421000	0.22030700	1.37404400
H	-1.59880200	0.13419400	2.25058400
H	-0.08193900	0.82499800	1.61667200
C	-0.58149100	-1.14772000	0.82651500
H	-0.33851600	-1.89342100	1.58093200
O	1.76611100	-1.02890500	0.47206200
C	2.51649400	0.09836400	0.02490000
O	1.53927700	1.01392200	-0.41968400
O	-1.78855500	-1.59977500	0.15385600
C	-2.50623100	-0.53081000	-0.19748100
O	-3.57746500	-0.59112500	-0.73461900

O	-2.61627000	1.78104200	0.47039000
H	-3.38549800	1.68596200	-0.10677300
C	3.25132100	0.69816600	1.19744700
H	2.54363600	0.97678500	1.97876700
H	3.80187100	1.58446500	0.87945400
H	3.96210400	-0.02448200	1.59997400
C	3.45328700	-0.31118000	-1.09966000
H	2.90195800	-0.74645500	-1.93467200
H	4.16490200	-1.05377300	-0.73584800
H	4.00731200	0.55702500	-1.46038000
H	0.76029300	0.04706600	-2.06769100
H	0.47330200	-1.93280400	-0.86663800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -764.882713

78) Conformer **6bC1**

C	-1.47709100	-0.96987100	-0.30872600
C	-1.23352900	-0.23052800	1.01361100
C	0.00519000	0.68314300	1.02734100
H	0.37835800	0.78828400	2.04781700
H	-0.27655900	1.67538000	0.67043500
C	1.12928900	0.17608300	0.12387600
C	0.60069000	0.04658700	-1.29515100
H	1.40233800	-0.11392800	-2.01305800
H	-0.01438000	0.89136300	-1.60047100
C	-0.20996000	-1.22085900	-1.10732700
H	-0.41124000	-1.76987100	-2.02483400
O	-2.33000200	-0.09521500	-1.00544800
C	-3.17573700	0.51048900	-0.04006200
O	-2.41883500	0.52397800	1.17456200
O	0.63268500	-2.06125500	-0.27622400
C	1.41847400	-1.28285600	0.48516500
O	2.14334400	-1.71515700	1.33216800
O	2.23479400	1.03437600	0.33028800
C	-3.46833200	1.92515900	-0.47968400
H	-2.53675200	2.47601800	-0.61312900
H	-4.07595800	2.42900700	0.27303700
H	-4.01885400	1.91933000	-1.42168900
C	-4.43594600	-0.30784800	0.16936500
H	-4.18880700	-1.33247000	0.45176400
H	-5.02984300	-0.32506800	-0.74596100
H	-5.03547300	0.13375600	0.96685700
H	-1.16626200	-0.94505300	1.83775300
H	-1.96949900	-1.93029400	-0.11316200

C	3.41451000	0.71903600	-0.23923100
O	3.57593100	-0.25958800	-0.92086700
C	4.45434000	1.73617300	0.09376000
H	4.58834700	1.78253100	1.17609000
H	4.12681400	2.72280300	-0.23861300
H	5.39303800	1.47284000	-0.38630100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -917.397116

79) Conformer **6bC2**

C	-1.48951000	1.00265200	0.38370000
C	-1.08561200	0.45571200	-0.98961300
C	0.28159600	-0.25149300	-1.02436500
H	0.69775400	-0.20298500	-2.03275700
H	0.14683800	-1.30066400	-0.76350000
C	1.28115600	0.34640800	-0.02970800
C	0.70844700	0.28017000	1.37624700
H	1.46428800	0.53165900	2.12271900
H	0.25528900	-0.67700600	1.61742600
C	-0.30776500	1.39803500	1.25207300
H	-0.62496100	1.82777000	2.19995800
O	-2.18456500	-0.07700500	0.95736400
C	-2.88604700	-0.72242900	-0.09505000
O	-2.13329200	-0.44815800	-1.28177900
O	0.39946900	2.43292900	0.52224000
C	1.34443000	1.86204200	-0.24046800
O	2.06724400	2.48682700	-0.95841400
O	2.59896000	-0.14122700	-0.21999400
C	-2.89982400	-2.20752500	0.17979700
H	-3.45029100	-2.41405100	1.09900000
H	-1.88017700	-2.57980300	0.28343400
H	-3.38928400	-2.73204700	-0.64181600
C	-4.27996100	-0.14548300	-0.25269000
H	-4.77337100	-0.59873600	-1.11387700
H	-4.23481200	0.93336200	-0.40990600
H	-4.87514900	-0.35022900	0.63873900
H	-1.10568500	1.25286500	-1.73666900
H	-2.14462600	1.87371400	0.25885100
C	2.88632900	-1.41730300	0.09563100
O	2.08354700	-2.19113400	0.54780900
C	4.32012600	-1.71926700	-0.19504600
H	4.55031000	-2.73599800	0.11218700
H	4.96441600	-1.01203000	0.32953200
H	4.50837000	-1.60279200	-1.26417000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -917.395664

80) Conformer **6bC3**

C	1.49684400	1.09034200	-0.12900600
C	1.30179600	0.13644300	1.07657500
C	-0.12755500	-0.31309100	1.39043700
H	-0.49402100	0.17719600	2.29411300
H	-0.09359100	-1.38458100	1.59645000
C	-1.12901800	-0.09286400	0.25112800
C	-0.43180100	-0.20032100	-1.09520300
H	-1.14633600	-0.23980600	-1.91437200
H	0.25531800	-1.04269300	-1.15501900
C	0.29260400	1.13399200	-1.06068800
H	0.57963300	1.52276800	-2.03563500
O	2.58408500	0.54284500	-0.84231600
C	3.14173500	-0.52984600	-0.08691800
O	2.06570600	-0.99783600	0.69790900
O	-0.67578300	2.05567900	-0.49853100
C	-1.52802400	1.38305300	0.28364100
O	-2.38181700	1.91143300	0.93403300
O	-2.21721400	-0.96316600	0.49885700
C	3.57113300	-1.62538900	-1.02990300
H	2.72104300	-1.95902500	-1.62566800
H	3.96743500	-2.47034700	-0.46542200
H	4.35239000	-1.25740700	-1.69594900
C	4.28493400	-0.02312700	0.77663200
H	4.68949500	-0.83855900	1.37843000
H	3.95332400	0.77360300	1.44446700
H	5.08000800	0.37162900	0.14251200
H	1.73373500	0.58846600	1.97418200
H	1.72475000	2.10766700	0.20486900
C	-3.32963800	-0.84029900	-0.25118700
O	-3.44274500	-0.03260600	-1.13617000
C	-4.36576900	-1.82835100	0.17000600
H	-3.95907500	-2.83957800	0.11677900
H	-5.23864700	-1.74130500	-0.47145700
H	-4.64675900	-1.64205600	1.20837600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -917.397524

81) Conformer **6bC4**

C	1.48466800	1.18084600	-0.08371800
C	1.06534800	0.23947600	1.07176900

C	-0.43351000	0.00665800	1.27610300
H	-0.78862400	0.56411300	2.14491800
H	-0.56434100	-1.05346800	1.49365000
C	-1.30094500	0.36249800	0.05832000
C	-0.52741400	0.20802000	-1.24064800
H	0.02875100	-0.72220300	-1.31171300
H	-1.19030800	0.30940000	-2.10207300
C	0.37339900	1.42167700	-1.09759200
H	0.78644800	1.79532200	-2.03254100
O	2.53446900	0.49929000	-0.73473100
C	2.86526000	-0.66803800	0.01478100
O	1.67610900	-0.98717600	0.70474600
O	-0.49967400	2.45131800	-0.57092300
C	-1.51492300	1.87699000	0.08331200
O	-2.39288400	2.49752100	0.60650800
O	-2.59038000	-0.22128100	0.12915900
C	3.19378900	-1.78942200	-0.93848900
H	2.34983400	-1.97332600	-1.60385100
H	3.41621300	-2.70032800	-0.38133000
H	4.06846300	-1.52622300	-1.53441900
C	4.00540700	-0.36714500	0.97364200
H	4.89592600	-0.08329400	0.41103400
H	4.23574200	-1.25124600	1.57037900
H	3.75119300	0.45330900	1.64675100
H	1.49532400	0.59880700	2.01157200
H	1.82847200	2.14726600	0.29863200
C	-2.72962000	-1.54450900	-0.07245100
O	-1.81161000	-2.28147400	-0.32119300
C	-4.16232700	-1.94696600	0.05609900
H	-4.26126000	-3.01415400	-0.12382400
H	-4.76956300	-1.38849800	-0.65833900
H	-4.52530800	-1.70156200	1.05586200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -917.396341

82) Conformer **6cC1**

C	1.98048000	-0.87149700	0.53856600
C	1.75082200	-0.52671400	-0.93745500
C	0.44396300	0.23470900	-1.22620400
H	0.11695700	0.03826000	-2.24863500
H	0.62420800	1.30685800	-1.13170400
C	-0.68371900	-0.12235900	-0.25755100
C	-0.22933900	0.16484100	1.16246200
H	0.29204700	1.11469800	1.26700200

H	-1.04693100	0.09972900	1.87929000
C	0.69549300	-1.02753700	1.33085100
H	0.88684200	-1.30075500	2.36619700
O	2.71345200	0.23222600	1.00873400
C	3.55947200	0.64626600	-0.05351400
O	2.87463300	0.26955300	-1.25329600
O	-0.03023600	-2.12643200	0.72036400
C	-0.84781200	-1.64496400	-0.22795300
O	-1.52404400	-2.33655500	-0.92832400
O	-1.84097000	0.54252700	-0.75910600
C	4.89409200	-0.07246200	0.00156400
H	5.49780300	0.20216600	-0.86473400
H	4.75124800	-1.15419100	-0.00759800
H	5.43471100	0.20684700	0.90738500
C	3.70460000	2.14784700	0.00684100
H	4.20301000	2.43982800	0.93244200
H	2.72332800	2.62151400	-0.03555000
H	4.30547700	2.49587800	-0.83424000
H	1.78618000	-1.43162800	-1.54861500
H	2.56139100	-1.79810900	0.61971700
S	-3.25126600	0.54199900	-0.01685300
O	-3.27092000	-0.49885300	0.96711600
C	-3.25472900	2.10873100	0.77171700
H	-3.13513300	2.87838700	0.01165600
H	-2.44830500	2.14761300	1.50164900
H	-4.22028900	2.20659800	1.26779800
O	-4.22094100	0.54667700	-1.06403200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1352.549503

83) Conformer 6cC2

C	1.99725700	0.92987300	-0.42459300
C	1.71799400	0.38680800	0.98267900
C	0.44175900	-0.46710800	1.10770800
H	0.05599600	-0.41333600	2.12717500
H	0.68522500	-1.50932400	0.89492600
C	-0.65378000	-0.04993500	0.12626200
C	-0.11345900	-0.13212800	-1.28948600
H	0.46752200	-1.03365700	-1.47514200
H	-0.90562200	-0.03555100	-2.02997500
C	0.74507600	1.11773700	-1.26194800
H	0.96899300	1.53348600	-2.24179800
O	2.81586300	-0.06391800	-0.98882000
C	3.63211800	-0.56754700	0.05754600

O	2.86768300	-0.38832600	1.25505800
O	-0.07197300	2.09154900	-0.55685600
C	-0.89869000	1.45310700	0.27992300
O	-1.63798000	2.01699000	1.03271500
O	-1.78263400	-0.86291000	0.43563800
C	3.86976900	-2.03854900	-0.18547700
H	4.44809300	-2.46125700	0.63700500
H	4.42985000	-2.18043000	-1.11100800
H	2.91762900	-2.56482000	-0.25951300
C	4.92228400	0.22234000	0.16937300
H	5.52193300	0.09278900	-0.73305100
H	5.49889600	-0.13016600	1.02590500
H	4.71464500	1.28453300	0.30803800
H	1.67620400	1.20720900	1.70315600
H	2.52587300	1.88831100	-0.35615300
S	-3.23540800	-0.64133800	-0.18763700
O	-3.69222300	-1.94198000	-0.56271700
C	-4.14163000	-0.09047000	1.20658700
H	-3.71198300	0.85134100	1.54138300
H	-4.08293900	-0.85483500	1.97928600
H	-5.17188200	0.03997600	0.87516200
O	-3.17174800	0.39389100	-1.17684800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1352.549892

84) Conformer **6cC3**

C	-2.06791600	1.08669800	-0.31713700
C	-1.53421700	-0.20084400	-0.98177300
C	-0.03008900	-0.46434100	-0.88740200
H	0.45158400	-0.23135300	-1.83559900
H	0.09778600	-1.53540600	-0.71986300
C	0.67229000	0.28147400	0.25767500
C	-0.29819000	0.55941100	1.39188100
H	0.23398400	0.93894500	2.26531500
H	-0.89723400	-0.30515800	1.66919000
C	-1.10877200	1.65350900	0.72126200
H	-1.63603000	2.31391900	1.40659100
O	-3.24558600	0.68176900	0.34573700
C	-3.49826600	-0.69280700	0.05396900
O	-2.23033900	-1.21743100	-0.27906200
O	-0.11026000	2.45323900	0.03741500
C	0.97660300	1.71170300	-0.19522400
O	1.97424000	2.15031200	-0.68897200
O	1.81122100	-0.39947100	0.78288200

C	-4.47342800	-0.80755800	-1.10538700
H	-5.42572100	-0.35051500	-0.83282300
H	-4.64574900	-1.85770600	-1.34669800
H	-4.09363900	-0.30110600	-1.99406800
C	-4.00028700	-1.37902800	1.29946700
H	-3.27349100	-1.27266400	2.10523900
H	-4.16354900	-2.43913900	1.10157300
H	-4.94665900	-0.93580000	1.61143300
H	-1.82128400	-0.21822000	-2.03730500
H	-2.28784200	1.86025900	-1.05922200
S	3.08930600	-0.90513500	-0.02821300
O	2.83898300	-0.85163300	-1.43594600
C	4.31093400	0.26995900	0.41761400
H	4.40409600	0.27575100	1.50202500
H	4.01065800	1.24199500	0.03397700
H	5.24008000	-0.06581200	-0.04321100
O	3.41575900	-2.15989500	0.57484500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1352.547836

85) Conformer **6cC4**

C	-2.01069200	0.92358500	0.41977900
C	-1.60883900	0.48027000	-0.99064100
C	-0.16301800	-0.03531100	-1.11343500
H	-0.14277400	-1.10275200	-0.89389200
H	0.19636800	0.10503400	-2.13457600
C	0.79593000	0.65219800	-0.14080100
C	0.31262700	0.46214600	1.28643200
H	-0.00200500	-0.55526300	1.50978900
H	1.05969300	0.78874400	2.01065900
C	-0.84805200	1.43930700	1.24843500
H	-1.16834500	1.78857800	2.22762400
O	-2.52915200	-0.25620700	0.98185700
C	-3.19520800	-0.95136300	-0.06231100
O	-2.53808900	-0.54769000	-1.26905000
O	-0.31383400	2.58283500	0.53363600
C	0.66541600	2.17192300	-0.28548200
O	1.27829700	2.90763300	-0.99856500
O	2.15576700	0.32598500	-0.43946300
C	-3.01170300	-2.43413800	0.15651900
H	-3.48930200	-2.73790800	1.08932500
H	-1.95000400	-2.67840400	0.20288800
H	-3.46989700	-2.98876300	-0.66333700
C	-4.65539200	-0.54843500	-0.13812700

H	-4.75200500	0.53220500	-0.25434700
H	-5.17814900	-0.85643000	0.76884900
H	-5.12828800	-1.03061700	-0.99504200
H	-1.77096900	1.29061200	-1.70521100
H	-2.77729200	1.70584300	0.36042000
S	2.84916400	-0.96752400	0.17554300
O	1.96585000	-2.08974000	0.05056800
C	4.17137400	-1.08911600	-0.96465400
H	4.74956200	-0.16786500	-0.93107200
H	3.76619200	-1.26974200	-1.95792700
H	4.77822600	-1.93244100	-0.63504800
O	3.35337300	-0.65242100	1.47826000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1352.549236

86) Conformer **6cC5**

C	2.01387700	1.05477900	-0.36134100
C	1.78504200	0.42333500	1.03338800
C	0.33516400	0.21980300	1.47818700
H	0.06089000	0.95019400	2.24104000
H	0.27223600	-0.76750400	1.93915200
C	-0.69370600	0.26574100	0.34140500
C	-0.07593100	-0.21630000	-0.95922700
H	0.52108700	-1.11965300	-0.84797400
H	-0.82226200	-0.34968200	-1.74102000
C	0.77504300	1.01104800	-1.24561700
H	1.04862400	1.13482800	-2.29125000
O	3.00622100	0.24912100	-0.95758200
C	3.48620500	-0.68587300	0.00647500
O	2.40573700	-0.84508500	0.90184200
O	-0.07616100	2.12961900	-0.88885300
C	-0.96470000	1.73942900	0.03072900
O	-1.76634800	2.47063600	0.53101200
O	-1.84919300	-0.39804200	0.84958400
C	4.71593200	-0.13152600	0.70592400
H	4.50323800	0.82691500	1.18222500
H	5.51666400	0.01838200	-0.01960600
H	5.06076700	-0.83246500	1.46779200
C	3.75437200	-2.00382400	-0.67506900
H	4.08577700	-2.74169900	0.05657400
H	4.53846100	-1.88223600	-1.42318900
H	2.84817700	-2.36416500	-1.16268900
H	2.30419000	1.01281800	1.79447600
H	2.35326400	2.09180900	-0.27691000

S	-3.17308600	-0.64363900	-0.00301100
O	-3.16200600	0.20292200	-1.15841600
C	-2.98941300	-2.31826600	-0.49109100
H	-2.11002100	-2.41373200	-1.12531500
H	-3.88888900	-2.58201900	-1.04723300
H	-2.89830800	-2.93153900	0.40326300
O	-4.24272800	-0.54693400	0.93694700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1352.549734

87) Conformer **6cC6**

C	-2.02874700	0.95970200	0.33659100
C	-1.52137700	0.39152200	-0.99299800
C	-0.06090900	-0.10112800	-0.97132700
H	0.35868300	-0.06129300	-1.97773000
H	-0.04952800	-1.14215300	-0.64357700
C	0.81214200	0.70670400	-0.01007200
C	0.23447600	0.64042100	1.39235100
H	0.93257400	1.04872400	2.12486600
H	-0.07395600	-0.35758800	1.69223000
C	-0.93629900	1.58211000	1.18780700
H	-1.33038200	2.01694300	2.10381200
O	-2.56537400	-0.17234900	0.97464800
C	-3.14557400	-0.97962900	-0.03936000
O	-2.41098700	-0.67955300	-1.23228900
O	-0.37769100	2.66532100	0.39994000
C	0.65529300	2.20119000	-0.31654100
O	1.29518600	2.87815800	-1.06336600
O	2.20665400	0.42834600	-0.13214000
C	-4.60280500	-0.61864800	-0.25422000
H	-5.18274600	-0.84780100	0.64127200
H	-5.00720100	-1.19301300	-1.08906000
H	-4.70779700	0.44297200	-0.48351500
C	-2.95448300	-2.42990500	0.33513100
H	-3.34485700	-3.07118100	-0.45607700
H	-3.49175000	-2.65299500	1.25818800
H	-1.89502600	-2.64477900	0.47810300
H	-1.64453600	1.12548100	-1.79287100
H	-2.80307500	1.71300800	0.14711100
S	2.78030500	-1.05139700	-0.00233200
O	2.76198800	-1.67592700	-1.29035500
C	4.42326800	-0.62890000	0.43017500
H	4.96776700	-1.56986200	0.50691800
H	4.41500500	-0.10770100	1.38497300

H	4.84464200	-0.00885600	-0.35870100
O	2.12490000	-1.72001900	1.08308100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1352.548823

88) Conformer **6cC7**

C	2.02007300	1.07220100	-0.27512100
C	1.78046200	0.31555700	1.05529800
C	0.33136200	-0.01729500	1.42107200
H	-0.01599800	0.61800600	2.23746300
H	0.31681700	-1.04683900	1.78320800
C	-0.65640900	0.07325400	0.25169400
C	0.03330700	-0.25668100	-1.05936300
H	-0.68455200	-0.37654400	-1.86877000
H	0.67866000	-1.13103300	-0.99728300
C	0.81822000	1.03517600	-1.20924200
H	1.11868400	1.26959100	-2.22819500
O	3.07666000	0.37390900	-0.89551100
C	3.58659400	-0.59835300	0.01432200
O	2.49006400	-0.89535300	0.85317200
O	-0.11009700	2.06931900	-0.78757200
C	-0.99727900	1.55229000	0.06387600
O	-1.84850300	2.19614000	0.60560300
O	-1.77040400	-0.73439500	0.62488100
C	4.75127000	-0.01955000	0.80002000
H	4.45694300	0.88355900	1.33722200
H	5.56402900	0.23788500	0.11943200
H	5.11721400	-0.75220800	1.52108100
C	3.96547500	-1.84015300	-0.75216500
H	4.76266700	-1.61090600	-1.46011600
H	3.10141300	-2.22083600	-1.29745100
H	4.32311600	-2.60815900	-0.06523300
H	2.22949800	0.87457300	1.88129300
H	2.29665600	2.11542700	-0.09297100
S	-3.16057800	-0.75368500	-0.15952200
O	-3.50626700	-2.13426400	-0.28614200
C	-4.23441200	0.00627900	0.99718500
H	-4.21285200	-0.57262200	1.91875400
H	-5.23080300	-0.01497600	0.55572100
H	-3.89418800	1.02712500	1.15726000
O	-3.05020800	0.05346500	-1.33874700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1352.550368

89) Conformer **6cC8**

C	-2.06791700	1.08669100	-0.31711400
C	-1.53421500	-0.20084700	-0.98176100
C	-0.03008800	-0.46436200	-0.88737300
H	0.45159400	-0.23141700	-1.83557500
H	0.09776700	-1.53542300	-0.71979000
C	0.67229400	0.28147900	0.25768000
C	-0.29818000	0.55942700	1.39189000
H	0.23399800	0.93896400	2.26532000
H	-0.89722500	-0.30514000	1.66920500
C	-1.10876400	1.65351900	0.72126600
H	-1.63601700	2.31393600	1.40659300
O	-3.24556500	0.68174800	0.34579300
C	-3.49827500	-0.69280900	0.05396300
O	-2.23035500	-1.21744100	-0.27907700
O	-0.11025900	2.45324300	0.03740300
C	0.97660200	1.71170400	-0.19523600
O	1.97424000	2.15030800	-0.68898500
O	1.81124000	-0.39944100	0.78289100
C	-4.47343000	-0.80749000	-1.10540500
H	-4.64576500	-1.85762400	-1.34676700
H	-4.09362800	-0.30100300	-1.99406100
H	-5.42571900	-0.35044500	-0.83282600
C	-4.00031900	-1.37906900	1.29942900
H	-4.16359600	-2.43917000	1.10149200
H	-4.94668800	-0.93583900	1.61140300
H	-3.27352900	-1.27274800	2.10521200
H	-1.82126700	-0.21820300	-2.03729700
H	-2.28787000	1.86024400	-1.05920100
S	3.08930700	-0.90513600	-0.02821700
O	2.83898000	-0.85162600	-1.43594800
C	4.31095400	0.26993900	0.41761100
H	4.40413000	0.27571700	1.50202100
H	4.01067800	1.24198200	0.03399100
H	5.24009200	-0.06582900	-0.04323100
O	3.41573900	-2.15990500	0.57483500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1352.547836

90) Conformer **7C1**

C	1.51012500	-1.36736700	1.54902200
H	1.53625400	-1.71269300	2.58507200
H	2.15039200	-2.05436700	0.98624700
C	2.08813000	0.04136700	1.44665800

H	1.66971600	0.69303300	2.22007900
H	3.16979200	0.01495000	1.60456400
C	1.78909300	0.68498100	0.08158500
C	0.28124700	0.80993300	-0.13253400
C	-0.08900300	-0.65698600	-0.28408300
C	0.08461500	-1.44886500	1.00905200
H	-0.63407100	-1.07419800	1.73729700
H	-0.18866900	-2.49046600	0.81738100
C	-0.66729800	1.53847400	0.79275600
H	-0.68114200	1.09926500	1.79300300
H	-0.37446500	2.58576200	0.90712200
C	-2.05316000	1.46123900	0.15039700
H	-2.03850400	2.04084300	-0.77896500
H	-2.80575800	1.93021500	0.79326200
C	-2.52945000	0.03723300	-0.17819500
C	-1.45795600	-0.78562700	-0.91494000
H	-1.39127400	-0.41734900	-1.94250500
H	-1.78782800	-1.82766800	-0.95500900
O	0.95686300	-1.11001100	-1.20413700
H	0.14951400	1.25963900	-1.12810000
C	-3.79190500	0.09405000	-1.02665400
H	-4.14904300	-0.91616400	-1.23862700
H	-3.61124400	0.60619800	-1.97396000
H	-4.58168500	0.63365800	-0.49565600
O	-2.81637100	-0.66865100	1.03268900
H	-3.51688600	-0.19197500	1.48973500
C	2.06425300	-0.37443400	-0.98812600
O	3.08739800	-0.58606700	-1.58310200
C	2.58636500	1.95130700	-0.13982200
H	2.32688900	2.42291600	-1.09080600
H	3.65701000	1.73715400	-0.14557100
H	2.38753300	2.66724900	0.66114100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -732.300441

91) Conformer 7C2

C	1.50011200	-1.38672700	1.53333600
H	2.13657900	-2.07202300	0.96426500
H	1.52323000	-1.74233400	2.56592900
C	2.08627100	0.01974900	1.44554100
H	1.67183700	0.66557900	2.22591400
H	3.16771900	-0.01488300	1.60327800
C	1.79148600	0.68007400	0.08731500
C	0.28428800	0.81457000	-0.12613500

C	-0.09239900	-0.64886900	-0.29428100
C	0.07454900	-1.45417000	0.99148200
H	-0.20487800	-2.49266300	0.79052000
H	-0.64120500	-1.07992200	1.72327400
C	-0.66010600	1.53605200	0.80883900
H	-0.66743200	1.09146300	1.80660700
H	-0.36615100	2.58257300	0.92775800
C	-2.05144000	1.46687100	0.17628300
H	-2.04302800	2.05462100	-0.74722000
H	-2.80018500	1.91796400	0.83282000
C	-2.53201500	0.05367000	-0.16947400
C	-1.46093300	-0.76159800	-0.92729600
H	-1.78863600	-1.80481300	-0.99404800
H	-1.39311900	-0.37844600	-1.94990700
O	0.95269800	-1.09807000	-1.21697800
H	0.15432500	1.27631000	-1.11638600
C	-3.79748200	0.12551000	-1.01240100
H	-3.61165400	0.62290300	-1.96660100
H	-4.57179200	0.67797000	-0.47566500
H	-4.17533000	-0.87945400	-1.22242700
O	-2.84360700	-0.56027200	1.08348200
H	-3.15248700	-1.45582300	0.91093600
C	2.06305200	-0.36916400	-0.99298200
O	3.08572800	-0.57933600	-1.58919600
C	2.59493600	1.94493900	-0.11936100
H	2.33806700	2.42843400	-1.06507200
H	3.66454600	1.72577600	-0.12715900
H	2.39912000	2.65274900	0.68951900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -732.300479

92) Conformer 8C1

H	0.90939500	2.01701200	-1.51287500
H	-3.15596400	2.90709900	0.36712000
H	-3.25450700	-3.11207300	1.35053600
C	0.77640400	-1.08152500	0.07183200
H	0.19424000	-2.90371700	-0.98746100
H	0.49993500	0.48154100	-2.23362900
H	0.19201700	-1.49192400	-2.02554200
O	-1.95407300	-0.91513200	-1.36729900
H	5.00593300	1.69890000	1.64766500
C	-4.16225400	2.47736900	0.28060700
C	-2.95922400	0.20010500	0.40093000
C	-5.03095600	-1.04654500	0.40706000

H	3.73061000	-2.29577400	1.49942200
H	2.89490500	2.32412900	0.38755000
H	1.29232400	0.89742200	0.67395500
H	0.36451100	-0.24174200	2.58267200
H	-5.56891000	-1.91594900	0.02239700
C	0.50360000	1.02794700	-1.28794200
C	2.90781100	0.38614500	-0.56861400
H	5.08233500	3.12664100	-0.33893800
H	1.35026800	-2.89680500	1.09752000
C	0.70301000	-1.96030300	-1.18954300
H	-4.20779600	1.84058400	2.37684300
H	7.03229400	-0.89465800	-0.13285800
H	-5.80310100	2.08988000	1.66032100
C	-3.98906500	1.08114300	-0.34095900
C	5.97116200	-0.93259700	-0.38740600
O	6.85899500	1.59606100	0.74543800
H	7.24412200	1.13458500	1.49668000
H	-5.50619800	-0.03402500	-1.44520000
H	3.25525500	0.15411900	1.49653800
H	-2.85287500	0.53976100	1.42940300
H	-3.04420600	-1.68679200	2.35816800
C	-0.92770500	1.21041400	-0.80330900
C	-1.58759200	-0.03415900	-0.24527500
H	3.37188900	-2.35101400	-0.20915500
H	-1.17490700	-2.89861300	0.28853300
C	-4.77421200	2.46089300	1.67785700
C	1.67955500	-1.85362800	1.05785300
H	5.86225000	-0.51925000	-1.38997200
C	4.85475600	2.06136200	-0.44223300
O	-3.49802700	-2.46504500	-1.78147700
C	-5.28892300	0.22861500	-0.40699400
H	-5.32022300	-0.91056300	1.45397400
C	-0.65644400	-0.83318000	0.72887700
C	-3.52702500	-1.21187800	0.33917700
H	-0.82400300	-2.59774100	1.96947900
H	3.41125200	-1.22912000	-1.98864700
C	3.26117800	-0.15026100	-1.96441300
H	-0.94300900	1.96606800	-0.01225400
H	-1.55152600	1.60487900	-1.60945800
C	5.46342600	1.31258000	0.72354800
H	-0.53711100	1.07179900	1.85420600
H	-5.98931700	3.01199500	-0.76917800
C	-0.54136600	-0.00444300	2.02845300
H	5.68050000	-1.98480900	-0.42798800

H	5.43970700	-0.60802300	1.63479700
H	4.17820400	0.30500200	-2.33999100
C	3.62337300	-0.35143900	0.58869000
H	1.57802300	-1.46414800	2.07281900
H	5.33312600	1.73341100	-1.37063300
C	1.37751500	0.31841600	-0.25422200
H	-4.51073900	3.45431600	-1.63150100
C	3.34350100	1.86582000	-0.50313900
C	-3.04161900	-1.62916100	-1.04317300
H	-1.37639400	-0.21750900	2.69734600
C	-2.83475400	-2.10193900	1.36721500
H	-3.64255300	1.24217300	-1.36627300
H	-6.16043900	0.77294100	-0.03914800
C	3.16089900	-1.79455800	0.70872900
C	5.15201800	-0.18578900	0.66049500
H	-5.03856800	4.39709800	-0.23045700
H	-4.80156100	3.47332200	2.08917400
H	2.47655600	0.08931900	-2.68416100
H	1.70809100	-2.21984000	-1.51706400
C	-1.32699600	-2.17885100	1.09449600
C	-4.96874400	3.38605800	-0.64070200
H	2.95304500	2.41334600	-1.36541700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1356.698239

93) Conformer **8C2**

H	0.90939500	2.01701200	-1.51287400
H	-3.15596400	2.90709900	0.36712000
H	-3.25450700	-3.11207300	1.35053600
C	0.77640400	-1.08152500	0.07183200
H	1.70809100	-2.21984000	-1.51706400
H	0.49993500	0.48154200	-2.23362900
H	0.19424000	-2.90371700	-0.98746100
O	-1.95407300	-0.91513200	-1.36729900
H	5.00593300	1.69890000	1.64766500
C	-4.16225400	2.47736900	0.28060700
C	-2.95922400	0.20010500	0.40093000
C	-5.03095600	-1.04654600	0.40706000
H	3.73061000	-2.29577400	1.49942100
H	2.89490500	2.32412900	0.38755000
H	1.29232400	0.89742100	0.67395500
H	-1.37639400	-0.21751000	2.69734600
H	-5.56891000	-1.91594900	0.02239700
C	0.50360000	1.02794700	-1.28794100

C	2.90781100	0.38614500	-0.56861400
H	5.08233500	3.12664100	-0.33893800
H	1.35026800	-2.89680500	1.09752000
C	0.70301000	-1.96030300	-1.18954300
H	-4.20779400	1.84058600	2.37684300
H	7.03229400	-0.89465900	-0.13285900
H	-5.80310000	2.08988100	1.66032200
C	-3.98906500	1.08114300	-0.34095900
C	5.97116200	-0.93259700	-0.38740600
O	6.85899500	1.59606100	0.74543800
H	7.24412200	1.13458400	1.49668000
H	-5.50619900	-0.03402400	-1.44519900
H	3.25525500	0.15411900	1.49653800
H	-2.85287500	0.53976100	1.42940300
H	-3.04420600	-1.68679300	2.35816800
C	-0.92770500	1.21041400	-0.80330800
C	-1.58759300	-0.03415900	-0.24527500
H	3.37188900	-2.35101400	-0.20915500
H	-1.17490700	-2.89861300	0.28853300
C	-4.77421100	2.46089400	1.67785700
C	1.67955500	-1.85362800	1.05785300
H	5.86225000	-0.51924900	-1.38997200
C	4.85475600	2.06136200	-0.44223200
O	-3.49802700	-2.46504500	-1.78147700
C	-5.28892400	0.22861500	-0.40699400
H	-5.32022300	-0.91056400	1.45397400
C	-0.65644400	-0.83318000	0.72887700
C	-3.52702500	-1.21187800	0.33917700
H	-0.82400300	-2.59774200	1.96947900
H	4.17820400	0.30500200	-2.33999100
C	3.26117800	-0.15026000	-1.96441300
H	-0.94300900	1.96606800	-0.01225400
H	-1.55152600	1.60487900	-1.60945700
C	5.46342600	1.31257900	0.72354800
H	0.36451000	-0.24174300	2.58267200
H	-4.51073900	3.45431500	-1.63150100
C	-0.54136600	-0.00444300	2.02845300
H	5.68050000	-1.98480900	-0.42798900
H	5.43970700	-0.60802300	1.63479700
H	2.47655600	0.08932000	-2.68416100
C	3.62337300	-0.35143900	0.58868900
H	1.57802300	-1.46414800	2.07281900
H	5.33312500	1.73341100	-1.37063300
C	1.37751500	0.31841600	-0.25422200

H	-5.03856700	4.39709800	-0.23045800
C	3.34350000	1.86582100	-0.50313800
C	-3.04161900	-1.62916100	-1.04317300
H	-0.53711100	1.07179900	1.85420600
C	-2.83475500	-2.10193900	1.36721400
H	-3.64255300	1.24217200	-1.36627200
H	-6.16043900	0.77294100	-0.03914600
C	3.16089900	-1.79455800	0.70872900
C	5.15201800	-0.18578900	0.66049400
H	-5.98931700	3.01199500	-0.76917800
H	-4.80156000	3.47332300	2.08917300
H	3.41125100	-1.22912000	-1.98864700
H	0.19201700	-1.49192300	-2.02554200
C	-1.32699600	-2.17885100	1.09449600
C	-4.96874300	3.38605800	-0.64070300
H	2.95304500	2.41334600	-1.36541600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1356.698239

94) Conformer **8C3**

H	0.91081300	2.01494000	-1.51476100
H	-3.15384700	2.90916400	0.36146600
H	-3.25580600	-3.10875300	1.35513000
C	0.77562700	-1.08269000	0.07151000
H	1.70541600	-2.22544700	-1.51532300
H	0.50123900	0.47939100	-2.23516600
H	0.18822500	-2.90334600	-0.98765800
O	-1.95487400	-0.91646600	-1.36647500
H	5.00670500	1.68881200	1.65173900
C	-4.16040500	2.47975800	0.27651100
C	-2.95877500	0.20185000	0.40047600
C	-5.03123100	-1.04363900	0.40921900
H	3.72861500	-2.29905100	1.49964500
H	2.89965500	2.32043200	0.38915700
H	1.29248300	0.89633300	0.67251300
H	-1.37423100	-0.21439600	2.69759900
H	-5.56975700	-1.91330900	0.02595200
C	0.50458200	1.02606500	-1.28964500
C	2.90840600	0.38312800	-0.56844000
H	5.08347400	3.11911000	-0.34568200
H	1.34810400	-2.89865500	1.09642300
C	0.70079700	-1.96195900	-1.18947400
H	-5.80034100	2.09552700	1.65823100
H	7.02953700	-0.90671000	-0.11471500

H	-4.79806000	3.47952100	2.08354000
C	-3.98835600	1.08227000	-0.34252400
C	5.97105600	-0.94122200	-0.37755700
O	6.87716800	1.47214400	0.80624300
H	7.05452600	2.41554200	0.86576300
H	-5.50701300	-0.03341200	-1.44418300
H	3.25171500	0.15079900	1.49732500
H	-2.85185500	0.54300900	1.42840100
H	-3.04419900	-1.68214000	2.36056900
C	-0.92694800	1.20931300	-0.80569000
C	-1.58749600	-0.03419900	-0.24587300
H	3.37037700	-2.35352600	-0.20899900
H	-1.17628900	-2.89845400	0.29236600
C	-4.77132700	2.46625800	1.67424000
C	1.67803400	-1.85564700	1.05753400
H	5.86841500	-0.52652400	-1.38039700
C	4.85792200	2.05091700	-0.44311300
O	-3.49978900	-2.46616900	-1.77784900
C	-5.28884000	0.23053300	-0.40650100
H	-5.32008200	-0.90607300	1.45604000
C	-0.65658000	-0.83247400	0.72900700
C	-3.52740700	-1.20988100	0.34106800
H	-0.82472300	-2.59476800	1.97263100
H	4.18291300	0.29540400	-2.33672500
C	3.26232100	-0.15445300	-1.96349200
H	-0.94234300	1.96611300	-0.01573700
H	-1.55045600	1.60275200	-1.61258800
C	5.46512900	1.30031300	0.72898600
H	0.36663000	-0.23863600	2.58072300
H	-5.98801500	3.01328000	-0.77288700
C	-0.54003300	-0.00208900	2.02741900
H	5.67345500	-1.99146200	-0.42108100
H	5.43799500	-0.60972600	1.64266100
H	2.48070300	0.08981100	-2.68499500
C	3.62243500	-0.35412000	0.59033700
H	1.57611300	-1.46671100	2.07268400
H	5.33642600	1.72017000	-1.37028900
C	1.37782700	0.31670600	-0.25522600
H	-4.50989600	3.45304100	-1.63728700
C	3.34530600	1.86233700	-0.50318100
C	-3.04275600	-1.62943800	-1.04090500
H	-0.53609600	1.07393600	1.85183800
C	-2.83537100	-2.09887800	1.37014700
H	-3.64213700	1.24118700	-1.36826700

H	-6.15972100	0.77598200	-0.03881500
C	3.15950100	-1.79719600	0.70895500
C	5.15122000	-0.19160500	0.66839400
H	-5.03609300	4.39894700	-0.23772100
H	-4.20456900	1.84717700	2.37403400
H	3.40637200	-1.23408500	-1.98762400
H	0.19277200	-1.49231300	-2.02658300
C	-1.32776400	-2.17715400	1.09707200
C	-4.96713700	3.38704200	-0.64598000
H	2.95439200	2.41196700	-1.36394500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1356.698226

95) Conformer 8C4

H	0.91081300	2.01494000	-1.51476100
H	-3.15384700	2.90916400	0.36146600
H	-3.25580600	-3.10875300	1.35513000
C	0.77562700	-1.08269000	0.07151100
H	1.70541600	-2.22544700	-1.51532300
H	0.50123900	0.47939000	-2.23516600
H	0.18822500	-2.90334600	-0.98765800
O	-1.95487400	-0.91646600	-1.36647600
H	5.00670500	1.68881200	1.65173900
C	-4.16040500	2.47975800	0.27651100
C	-2.95877500	0.20185100	0.40047600
C	-5.03123100	-1.04363900	0.40921900
H	3.72861500	-2.29905100	1.49964500
H	2.89965500	2.32043200	0.38915700
H	1.29248300	0.89633300	0.67251300
H	-0.53609700	1.07393700	1.85183700
H	-5.56975700	-1.91330900	0.02595300
C	0.50458200	1.02606500	-1.28964500
C	2.90840600	0.38312800	-0.56844000
H	5.08347400	3.11911000	-0.34568200
H	1.34810400	-2.89865500	1.09642300
C	0.70079700	-1.96195900	-1.18947400
H	-4.79805900	3.47952100	2.08354000
H	5.67345500	-1.99146200	-0.42108100
H	-4.20456900	1.84717600	2.37403400
C	-3.98835600	1.08227000	-0.34252400
C	5.97105600	-0.94122200	-0.37755600
O	6.87716800	1.47214400	0.80624300
H	7.05452600	2.41554300	0.86576200
H	-5.50701300	-0.03341200	-1.44418300

H	3.25171500	0.15079900	1.49732500
H	-2.85185500	0.54300900	1.42840100
H	-3.04419900	-1.68214000	2.36056900
C	-0.92694700	1.20931300	-0.80569000
C	-1.58749600	-0.03419900	-0.24587300
H	3.37037700	-2.35352600	-0.20899800
H	-1.17629000	-2.89845400	0.29236600
C	-4.77132700	2.46625800	1.67424000
C	1.67803400	-1.85564700	1.05753400
H	7.02953700	-0.90671000	-0.11471500
C	4.85792200	2.05091700	-0.44311300
O	-3.49978900	-2.46616900	-1.77784900
C	-5.28884000	0.23053300	-0.40650100
H	-5.32008200	-0.90607300	1.45604000
C	-0.65658000	-0.83247400	0.72900700
C	-3.52740700	-1.20988100	0.34106800
H	-0.82472300	-2.59476800	1.97263100
H	3.40637200	-1.23408500	-1.98762400
C	3.26232200	-0.15445300	-1.96349200
H	-0.94234300	1.96611300	-0.01573800
H	-1.55045600	1.60275200	-1.61258800
C	5.46512900	1.30031300	0.72898600
H	-1.37423100	-0.21439600	2.69759900
H	-4.50989600	3.45304100	-1.63728700
C	-0.54003300	-0.00208900	2.02741900
H	5.86841500	-0.52652400	-1.38039700
H	5.43799500	-0.60972600	1.64266100
H	4.18291300	0.29540400	-2.33672500
C	3.62243500	-0.35412000	0.59033700
H	1.57611300	-1.46671000	2.07268500
H	5.33642600	1.72017000	-1.37028900
C	1.37782700	0.31670500	-0.25522600
H	-5.03609300	4.39894700	-0.23772100
C	3.34530600	1.86233700	-0.50318200
C	-3.04275600	-1.62943800	-1.04090500
H	0.36663000	-0.23863600	2.58072300
C	-2.83537100	-2.09887800	1.37014700
H	-3.64213700	1.24118700	-1.36826700
H	-6.15972100	0.77598300	-0.03881500
C	3.15950100	-1.79719600	0.70895500
C	5.15122000	-0.19160400	0.66839400
H	-5.98801500	3.01328000	-0.77288700
H	-5.80034100	2.09552700	1.65823100
H	2.48070300	0.08981100	-2.68499500

H	0.19277200	-1.49231400	-2.02658200
C	-1.32776400	-2.17715400	1.09707200
C	-4.96713700	3.38704300	-0.64598000
H	2.95439200	2.41196700	-1.36394500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1356.698226

96) Conformer **8C5**

H	0.90982100	2.02022000	-1.50561800
H	-3.15656900	2.90708900	0.36464200
H	-3.25705600	-3.11439000	1.34394800
C	0.77506500	-1.08134200	0.07284900
H	1.70848200	-2.21604300	-1.51785900
H	0.50252400	0.48567200	-2.22950600
H	0.19413200	-2.90099800	-0.99131700
O	-1.95380600	-0.91317100	-1.36895800
H	5.04564500	1.69097800	1.66939200
C	-4.16290300	2.47746700	0.27826100
C	-2.96098300	0.19936600	0.39973500
C	-5.03256300	-1.04753800	0.40235300
H	3.72764900	-2.30050800	1.49857600
H	2.89469500	2.31883100	0.41391500
H	1.28830900	0.89621600	0.68056400
H	-0.54127400	1.06837900	1.85794200
H	-5.57005500	-1.91635600	0.01573900
C	0.50414400	1.03057800	-1.28295500
C	2.90737600	0.38985400	-0.55891500
H	5.08008100	3.13027900	-0.30616000
H	1.34739600	-2.89864300	1.09569600
C	0.70310300	-1.95712800	-1.19067900
H	-5.80381300	2.09077600	1.65816200
H	7.02610800	-0.94690100	-0.10104400
H	-4.80231400	3.47451600	2.08613100
C	-3.98995400	1.08095600	-0.34268800
C	5.96945600	-0.93447900	-0.38151300
O	6.86995700	1.56474200	0.85850900
H	7.29108200	1.31914300	0.02870100
H	-5.50819800	-0.03164700	-1.44808100
H	3.25513100	0.14901600	1.50497700
H	-2.85600800	0.53782700	1.42874900
H	-3.04751000	-1.69079000	2.35407400
C	-0.92811200	1.21162800	-0.80048600
C	-1.58858700	-0.03394700	-0.24521800
H	3.36845500	-2.34990500	-0.21020900

H	-1.17634500	-2.89924800	0.28411000
C	-4.77493400	2.46182000	1.67547500
C	1.67698200	-1.85550300	1.05815400
H	5.89345200	-0.49566600	-1.37744300
C	4.85282300	2.06598600	-0.41959100
O	-3.49745100	-2.46232800	-1.78725000
C	-5.29023100	0.22908200	-0.40955000
H	-5.32267200	-0.91353100	1.44928500
C	-0.65852500	-0.83448000	0.72870100
C	-3.52856300	-1.21257400	0.33543400
H	-0.82711100	-2.60126500	1.96594200
H	4.18897800	0.31044500	-2.32273100
C	3.26508900	-0.13841000	-1.95633300
H	-0.94495500	1.96613100	-0.00837700
H	-1.55074500	1.60701400	-1.60709900
C	5.47456900	1.30449700	0.73795800
H	-1.38054600	-0.22307800	2.69769700
H	-4.51115900	3.45330400	-1.63446700
C	-0.54503800	-0.00822000	2.02998800
H	5.65109800	-1.97614000	-0.45867300
H	5.44066300	-0.61558000	1.64147300
H	2.48776000	0.11461100	-2.67940700
C	3.62235200	-0.35301300	0.59474900
H	1.57501200	-1.46779200	2.07375900
H	5.32436200	1.75144700	-1.35823300
C	1.37631900	0.31953700	-0.24875900
H	-5.03873700	4.39711400	-0.23401900
C	3.34125500	1.86914900	-0.48215500
C	-3.04183900	-1.62765600	-1.04711300
H	0.36048500	-0.24614800	2.58454200
C	-2.83722900	-2.10432700	1.36262500
H	-3.64267000	1.24153300	-1.36782300
H	-6.16127400	0.77319500	-0.04027800
C	3.15834400	-1.79622200	0.70960900
C	5.15106400	-0.19106300	0.67106300
H	-5.98983800	3.01190700	-0.77185300
H	-4.20850100	1.84199200	2.37486900
H	3.40461400	-1.21848000	-1.98810700
H	0.19296400	-1.48686500	-2.02611800
C	-1.32924200	-2.18088700	1.09118000
C	-4.96917200	3.38579600	-0.64361700
H	2.94847500	2.42482400	-1.33824500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1356.698430

97) Conformer 8C6

H	0.90982100	2.02022100	-1.50561700
H	-3.15657000	2.90708900	0.36464300
H	-3.25705600	-3.11439000	1.34394900
C	0.77506500	-1.08134100	0.07284900
H	0.19296600	-1.48686300	-2.02611900
H	0.50252500	0.48567300	-2.22950600
H	1.70848100	-2.21604500	-1.51785800
O	-1.95380600	-0.91317100	-1.36895800
H	5.04564600	1.69097800	1.66939200
C	-4.16290400	2.47746700	0.27826100
C	-2.96098300	0.19936600	0.39973500
C	-5.03256300	-1.04753800	0.40235300
H	3.72764900	-2.30050800	1.49857600
H	2.89469600	2.31883100	0.41391500
H	1.28830900	0.89621600	0.68056400
H	-1.38054500	-0.22307700	2.69769700
H	-5.57005400	-1.91635700	0.01573800
C	0.50414500	1.03057900	-1.28295400
C	2.90737600	0.38985400	-0.55891500
H	5.08008200	3.13027900	-0.30615900
H	1.34739500	-2.89864300	1.09569500
C	0.70310300	-1.95712700	-1.19067900
H	-4.20850300	1.84199000	2.37486900
H	7.02610800	-0.94690200	-0.10104400
H	-5.80381500	2.09077400	1.65816100
C	-3.98995500	1.08095600	-0.34268800
C	5.96945600	-0.93448000	-0.38151300
O	6.86995800	1.56474200	0.85850900
H	7.29108200	1.31914200	0.02870100
H	-5.50819700	-0.03164900	-1.44808300
H	3.25513200	0.14901700	1.50497700
H	-2.85600800	0.53782700	1.42874900
H	-3.04751000	-1.69078900	2.35407400
C	-0.92811200	1.21162800	-0.80048600
C	-1.58858700	-0.03394700	-0.24521800
H	3.36845500	-2.34990500	-0.21020900
H	-1.17634500	-2.89924800	0.28411100
C	-4.77493600	2.46181800	1.67547600
C	1.67698200	-1.85550300	1.05815400
H	5.89345200	-0.49566600	-1.37744300
C	4.85282300	2.06598600	-0.41959100
O	-3.49745000	-2.46232900	-1.78724900

C	-5.29023100	0.22908100	-0.40955200
H	-5.32267200	-0.91353100	1.44928400
C	-0.65852500	-0.83447900	0.72870100
C	-3.52856300	-1.21257400	0.33543400
H	-0.82711100	-2.60126400	1.96594200
H	2.48776100	0.11461200	-2.67940700
C	3.26508900	-0.13841000	-1.95633300
H	-0.94495600	1.96613200	-0.00837700
H	-1.55074500	1.60701400	-1.60709900
C	5.47456900	1.30449700	0.73795800
H	0.36048500	-0.24614800	2.58454200
H	-4.51115900	3.45330500	-1.63446700
C	-0.54503800	-0.00821900	2.02998800
H	5.65109800	-1.97614000	-0.45867300
H	5.44066300	-0.61558000	1.64147300
H	3.40461300	-1.21848000	-1.98810700
C	3.62235200	-0.35301300	0.59474900
H	1.57501100	-1.46779300	2.07375800
H	5.32436200	1.75144700	-1.35823300
C	1.37631900	0.31953800	-0.24875900
H	-5.03873900	4.39711300	-0.23401700
C	3.34125500	1.86914900	-0.48215400
C	-3.04183900	-1.62765600	-1.04711300
H	-0.54127400	1.06838000	1.85794200
C	-2.83722900	-2.10432700	1.36262600
H	-3.64267000	1.24153400	-1.36782300
H	-6.16127400	0.77319400	-0.04028000
C	3.15834400	-1.79622200	0.70960900
C	5.15106400	-0.19106300	0.67106300
H	-5.98983800	3.01190600	-0.77185300
H	-4.80231600	3.47451400	2.08613200
H	4.18897900	0.31044500	-2.32273000
H	0.19413000	-2.90099600	-0.99131800
C	-1.32924200	-2.18088700	1.09118100
C	-4.96917300	3.38579600	-0.64361700
H	2.94847500	2.42482400	-1.33824500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1356.698430

98) Conformer 9C1

C	2.97658800	-0.05206300	0.96769200
C	2.55875700	-2.37227200	-0.54330300
H	2.96167600	-2.63333600	0.44005600
H	2.65639100	-3.27202300	-1.15521100

C	3.39209400	-1.24261400	-1.13322400
H	3.24222100	-1.17113300	-2.21540500
H	4.45538900	-1.43775500	-0.96809400
C	3.02348200	0.13310600	-0.53809600
C	1.54033900	0.37713500	-0.83923000
C	0.88782900	-0.59934500	0.16452700
C	1.08115900	-2.01919400	-0.38086500
H	0.62463700	-2.74902700	0.28774900
H	0.55841300	-2.09200700	-1.33958300
C	1.07837400	1.81959100	-0.73968600
H	1.53206200	2.36895200	-1.57328200
C	-0.44910100	1.89746600	-0.85850800
H	-0.80596700	2.65682900	-0.15503100
H	-0.71988300	2.25619700	-1.85574900
C	-1.18068400	0.57794600	-0.60756300
C	-0.58614600	-0.23503100	0.56730700
C	-2.67470000	0.85514400	-0.45309300
H	-3.02278200	1.39115200	-1.34361200
H	-2.81732500	1.54288600	0.38729500
C	-3.53714600	-0.38559800	-0.22779000
C	-2.93698200	-1.18570600	0.94222100
H	-3.09567200	-0.62496900	1.86827200
H	-3.48609500	-2.12660100	1.05646900
C	-1.45757300	-1.49090800	0.75301600
H	-1.35741300	-2.14502700	-0.11510500
H	-1.09655000	-2.06330000	1.61378400
C	4.01040200	1.18814100	-0.99184400
H	5.01675100	0.91916800	-0.66441700
H	4.01765400	1.25100800	-2.08285300
H	3.76874300	2.16925500	-0.58517900
H	1.30511400	0.05262000	-1.85632200
H	-1.05148500	-0.04240600	-1.50419900
C	-3.60219200	-1.24856900	-1.49538400
H	-4.23253500	-2.12672600	-1.33026800
H	-2.61751100	-1.60116600	-1.80677700
H	-4.03004500	-0.67664700	-2.32266300
O	1.76392100	-0.48978500	1.33074300
O	3.86341900	0.09130600	1.76893600
O	1.56342600	2.37776600	0.47717300
H	1.36016200	3.31740100	0.47629400
C	-0.61085800	0.56504000	1.87378900
H	-0.32155500	-0.07147100	2.71186300
H	-1.61475800	0.93919700	2.07609700
H	0.06871700	1.41324400	1.84530900

C	-4.95647900	-0.03744700	0.13172600
H	-5.57820100	-0.90525200	0.35512900
C	-5.51212700	1.16647300	0.19198800
H	-4.96017900	2.07523300	-0.02189200
H	-6.55631500	1.28366000	0.46041000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.652813

99) Conformer 9C2

C	2.94808400	-0.16488400	1.02213700
C	2.46452100	-2.42871300	-0.55362200
H	2.82071800	-2.73053400	0.43608400
H	2.53736000	-3.31920400	-1.18228500
C	3.37259300	-1.33071000	-1.09051000
H	3.26270800	-1.22899200	-2.17503900
H	4.41868100	-1.58293900	-0.89554800
C	3.05374100	0.04925800	-0.47663800
C	1.59568000	0.37483400	-0.81911100
C	0.86228100	-0.58860500	0.14072500
C	1.00190400	-2.00442300	-0.43089000
H	0.48707200	-2.72401800	0.20567600
H	0.50810000	-2.02970600	-1.40729100
C	1.20379500	1.83676700	-0.70243300
H	1.71089400	2.37861700	-1.50973400
C	-0.31346700	1.99477300	-0.86683800
H	-0.65475800	2.75339100	-0.15501600
H	-0.53396600	2.39060600	-1.86240700
C	-1.11534000	0.70737300	-0.67204700
C	-0.60380000	-0.15819500	0.50396900
C	-2.59884000	1.05066600	-0.56257700
H	-2.89827600	1.60747500	-1.45839500
H	-2.74508200	1.73542300	0.27998200
C	-3.53347100	-0.15707000	-0.37811200
C	-3.01202400	-0.99508100	0.78957300
H	-3.16047100	-0.44151100	1.72133800
H	-3.60530200	-1.91104000	0.88016000
C	-1.54422200	-1.37076700	0.63447100
H	-1.44990100	-2.01055100	-0.24505000
H	-1.23761400	-1.97870900	1.49186700
C	4.10716600	1.06175800	-0.87421100
H	5.08694700	0.73462300	-0.52028200
H	4.15425800	1.14705400	-1.96271300
H	3.90199700	2.04523700	-0.45343500
H	1.37842400	0.08406800	-1.85022900

H	-0.98485600	0.10091700	-1.57785600
C	-3.60040600	-0.98598800	-1.66821100
H	-4.25100100	-1.85346600	-1.53099700
H	-2.61896600	-1.34788800	-1.97918300
H	-4.00598800	-0.38597500	-2.48747800
O	1.70385300	-0.54848400	1.33644500
O	3.81420600	-0.08284500	1.85404300
O	1.67676300	2.34595100	0.54034200
H	1.51947400	3.29433200	0.55291800
C	-0.63155600	0.61701200	1.82553500
H	-1.61943300	1.04440500	1.99954600
H	0.09546600	1.42531200	1.84004300
H	-0.41032600	-0.05100300	2.65989000
C	-4.92049700	0.37288300	-0.13150800
H	-5.29152100	1.02433100	-0.92367300
C	-5.71230200	0.12865700	0.90531300
H	-5.41443600	-0.51293800	1.72738200
H	-6.70182000	0.56844000	0.96500800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.652891

100) Conformer **9C3**

C	3.01608500	-0.14573700	0.93171100
C	2.46284100	-2.43126600	-0.58938500
H	2.86998800	-2.71936100	0.38466500
H	2.50759600	-3.32933600	-1.20983000
C	3.33783400	-1.33670600	-1.18519300
H	3.17279600	-1.24911900	-2.26399300
H	4.39353800	-1.58258600	-1.04044000
C	3.04442300	0.04975600	-0.57316500
C	1.56928600	0.36498000	-0.84526100
C	0.89015300	-0.58880600	0.16278400
C	1.00643900	-2.01097300	-0.39798000
H	0.52732300	-2.72479800	0.27209500
H	0.46433700	-2.04963300	-1.34796000
C	1.17660900	1.82642300	-0.72698100
H	1.64023900	2.36080900	-1.56478000
C	-0.34761900	1.97558700	-0.81776000
H	-0.65605700	2.74536800	-0.10292600
H	-0.61945100	2.35363700	-1.80752500
C	-1.13393500	0.68874300	-0.56168100
C	-0.55687200	-0.15889600	0.59639700
C	-2.61021100	1.03297500	-0.37848500
H	-2.95680400	1.58054100	-1.26233200

H	-2.70887800	1.72872900	0.46254800
C	-3.53929100	-0.16944500	-0.13449800
C	-2.94267800	-1.00136800	1.01602600
H	-3.05091500	-0.44183000	1.95051000
H	-3.53230200	-1.91571600	1.13916400
C	-1.48357000	-1.37317700	0.79057300
H	-1.43312100	-2.02370600	-0.08467400
H	-1.13200400	-1.96977200	1.63877600
C	4.07111200	1.06143000	-1.03746500
H	5.06981900	0.74268400	-0.73204100
H	4.06043000	1.13344600	-2.12789300
H	3.88385300	2.04926300	-0.61849800
H	1.30110800	0.06025400	-1.86032500
H	-1.05071300	0.06975700	-1.46468400
C	-3.68380500	-1.00934800	-1.39823700
H	-4.33495900	-1.86981000	-1.22383300
H	-2.72144400	-1.38931300	-1.74272800
H	-4.11322600	-0.41839400	-2.21127500
O	1.79130400	-0.53073200	1.31342600
O	3.92276100	-0.05042100	1.71774300
O	1.70846400	2.35242700	0.48481500
H	1.55454300	3.30140400	0.49088200
C	-0.51920800	0.63265700	1.90774300
H	-1.49979700	1.05410100	2.13043700
H	0.20017300	1.44709400	1.87192200
H	-0.24659900	-0.02270200	2.73680900
C	-4.86748200	0.36676600	0.32673800
H	-4.80839700	0.97617800	1.22909600
C	-6.05911900	0.18023500	-0.22767400
H	-6.19826400	-0.41308600	-1.12464900
H	-6.94900300	0.62273300	0.20637200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.653246

101) Conformer **10C1**

H	-0.46404200	1.05064800	-1.29626200
O	-1.24992200	-1.40107500	2.19716800
H	1.25959600	3.02875100	0.06371500
C	-0.43557400	0.80340800	-0.22602000
H	3.60965900	3.07278500	-0.71392800
C	-4.63963800	-0.58390900	-2.01018400
H	-4.25432800	-0.91519600	1.45619500
H	1.45766100	2.19321200	-1.47196700
C	3.21415200	2.17184000	-0.23505500

H	3.43215000	-1.33350600	-2.35950900
H	2.24742800	1.17823200	1.99578700
H	-0.94713300	2.80673300	0.38944100
H	-3.40286800	2.46527100	0.27975900
C	-2.72333700	1.73751700	-0.17075700
C	1.78493800	-0.32258600	-0.51946400
C	1.00469000	-1.63048200	-0.37233800
O	0.55761600	-1.86554700	0.99202800
C	3.88558900	0.94980800	-0.84428200
H	1.65940100	-0.09006700	-1.58689800
H	-3.86733600	-1.30482700	-2.24999100
H	-2.63431800	1.99163800	-1.23195900
C	-1.35165800	1.79533200	0.47413300
H	4.89975300	-1.05071400	0.94014100
O	-2.42525100	-0.67701600	-0.43075400
H	0.92026900	0.08028500	2.26697000
C	1.22032600	0.96627100	1.71412200
H	-3.08547700	0.22931400	2.11763200
H	3.76695900	1.00109600	-1.93425000
C	3.85694500	-1.46140100	-1.35950000
H	-5.52580200	-0.56749500	-2.63438200
H	3.75488000	0.01561300	1.73750000
H	4.94315200	-1.36640300	-1.44250300
C	3.32490200	-0.40714300	-0.38166200
C	1.06960000	0.86692500	0.18696100
H	-0.81257600	-2.49781100	-1.17545500
H	-0.22078000	-1.10625600	-2.11702700
C	3.84027800	-0.78752800	1.00799400
C	-0.31266700	-1.52770200	-1.11736300
C	-1.05361100	-0.61598300	-0.15239600
H	3.47706800	2.26332700	0.82282200
C	-0.65212000	-1.30808700	1.16137700
H	-5.30816500	0.96202700	-0.77259500
C	-4.51332800	0.25160000	-0.98975700
C	1.69895700	2.14207400	-0.40302700
H	4.96362700	0.97451000	-0.65148100
H	-1.42768300	1.57387700	1.54187300
H	3.64996000	-2.48128700	-1.02668500
C	-3.86966500	0.10260600	1.37332900
H	-4.68247300	0.79915900	1.59153500
C	-3.34839700	0.34542000	-0.04282800
H	0.62542300	1.80609400	2.07764000
H	3.30926500	-1.65687300	1.40453500
H	1.59490000	-2.50090600	-0.64789000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.630784

102) Conformer **10C2**

H	-0.49269500	1.22247100	-1.06391000
O	-1.14178200	-1.99443200	1.77482300
H	1.35617300	2.48404500	-0.94394800
C	-0.45318100	0.74170700	-0.07664000
H	3.45134100	3.28983800	0.02555700
C	-5.18989000	1.06444600	-1.49094800
H	-4.20385500	-1.50357900	1.10704900
H	1.10668800	2.93598500	0.73812600
C	3.10892600	2.28265000	0.28201900
H	5.04692400	-0.78661000	-1.66642800
H	0.95127200	-0.45466900	2.20727400
H	-1.08344700	2.51978900	0.96808700
H	-3.50646900	2.08953100	0.74529200
C	-2.79449800	1.51362000	0.14933300
C	1.83034300	-0.16038100	-0.58061000
C	1.12850500	-1.51022600	-0.74526500
O	0.69132400	-2.07326100	0.52303800
C	3.85225400	1.27100300	-0.57777500
H	1.69373100	0.30012500	-1.56973400
H	-4.99407400	2.09067500	-1.19995900
H	-2.71147600	2.00664100	-0.82431300
C	-1.42977100	1.49532400	0.81305200
H	3.43164100	-1.80773200	1.01278800
O	-2.35088500	-0.75854700	-0.64703000
H	0.53043300	1.24343300	2.41211300
C	1.18531200	0.55361900	1.87686400
H	-3.05431600	-0.52798400	2.01904300
H	3.73222900	1.56074300	-1.62960700
C	3.96785100	-0.95864500	-1.62427500
H	-6.01331600	0.90141400	-2.17703700
H	4.98113800	-1.01421000	0.72684500
H	3.81943300	-2.03740700	-1.53456600
C	3.37237600	-0.18528400	-0.44188600
C	1.04423800	0.79555500	0.36491400
H	-0.63240900	-2.27430700	-1.75334000
H	-0.11997500	-0.67446900	-2.34600100
C	3.90669400	-0.83956400	0.83386100
C	-0.19011200	-1.31615800	-1.46921900
C	-0.98646300	-0.68961800	-0.33568700
H	3.36447700	2.14633700	1.33686100

C	-0.54918100	-1.63699800	0.79490400
H	-4.71848700	-0.96624800	-1.35254400
C	-4.47616600	0.04592900	-1.03448000
C	1.59831900	2.20515600	0.08902400
H	4.92667800	1.31317900	-0.36853100
H	-1.49749500	1.03265300	1.80110200
H	3.53898900	-0.63110000	-2.57593500
C	-3.84321500	-0.48611200	1.26986100
H	-4.67026700	0.11797600	1.64912500
C	-3.34127500	0.10669600	-0.04571100
H	2.19407200	0.76844900	2.21683300
H	3.76704400	-0.23077600	1.72515000
H	1.77036500	-2.26058700	-1.20005500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.629367

103) Conformer **10C3**

H	-0.40531900	1.15898900	-1.22500700
O	-1.22172900	-1.69899100	1.93631800
H	1.23567400	2.99804100	0.40550900
C	-0.39870200	0.78852200	-0.19049600
H	3.60252700	3.18172900	-0.29665500
C	-5.67326300	0.09599000	-1.07099100
H	-4.26936600	-1.16858500	1.15390000
H	1.49131400	2.35370100	-1.21152600
C	3.21663900	2.22264400	0.06209700
H	5.05850700	-1.11358800	-1.50234000
H	0.91096300	-0.19526700	2.23776600
H	-1.45391400	1.32495800	1.62649400
H	-3.41510200	2.32423700	0.42502800
C	-2.70920100	1.66786200	-0.08937600
C	1.85429300	-0.25006900	-0.55095400
C	1.10157800	-1.58200800	-0.57922700
O	0.62482200	-1.98464200	0.73513000
C	3.93183100	1.09504100	-0.66742000
H	1.74958600	0.10304300	-1.58704200
H	-6.33975700	0.12584400	-1.92556800
H	-2.59615500	2.05236100	-1.10876000
C	-1.35487100	1.67271400	0.59496600
H	3.36299700	-1.76926400	1.24435500
O	-2.34771700	-0.69702300	-0.62532500
H	0.57824800	1.53396500	2.24356600
C	1.20288600	0.75587500	1.80115800
H	-3.08407000	-0.14871800	1.96399500

H	3.83947100	1.27186300	-1.74673600
C	3.97297700	-1.23907100	-1.46144700
H	-6.13093300	-0.05638700	-0.10012200
H	4.94886300	-1.07774600	0.89887600
H	3.78078900	-2.29491500	-1.25640400
C	3.39203800	-0.31800000	-0.38217400
C	1.09350000	0.83352200	0.26926900
H	-0.67416400	-2.38468000	-1.52977300
H	-0.09023800	-0.88046000	-2.28447700
C	3.88172000	-0.84779400	0.96726500
C	-0.19807900	-1.41863900	-1.34411500
C	-0.98482200	-0.64148800	-0.30060300
H	3.45091200	2.19412900	1.13020800
C	-0.60114200	-1.47442000	0.93452000
H	-3.95886800	0.39310100	-2.22520200
C	-4.36593800	0.24540800	-1.22683900
C	1.70719900	2.18173100	-0.14977200
H	5.00380200	1.11880200	-0.44325300
H	-0.97096400	2.69465900	0.64155200
H	3.57102100	-1.00270100	-2.45111600
C	-3.86456800	-0.15675800	1.20629600
H	-4.66042800	0.52288300	1.51745300
C	-3.31609000	0.26388900	-0.14617400
H	2.21684700	0.95549500	2.13479100
H	3.75763200	-0.13806200	1.78302000
H	1.71919800	-2.40187900	-0.93740000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.630241

104) Conformer **11aC1**

C	3.15551200	-2.03978800	-0.71652400
H	3.36617400	-2.30328800	0.32325900
H	3.50898500	-2.87467600	-1.32873600
C	3.88732200	-0.76823300	-1.10154300
H	3.69050400	-0.55229400	-2.16000200
H	4.97010300	-0.90304500	-1.00746200
C	3.47120800	0.45016600	-0.26796800
C	1.93181300	0.62528600	-0.37241900
C	1.07308900	-0.67046000	-0.18651200
C	1.65983100	-1.87129100	-0.91697200
H	1.12740900	-2.77845400	-0.61987100
H	1.46469600	-1.73041700	-1.98705200
C	1.40031200	1.75422200	0.51688300
H	1.83376400	2.71162500	0.22189800

H	1.70970400	1.58283900	1.55043600
C	-0.11173900	1.90835800	0.51495100
H	-0.41136100	2.46452400	1.41410800
C	-0.79809500	0.53514100	0.55572400
C	-0.35510800	-0.30821200	-0.63123600
C	-2.27068800	0.65696000	0.73002200
H	-2.61028100	1.34096900	1.50579800
C	-3.16315200	0.01955000	-0.03132000
C	-2.71865600	-0.94891500	-1.08986500
H	-3.42195300	-1.78453800	-1.14283500
H	-2.77289900	-0.45714300	-2.06954700
C	-1.31057400	-1.46966100	-0.84789000
H	-0.98581200	-2.07502700	-1.69675700
H	-1.31713400	-2.12693300	0.02926600
C	-4.64202000	0.24482500	0.15737300
H	-4.75006000	1.06214300	0.87852100
C	-5.32784100	-0.98651700	0.74911700
H	-4.86578700	-1.28256900	1.69346000
H	-5.28467400	-1.83925900	0.06666500
H	-6.38234900	-0.77143600	0.93900200
C	-5.32126600	0.67051300	-1.14254200
H	-6.37424800	0.89729700	-0.95930300
H	-5.28043500	-0.12388700	-1.89247100
H	-4.85091200	1.56131000	-1.56584800
C	4.14939100	1.67969400	-0.87564300
H	5.23211900	1.52793200	-0.90842300
H	3.96414700	2.58407300	-0.29197200
H	3.80478600	1.85659100	-1.89875300
C	3.98128400	0.28926100	1.16617100
H	5.06165700	0.11927600	1.14654900
H	3.52000100	-0.54918600	1.68790100
H	3.80909000	1.19064000	1.75840400
C	0.81693600	-0.92105300	1.29311000
O	-0.22875800	-0.17963500	1.70138200
O	1.38604500	-1.65725800	2.05515900
H	1.74976100	0.90523100	-1.41794900
H	-0.32962800	0.30681000	-1.53407700
O	-0.50173000	2.62277700	-0.64259200
H	-1.46519800	2.65475900	-0.66331800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.678801

105) Conformer **11aC2**

C	3.31968300	-1.96224000	-0.40378000
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H	3.75169500	-2.84403700	-0.88604000
H	3.53300500	-2.05385700	0.66440400
C	3.95049100	-0.70252700	-0.96598400
H	3.75549300	-0.65976600	-2.04572600
H	5.03885200	-0.73035400	-0.84717300
C	3.42007200	0.58449200	-0.32181200
C	1.87358600	0.61164100	-0.45952100
C	1.12242500	-0.71119100	-0.08973700
C	1.81890000	-1.95127200	-0.63433800
H	1.35806000	-2.84742300	-0.21094700
H	1.63136200	-1.98371400	-1.71451400
C	1.23425900	1.80946300	0.25064000
H	1.59159700	2.74661200	-0.18012500
H	1.53893200	1.81827800	1.29960200
C	-0.28523700	1.83316200	0.21899700
H	-0.64498600	2.48729500	1.02539300
C	-0.85517100	0.42702600	0.45802200
C	-0.32272700	-0.53897000	-0.58973600
C	-2.33530300	0.44818100	0.61464700
H	-2.72553900	1.19498400	1.29994600
C	-3.16084400	-0.35697800	-0.05837700
C	-2.61495300	-1.42189900	-0.96962000
H	-3.25806200	-2.30571800	-0.90906800
H	-2.67855800	-1.08007500	-2.01018000
C	-1.17834700	-1.79324700	-0.63922900
H	-0.79115600	-2.48919600	-1.38640600
H	-1.15231100	-2.31230300	0.32580400
C	-4.66262600	-0.27970300	0.05142700
H	-4.99376500	-1.28984800	0.33137500
C	-5.28942200	0.03478900	-1.30967900
H	-4.97961900	1.02608100	-1.65323300
H	-6.37902500	0.02925400	-1.23230200
H	-5.00539100	-0.69283400	-2.07180800
C	-5.17474300	0.68654700	1.10651700
H	-6.26361700	0.62554500	1.16662100
H	-4.91617000	1.72056900	0.86088200
H	-4.77068300	0.46083900	2.09588200
C	4.00504000	1.76552600	-1.09893900
H	3.73568200	2.72616800	-0.65453700
H	3.66512500	1.76254200	-2.13877400
H	5.09700900	1.70225500	-1.10341900
C	3.91620100	0.67729700	1.12321200
H	5.00725400	0.60013400	1.13428900
H	3.51823900	-0.11362400	1.75881600

H	3.65784400	1.63659300	1.57699800
C	0.86270800	-0.76412500	1.40924100
O	-0.24668200	-0.06073400	1.69909200
O	1.47726700	-1.33118900	2.27380800
H	1.68801700	0.71892600	-1.53597900
H	-0.33209000	-0.06220800	-1.57291800
O	-0.71370700	2.33546300	-1.03260900
H	-1.67616700	2.28472100	-1.06088900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.678344

106) Conformer **11aC3**

C	3.13619500	-2.05798300	-0.70998800
H	3.33743300	-2.32452400	0.33090800
H	3.48453900	-2.89615400	-1.32065600
C	3.88340300	-0.79389500	-1.08919200
H	3.69306900	-0.57343400	-2.14791800
H	4.96432900	-0.94030000	-0.99111600
C	3.47672900	0.42627700	-0.25392000
C	1.93970900	0.61980700	-0.36194700
C	1.06398000	-0.66699900	-0.19270700
C	1.64396500	-1.87304400	-0.92004700
H	1.10028400	-2.77482500	-0.62731700
H	1.45770100	-1.72963700	-1.99137700
C	1.41464800	1.74079400	0.53920500
H	1.88036800	2.69350200	0.27509300
H	1.69668300	1.54641100	1.57731600
C	-0.09855200	1.92108200	0.49517400
H	-0.41512600	2.49168100	1.37851200
C	-0.80393600	0.56115200	0.53175900
C	-0.35917800	-0.29336200	-0.64804000
C	-2.27604200	0.68177600	0.70896700
H	-2.61232000	1.38125600	1.47143200
C	-3.16972900	0.02491200	-0.03079900
C	-2.72859100	-0.94575400	-1.08881800
H	-2.79366100	-0.45813300	-2.07004500
H	-3.42485400	-1.78786800	-1.13355100
C	-1.31569700	-1.45642200	-0.85635900
H	-0.99324400	-2.06261500	-1.70561100
H	-1.31325600	-2.11227300	0.02197200
C	-4.64877800	0.24203500	0.16892900
H	-4.75536700	1.05974000	0.89004500
C	-5.32671100	-0.99087600	0.76594800
H	-6.38141700	-0.78116100	0.96139000

H	-4.85814600	-1.28387300	1.70812500
H	-5.28319500	-1.84459500	0.08455700
C	-5.33928400	0.66455500	-1.12624700
H	-4.87497100	1.55682400	-1.55304900
H	-6.39220700	0.88704900	-0.93673100
H	-5.29993500	-0.13002800	-1.87621300
C	4.17094600	1.65004300	-0.85505900
H	5.25230600	1.48767200	-0.88128800
H	3.99148800	2.55547900	-0.27111600
H	3.83468600	1.83193300	-1.88007000
C	3.97833000	0.25568300	1.18207900
H	5.05644400	0.07140300	1.16753800
H	3.50313100	-0.57749500	1.69988700
H	3.81440200	1.15814700	1.77502300
C	0.79201000	-0.91443300	1.28384700
O	-0.24351400	-0.15521800	1.68312900
O	1.34393100	-1.65888100	2.05090100
H	1.76263400	0.91691700	-1.40369800
H	-0.32629000	0.31283100	-1.55614200
O	-0.53913200	2.57429900	-0.68196400
H	-0.19628700	3.47238800	-0.66912500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.677675

107) Conformer **11aC4**

C	3.30155100	-1.98137800	-0.39705800
H	3.50703100	-2.07844700	0.67221200
H	3.72781900	-2.86606200	-0.87916400
C	3.94828200	-0.72642800	-0.95125400
H	3.75889600	-0.67747000	-2.03173200
H	5.03572000	-0.76582700	-0.82735300
C	3.42787200	0.56290700	-0.30404200
C	1.88234800	0.60877400	-0.44796100
C	1.11321400	-0.70904900	-0.09675700
C	1.80274000	-1.95452900	-0.63817800
H	1.62312800	-1.98362500	-1.71979700
H	1.33026900	-2.84691400	-0.21988300
C	1.25018700	1.80079200	0.27593700
H	1.63945300	2.74108300	-0.12255000
H	1.52934900	1.78447900	1.33267200
C	-0.27185600	1.84450000	0.19847300
H	-0.64942000	2.50891100	0.98726900
C	-0.86233700	0.44939400	0.43077100
C	-0.32757700	-0.52601400	-0.60880500

C	-2.34192900	0.47020800	0.59067300
H	-2.72973200	1.23010300	1.26199300
C	-3.16755200	-0.35067000	-0.05899500
C	-2.62521400	-1.41711800	-0.97037900
H	-3.26166000	-2.30533200	-0.90153400
H	-2.69901600	-1.07935600	-2.01174000
C	-1.18457400	-1.78046000	-0.65080100
H	-0.79971200	-2.47702100	-1.39871700
H	-1.15004700	-2.29790800	0.31490600
C	-4.66919100	-0.28230000	0.06516600
H	-4.99341000	-1.29277100	0.35236800
C	-5.31153900	0.02469200	-1.29027600
H	-5.03059700	-0.70369900	-2.05295700
H	-5.00984100	1.01631000	-1.63992400
H	-6.40050800	0.01357700	-1.20300900
C	-5.17635500	0.68523500	1.12163800
H	-4.75808800	0.46751200	2.10694000
H	-6.26406100	0.61676900	1.19540500
H	-4.92819100	1.71983300	0.86789300
C	4.02969900	1.74117000	-1.07244300
H	5.12101500	1.66758700	-1.06934600
H	3.76674700	2.70293500	-0.62650900
H	3.69735000	1.74511700	-2.11471600
C	3.91651200	0.64380300	1.14425500
H	5.00640400	0.55270500	1.16215500
H	3.50408900	-0.14429000	1.77422900
H	3.66668700	1.60455000	1.59977500
C	0.83766000	-0.76102700	1.39868900
O	-0.26296200	-0.04058600	1.67733400
O	1.43565700	-1.33703600	2.26921200
H	1.70041800	0.73472700	-1.52310000
H	-0.32847200	-0.05746600	-1.59552300
O	-0.74458800	2.28034400	-1.06369700
H	-0.46811500	3.19319000	-1.18498100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.677130

108) Conformer **11aC5**

C	3.23245500	-2.04411200	-0.42022900
H	3.36895600	-2.21940300	0.65013700
H	3.64759200	-2.91552300	-0.93513800
C	3.96619400	-0.78881900	-0.85121000
H	3.84455000	-0.66139000	-1.93505600
H	5.04139600	-0.88817400	-0.66820800

C	3.46485600	0.47945800	-0.14986900
C	1.93455500	0.60872200	-0.37988000
C	1.08733100	-0.69001200	-0.16333800
C	1.75363300	-1.93021600	-0.74499300
H	1.63912200	-1.88205800	-1.83479900
H	1.21809500	-2.82390700	-0.41488300
C	1.31261800	1.78029700	0.38456900
H	1.52362900	1.68124900	1.45259700
H	1.76776200	2.72456800	0.07522500
C	-0.19781900	1.90186100	0.21897100
H	-0.59476000	2.53293500	1.02542200
C	-0.86448800	0.52567800	0.32280900
C	-0.31024800	-0.40722700	-0.74566900
C	-2.34892000	0.61420200	0.39051100
H	-2.74472000	1.37375200	1.05816400
C	-3.16730400	-0.14003700	-0.34267900
C	-2.62144000	-1.18096800	-1.27800000
H	-3.28940100	-2.04699700	-1.29463300
H	-2.64420300	-0.77453900	-2.29833500
C	-1.21208000	-1.61895500	-0.91866000
H	-0.81452000	-2.27791200	-1.69354300
H	-1.24590400	-2.20285300	0.00847300
C	-4.67050100	-0.01348800	-0.30351300
H	-5.01159700	-0.12192500	-1.34236500
C	-5.17951300	1.32160100	0.21757800
H	-6.26662400	1.37021200	0.12061000
H	-4.74974500	2.16010600	-0.33488600
H	-4.94168400	1.45514300	1.27647200
C	-5.28588100	-1.16397700	0.49795000
H	-4.95601700	-2.14075900	0.13858600
H	-6.37610200	-1.13426200	0.42980900
H	-5.00923100	-1.08050600	1.55255200
C	4.16397100	1.67444500	-0.80110400
H	3.91616900	2.61718900	-0.30838500
H	3.89733600	1.76078100	-1.85856600
H	5.24874000	1.54893000	-0.73853700
C	3.86683500	0.44333700	1.32660500
H	3.63471700	1.38473500	1.82946100
H	4.94811700	0.29615700	1.40205900
H	3.37993300	-0.36099700	1.87802200
C	0.71699000	-0.82437100	1.30651500
O	-0.36702100	-0.07248800	1.56709800
O	1.23420600	-1.48268000	2.17044700
H	1.82429700	0.81246400	-1.45284000

H	-0.23095900	0.12171700	-1.69804000
O	-0.57029100	2.43817300	-1.03818400
H	-0.24755200	3.34270800	-1.08245600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.677083

109) Conformer **11aC6**

C	3.13768200	-2.05820700	-0.70503600
H	3.48634900	-2.89757100	-1.31370900
H	3.34057200	-2.32141400	0.33632100
C	3.88270300	-0.79431900	-1.08916900
H	4.96378300	-0.93887300	-0.99158000
H	3.69138900	-0.57745900	-2.14844800
C	3.47605200	0.42809000	-0.25717800
C	1.93790600	0.61831100	-0.36397700
C	1.06398300	-0.66900800	-0.18984500
C	1.64489400	-1.87661700	-0.91398200
H	1.10300000	-2.77793100	-0.61685700
H	1.45687100	-1.73769400	-1.98559500
C	1.41515400	1.74356200	0.53632700
H	1.87559800	2.69737300	0.27144300
H	1.70296700	1.54284700	1.57083600
C	-0.09782000	1.92726300	0.50089600
H	-0.40840100	2.48505300	1.38947900
C	-0.80563800	0.56177600	0.53101000
C	-0.36038600	-0.29989600	-0.64333600
C	-2.27736900	0.68385100	0.70527100
H	-2.61464200	1.38704000	1.46377300
C	-3.17091100	0.02490600	-0.03299000
C	-2.72945000	-0.95293200	-1.08431300
H	-2.79330800	-0.47251300	-2.06916100
H	-3.42589800	-1.79501600	-1.12397300
C	-1.31763100	-1.46380200	-0.84663000
H	-0.99378900	-2.07586000	-1.69094700
H	-1.31583200	-2.11219800	0.03688900
C	-4.64993300	0.24499100	0.16302600
H	-4.75649000	1.06611400	0.88018300
C	-5.33044500	-0.98430400	0.76461300
H	-5.28824100	-1.84090600	0.08678000
H	-6.38483600	-0.77165300	0.95842300
H	-4.86313500	-1.27427300	1.70833700
C	-5.33755600	0.66259200	-1.13524700
H	-4.87160400	1.55261100	-1.56493500
H	-6.39051800	0.88705500	-0.94842500

H	-5.29789000	-0.13529400	-1.88168400
C	4.16729700	1.65128400	-0.86276200
H	5.24865300	1.48984300	-0.88976400
H	3.98739200	2.55802500	-0.28118400
H	3.83004900	1.82978000	-1.88806900
C	3.97828700	0.26265600	1.17910300
H	3.81633700	1.16741100	1.76894400
H	5.05614700	0.07764600	1.16323600
H	3.50351900	-0.56849200	1.70046000
C	0.79221200	-0.91208500	1.28846800
O	-0.24669200	-0.15715700	1.68432900
O	1.34860300	-1.65201400	2.05617500
H	1.76982900	0.90316300	-1.41251300
H	-0.33028000	0.28454400	-1.56767500
O	-0.54235500	2.70453700	-0.59471600
H	-0.08823100	2.41705400	-1.39236600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1004.676424

110) Conformer **11bC1**

C	3.15211400	-2.06376400	-0.69679100
H	3.49564600	-2.88254400	-1.33549800
H	3.34131400	-2.37121500	0.33489400
C	3.91380600	-0.79417500	-1.02167600
H	4.99210900	-0.95503600	-0.91924200
H	3.73578800	-0.53134300	-2.07280400
C	3.50953700	0.39515200	-0.14291900
C	1.97629500	0.61497300	-0.26551600
C	1.08843400	-0.66734500	-0.15346900
C	1.66290400	-1.85811800	-0.91068900
H	1.11197500	-2.76397800	-0.64724700
H	1.49298900	-1.68750300	-1.98162200
C	1.45543800	1.71047800	0.66912600
H	1.92382700	2.66792400	0.43503700
H	1.73576100	1.47502400	1.69910700
C	-0.05757600	1.92266000	0.63553200
H	-0.35378900	2.41306600	1.56846000
C	-0.78924600	0.57024200	0.59152100
C	-0.34932600	-0.28070500	-0.61033300
C	-2.26187900	0.70887800	0.74997700
H	-2.59640800	1.45603300	1.46578400
C	-3.15829600	0.00404800	0.05949700
C	-2.72791900	-1.02131100	-0.94716300
H	-2.86810000	-0.60709700	-1.95201700

H	-3.38607600	-1.89299400	-0.89609500
C	-1.28720900	-1.47086300	-0.76224700
H	-0.96894200	-2.07729100	-1.61525000
H	-1.21481400	-2.11268600	0.12046800
C	-4.63644800	0.22790900	0.25933600
H	-4.73847900	1.09207300	0.92457300
C	-5.29839400	-0.96541100	0.94806200
H	-4.81563800	-1.19104300	1.90150100
H	-5.25845200	-1.86301900	0.32538100
H	-6.35164600	-0.74837300	1.14295400
C	-5.34662800	0.55769100	-1.05180700
H	-6.39593000	0.79519800	-0.86101900
H	-5.32091600	-0.28855800	-1.74347400
H	-4.88908100	1.41654400	-1.54867400
C	4.22565400	1.63389700	-0.68497200
H	3.90602200	1.86039100	-1.70636900
H	5.30534500	1.45988200	-0.70263100
H	4.04740600	2.51701900	-0.06773200
C	3.99057700	0.16128600	1.29121300
H	5.06629400	-0.03662100	1.28212300
H	3.49874000	-0.68494600	1.77080200
H	3.83119400	1.04191000	1.91711000
C	0.78529800	-0.95993300	1.30363600
O	-0.25565700	-0.20935200	1.70908600
O	1.31434400	-1.73524700	2.05378200
H	1.82080300	0.94778000	-1.29758500
O	-0.38931700	0.50609400	-1.78248500
H	-0.25741000	-0.05458400	-2.55380700
O	-0.48682000	2.78456500	-0.39622700
H	-0.43275400	2.28398400	-1.22228600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1079.851620

111) Conformer **11bC2**

C	3.14575300	-2.05948900	-0.73886000
H	3.34282900	-2.39015200	0.28441400
H	3.48580600	-2.86390300	-1.39767200
C	3.90792400	-0.78432800	-1.03998300
H	3.72691700	-0.49973900	-2.08481600
H	4.98654200	-0.94711400	-0.94341500
C	3.50683600	0.38737800	-0.13647300
C	1.97354500	0.60819000	-0.25238500
C	1.08374800	-0.67175800	-0.16027000
C	1.65573700	-1.84784700	-0.93967900

H	1.10656200	-2.75804900	-0.68759600
H	1.46938300	-1.64929500	-2.00192000
C	1.45886100	1.68873400	0.70259300
H	1.94641600	2.64536300	0.49795100
H	1.72427000	1.43479300	1.73171900
C	-0.04809400	1.90208400	0.66170700
H	-0.36396900	2.41243300	1.57985800
C	-0.79100300	0.56097600	0.59282600
C	-0.35265200	-0.27278900	-0.62724600
C	-2.26297200	0.71011200	0.74938000
H	-2.59819700	1.45626300	1.46633000
C	-3.15798400	0.00662700	0.05485400
C	-2.72632900	-1.01894600	-0.95083200
H	-3.38842200	-1.88809100	-0.90138000
H	-2.86022400	-0.60114300	-1.95458800
C	-1.28581500	-1.46851200	-0.76985700
H	-0.96783100	-2.05913000	-1.63158500
H	-1.21059900	-2.11510700	0.10927100
C	-4.63603700	0.23322300	0.25269700
H	-4.73844100	1.09991500	0.91470200
C	-5.29912700	-0.95719300	0.94546500
H	-6.35259000	-0.73917200	1.13823600
H	-4.81753000	-1.17909400	1.90038600
H	-5.25815700	-1.85711800	0.32630600
C	-5.34502800	0.55804500	-1.06027300
H	-5.31850500	-0.29093300	-1.74842000
H	-4.88670600	1.41466300	-1.56030100
H	-6.39440600	0.79672500	-0.87121300
C	3.98586900	0.12307400	1.29294200
H	3.49042500	-0.73123300	1.75426900
H	3.82899200	0.99124100	1.93690100
H	5.06089600	-0.07814900	1.28130700
C	4.22484200	1.63560700	-0.65370000
H	3.90213300	1.88564900	-1.66860000
H	5.30373600	1.45801900	-0.67979900
H	4.05428900	2.50613600	-0.01643800
C	0.77459100	-0.98338600	1.28848600
O	-0.26288900	-0.22760200	1.70322700
O	1.28960600	-1.77442400	2.03232000
H	1.81617500	0.95573100	-1.28007600
O	-0.38712000	0.41348600	-1.84874000
H	-0.34871800	1.36795300	-1.66491400
O	-0.46896700	2.66688800	-0.46476700
H	0.01790700	3.49695300	-0.47357300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1079.852608

112) Conformer **11bC3**

C	3.14575300	-2.05948900	-0.73886000
H	3.34282900	-2.39015200	0.28441400
H	3.48580600	-2.86390300	-1.39767200
C	3.90792400	-0.78432800	-1.03998300
H	3.72691700	-0.49973900	-2.08481600
H	4.98654200	-0.94711400	-0.94341500
C	3.50683600	0.38737800	-0.13647300
C	1.97354500	0.60819000	-0.25238500
C	1.08374800	-0.67175800	-0.16027000
C	1.65573700	-1.84784700	-0.93967900
H	1.10656200	-2.75804900	-0.68759600
H	1.46938300	-1.64929500	-2.00192000
C	1.45886100	1.68873400	0.70259300
H	1.94641600	2.64536300	0.49795100
H	1.72427000	1.43479300	1.73171900
C	-0.04809400	1.90208400	0.66170700
H	-0.36396900	2.41243300	1.57985800
C	-0.79100300	0.56097600	0.59282600
C	-0.35265200	-0.27278900	-0.62724600
C	-2.26297200	0.71011200	0.74938000
H	-2.59819700	1.45626300	1.46633000
C	-3.15798400	0.00662700	0.05485400
C	-2.72632900	-1.01894600	-0.95083200
H	-3.38842200	-1.88809100	-0.90138000
H	-2.86022400	-0.60114300	-1.95458800
C	-1.28581500	-1.46851200	-0.76985700
H	-0.96783100	-2.05913000	-1.63158500
H	-1.21059900	-2.11510700	0.10927100
C	-4.63603700	0.23322300	0.25269700
H	-4.73844100	1.09991500	0.91470200
C	-5.29912700	-0.95719300	0.94546500
H	-6.35259000	-0.73917200	1.13823600
H	-4.81753000	-1.17909400	1.90038600
H	-5.25815700	-1.85711800	0.32630600
C	-5.34502800	0.55804500	-1.06027300
H	-5.31850500	-0.29093300	-1.74842000
H	-4.88670600	1.41466300	-1.56030100
H	-6.39440600	0.79672500	-0.87121300
C	3.98586900	0.12307400	1.29294200
H	3.49042500	-0.73123300	1.75426900

H	3.82899200	0.99124100	1.93690100
H	5.06089600	-0.07814900	1.28130700
C	4.22484200	1.63560700	-0.65370000
H	3.90213300	1.88564900	-1.66860000
H	5.30373600	1.45801900	-0.67979900
H	4.05428900	2.50613600	-0.01643800
C	0.77459100	-0.98338600	1.28848600
O	-0.26288900	-0.22760200	1.70322700
O	1.28960600	-1.77442400	2.03232000
H	1.81617500	0.95573100	-1.28007600
O	-0.38712000	0.41348600	-1.84874000
H	-0.34871800	1.36795300	-1.66491400
O	-0.46896700	2.66688800	-0.46476700
H	0.01790700	3.49695300	-0.47357300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1079.852608

113) Conformer **11bC4**

C	3.31127100	-1.99906700	-0.33247500
H	3.72585400	-2.88412400	-0.82395300
H	3.52251600	-2.10738500	0.73474800
C	3.96747300	-0.74660600	-0.87886400
H	5.05461100	-0.79552800	-0.75654500
H	3.77673900	-0.68701000	-1.95844200
C	3.45803800	0.54034400	-0.21972400
C	1.91329300	0.60356300	-0.37079700
C	1.13330700	-0.70483800	-0.02702600
C	1.81134100	-1.95735400	-0.56467800
H	1.62252200	-1.98573000	-1.64447900
H	1.33685300	-2.84416600	-0.13793500
C	1.29699700	1.80197400	0.35653000
H	1.70408200	2.73858800	-0.03324200
H	1.57066400	1.77745600	1.41410100
C	-0.22225500	1.87425700	0.28240100
H	-0.59063500	2.52419600	1.08555700
C	-0.84794400	0.48652200	0.47952200
C	-0.32512600	-0.52674800	-0.55661100
C	-2.32888200	0.53779900	0.62096700
H	-2.71623500	1.36793200	1.20304700
C	-3.15544800	-0.35190900	0.06981500
C	-2.62220700	-1.50624900	-0.72941300
H	-3.22290600	-2.39670100	-0.51722400
H	-2.76248600	-1.29760900	-1.79506800
C	-1.15602000	-1.79973400	-0.46059800

H	-0.77913400	-2.52071200	-1.18911400
H	-1.04473700	-2.25241200	0.52902400
C	-4.65660200	-0.26914800	0.19583200
H	-4.97795600	-1.24308600	0.59143000
C	-5.31102400	-0.10715600	-1.17890000
H	-5.04304500	-0.91601700	-1.86053500
H	-5.00800000	0.83866500	-1.63726500
H	-6.39889300	-0.10131100	-1.07906500
C	-5.15596600	0.80542000	1.14751100
H	-4.72880900	0.69484300	2.14672800
H	-6.24276700	0.74373700	1.23778300
H	-4.91268400	1.80727000	0.78217100
C	3.93973800	0.60083000	1.23177000
H	3.51319400	-0.18727000	1.85232700
H	3.70139000	1.56064300	1.69548200
H	5.02808700	0.49455700	1.25485100
C	4.07548900	1.72011200	-0.97334400
H	3.82491200	2.68037300	-0.51716400
H	3.74552400	1.73988800	-2.01615100
H	5.16569300	1.63252000	-0.96885600
C	0.83438400	-0.75337400	1.45601200
O	-0.26717600	-0.02145800	1.72020000
O	1.40537900	-1.33790300	2.33727900
H	1.74072500	0.72916500	-1.44600600
O	-0.40037000	-0.09530000	-1.88814200
H	-0.44688800	0.87639800	-1.89269800
O	-0.69324800	2.36776300	-0.96898800
H	-0.27398600	3.21621000	-1.14387600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1079.851989

114) Conformer **11bC5**

C	3.25415500	-2.03413000	-0.44416200
H	3.66721400	-2.87439200	-1.00996200
H	3.39274400	-2.27278500	0.61375500
C	3.98888900	-0.75714800	-0.80050100
H	3.87033800	-0.56634200	-1.87520500
H	5.06339400	-0.86653500	-0.61974700
C	3.48430200	0.46653900	-0.02727500
C	1.95601500	0.61350400	-0.26370700
C	1.10818900	-0.68998700	-0.12235600
C	1.77473300	-1.90160500	-0.75923300
H	1.24263200	-2.81001600	-0.46724900
H	1.65509900	-1.79919100	-1.84446300

C	1.33756800	1.74662600	0.55948100
H	1.80441200	2.70260300	0.30866100
H	1.53828200	1.58865100	1.62193800
C	-0.16926500	1.89307600	0.39893800
H	-0.56715200	2.46478300	1.24637000
C	-0.85824500	0.52141200	0.39572500
C	-0.30565700	-0.39176400	-0.71612900
C	-2.34229800	0.62800800	0.44341700
H	-2.73889400	1.42773900	1.06137700
C	-3.16063400	-0.17300200	-0.23898900
C	-2.62197400	-1.26140200	-1.11932200
H	-3.25627200	-2.14878100	-1.03714600
H	-2.71378500	-0.92904000	-2.16014100
C	-1.18120500	-1.63440600	-0.81709200
H	-0.78609500	-2.27677700	-1.60690000
H	-1.13783600	-2.20602800	0.11458300
C	-4.66377000	-0.04612400	-0.19972300
H	-5.01097600	-0.22560300	-1.22636800
C	-5.17240800	1.32029800	0.23307800
H	-6.25988700	1.36066900	0.13694200
H	-4.74616600	2.12051300	-0.37597700
H	-4.93137800	1.52469300	1.27985400
C	-5.27044100	-1.14109000	0.68226400
H	-4.94330200	-2.13940000	0.38514200
H	-6.36117600	-1.11564200	0.62203100
H	-4.98438700	-0.98779300	1.72643600
C	4.19200900	1.69698900	-0.59831400
H	3.94666400	2.60864600	-0.04908200
H	3.93235900	1.85038300	-1.64985400
H	5.27569200	1.56227900	-0.53730900
C	3.87116100	0.33915800	1.44807300
H	4.95058300	0.18018200	1.52508200
H	3.37383800	-0.49338800	1.94573700
H	3.64069100	1.25016200	2.00487900
C	0.70927500	-0.89374100	1.32363500
O	-0.38116900	-0.15030700	1.60228300
O	1.19879200	-1.59923900	2.16447900
H	1.85878700	0.86836700	-1.32547400
O	-0.28032800	0.18795100	-1.99186700
H	-0.28665400	1.15520800	-1.88834800
O	-0.53656100	2.54314200	-0.81508400
H	-0.07703400	3.38719300	-0.86489000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1079.851889

115) Conformer **11bC6**

C	3.32361800	-1.98762600	-0.33546000
H	3.53601300	-2.09522100	0.73157800
H	3.74242000	-2.87039100	-0.82749800
C	3.97365300	-0.73169600	-0.88185900
H	3.78463800	-0.67426900	-1.96185500
H	5.06083000	-0.77471100	-0.75752900
C	3.45601000	0.55370800	-0.22563000
C	1.91124200	0.60599100	-0.38041900
C	1.14054400	-0.70473500	-0.02594800
C	1.82304800	-1.95378300	-0.56594800
H	1.35358200	-2.84336200	-0.13922300
H	1.63261500	-1.98195600	-1.64548500
C	1.28814700	1.81218500	0.33009600
H	1.66855900	2.74498200	-0.08929900
H	1.57793700	1.80847000	1.38295200
C	-0.22948700	1.86961500	0.28334700
H	-0.58660300	2.52157000	1.08904000
C	-0.84204600	0.47492500	0.49270000
C	-0.32023800	-0.53205200	-0.54887800
C	-2.32297800	0.52432700	0.63536600
H	-2.71214200	1.34180500	1.23544100
C	-3.15050100	-0.35740700	0.06985500
C	-2.61499500	-1.50736100	-0.73403300
H	-3.21965200	-2.39687900	-0.52998800
H	-2.74972600	-1.29173200	-1.79890600
C	-1.15029500	-1.80535400	-0.45980800
H	-0.77240700	-2.52511200	-1.18898400
H	-1.04330400	-2.26016100	0.52927600
C	-4.65138600	-0.27428800	0.19266100
H	-4.97274300	-1.25032900	0.58284100
C	-5.30195300	-0.10679400	-1.18334200
H	-6.38991100	-0.10185300	-1.08574100
H	-5.03205300	-0.91261900	-1.86768300
H	-4.99857500	0.84125700	-1.63686800
C	-5.15299300	0.79572100	1.14815700
H	-4.90757500	1.79940300	0.78925900
H	-4.73040000	0.67918700	2.14859700
H	-6.24011500	0.73449400	1.23365900
C	4.06678000	1.73583200	-0.98110100
H	5.15740200	1.65330900	-0.97822200
H	3.81169800	2.69487000	-0.52501900
H	3.73496700	1.75352200	-2.02336400

C	3.93676500	0.62027400	1.22590000
H	5.02629500	0.52663800	1.24848500
H	3.51985800	-0.17255500	1.84682600
H	3.68804300	1.57744700	1.68961100
C	0.85077900	-0.75472500	1.45921900
O	-0.25443600	-0.03097700	1.73026000
O	1.43072500	-1.33600200	2.33676200
H	1.74290400	0.71661500	-1.45780900
O	-0.40045700	-0.09209700	-1.87787800
H	-0.43457500	0.88025400	-1.87558200
O	-0.63402200	2.41444900	-0.97210000
H	-1.58474000	2.57378400	-0.94411600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1079.852890

116) Conformer **11bC7**

C	3.26640000	-2.02247300	-0.44761100
H	3.68379400	-2.86033100	-1.01380300
H	3.40585200	-2.26096900	0.61020000
C	3.99530800	-0.74166100	-0.80300000
H	3.87814000	-0.55212600	-1.87807700
H	5.06996500	-0.84580800	-0.61998400
C	3.48323200	0.48063400	-0.03209600
C	1.95457800	0.61764800	-0.27221200
C	1.11505700	-0.68998600	-0.12211100
C	1.78606400	-1.89735700	-0.76223900
H	1.25856900	-2.80894300	-0.47150300
H	1.66510500	-1.79334200	-1.84718200
C	1.33106300	1.75865400	0.53804600
H	1.77318100	2.71634700	0.25873600
H	1.54871900	1.61781600	1.59889800
C	-0.17647100	1.88805000	0.40273000
H	-0.56334800	2.45949900	1.25459300
C	-0.85387300	0.50760200	0.40895100
C	-0.30175100	-0.39651000	-0.70947700
C	-2.33810100	0.61133300	0.45870000
H	-2.73900800	1.39349600	1.09779100
C	-3.15597600	-0.17848300	-0.23954900
C	-2.61484300	-1.26024100	-1.12604300
H	-3.25294800	-2.14565300	-1.05280900
H	-2.70187600	-0.91988300	-2.16454500
C	-1.17587800	-1.63860000	-0.81992800
H	-0.77945600	-2.27813700	-1.61134700
H	-1.13676300	-2.21386300	0.10965600

C	-4.65870500	-0.05227500	-0.20168500
H	-5.00503800	-0.23470000	-1.22790700
C	-5.16874300	1.31445000	0.22857400
H	-4.74386300	2.11397000	-0.38252600
H	-4.92860600	1.52163400	1.27492100
H	-6.25616100	1.35314700	0.13195800
C	-5.26270600	-1.14699600	0.68279200
H	-6.35334900	-1.12337900	0.62203000
H	-4.97701400	-0.99096300	1.72657000
H	-4.93350100	-2.14508200	0.38735200
C	3.87022900	0.35830500	1.44362300
H	3.38161100	-0.47902900	1.94172300
H	3.63067500	1.26730500	1.99985900
H	4.95123600	0.21061900	1.52101000
C	4.18418800	1.71426800	-0.60473100
H	5.26861300	1.58508100	-0.54460800
H	3.93393300	2.62474500	-0.05589400
H	3.92265300	1.86569000	-1.65609200
C	0.72544600	-0.89816200	1.32613500
O	-0.36943700	-0.16421900	1.61184200
O	1.22469900	-1.60160400	2.16297100
H	1.86046400	0.85994000	-1.33709500
O	-0.28124700	0.19420100	-1.98082000
H	-0.27381600	1.16049700	-1.86770000
O	-0.47370100	2.58979300	-0.80390700
H	-1.41737600	2.78787300	-0.81813000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1079.852791

117) Conformer **11bC8**

C	3.15211100	-2.06376800	-0.69678800
H	3.34130800	-2.37122000	0.33489700
H	3.49564300	-2.88254900	-1.33549300
C	3.91380600	-0.79418100	-1.02167200
H	3.73579100	-0.53134700	-2.07280000
H	4.99210900	-0.95504300	-0.91923600
C	3.50953800	0.39514700	-0.14291500
C	1.97629700	0.61497100	-0.26551500
C	1.08843200	-0.66734400	-0.15346900
C	1.66290200	-1.85811900	-0.91068800
H	1.11197000	-2.76397800	-0.64724800
H	1.49298800	-1.68750300	-1.98162200
C	1.45544000	1.71047900	0.66912400
H	1.92383100	2.66792300	0.43503600

H	1.73576100	1.47502500	1.69910600
C	-0.05757400	1.92266400	0.63552700
H	-0.35378600	2.41307100	1.56845500
C	-0.78924700	0.57024800	0.59151500
C	-0.34932500	-0.28070200	-0.61033600
C	-2.26187900	0.70888500	0.74997000
H	-2.59640800	1.45603900	1.46577800
C	-3.15829600	0.00405500	0.05949200
C	-2.72791900	-1.02130200	-0.94717200
H	-3.38607900	-1.89298300	-0.89611000
H	-2.86809600	-0.60708200	-1.95202400
C	-1.28721100	-1.47085700	-0.76225300
H	-1.21481900	-2.11268100	0.12046200
H	-0.96894300	-2.07728600	-1.61525500
C	-4.63644800	0.22791000	0.25933600
H	-4.73848100	1.09208200	0.92456100
C	-5.29837800	-0.96540700	0.94808500
H	-6.35163200	-0.74837900	1.14297700
H	-4.81561500	-1.19101600	1.90152700
H	-5.25842500	-1.86302500	0.32542000
C	-5.34664200	0.55766600	-1.05180500
H	-6.39594500	0.79516600	-0.86101200
H	-5.32092800	-0.28859200	-1.74346100
H	-4.88910700	1.41651600	-1.54868900
C	4.22565900	1.63389100	-0.68496600
H	3.90602900	1.86038700	-1.70636400
H	5.30535000	1.45987400	-0.70262300
H	4.04741200	2.51701400	-0.06772600
C	3.99057400	0.16128000	1.29121800
H	3.83119000	1.04190500	1.91711500
H	5.06629100	-0.03662800	1.28213100
H	3.49873500	-0.68495100	1.77080600
C	0.78529300	-0.95993100	1.30363500
O	-0.25566000	-0.20934800	1.70908300
O	1.31433600	-1.73524700	2.05378200
H	1.82080800	0.94777800	-1.29758600
O	-0.38931100	0.50609700	-1.78249000
H	-0.25740600	-0.05458300	-2.55381100
O	-0.48681400	2.78456900	-0.39623200
H	-0.43274600	2.28399000	-1.22229200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1079.851620

118) Conformer **12aC1**

C	3.03522800	1.52725700	0.40253100
H	3.16235100	1.43613700	1.48687700
C	3.67888400	0.32758600	-0.27364900
H	4.72350100	0.26082200	0.06875800
C	2.98084400	-0.99353800	0.08138400
C	1.45006200	-0.85290800	-0.14770100
C	0.75026500	0.40034000	0.44644800
C	1.56535500	1.63969300	0.04960100
H	1.49003200	1.79341400	-1.03209800
H	1.15506700	2.53193900	0.53419000
C	0.65213600	-2.10666700	0.19239600
H	1.16262800	-3.00066100	-0.17096700
H	0.55802700	-2.22580400	1.27509600
C	-0.72035900	-2.04457800	-0.45405100
H	-1.34363600	-2.89338300	-0.15739200
H	-0.59989200	-2.10457000	-1.54142500
C	-1.49119600	-0.77213500	-0.18485900
C	-0.64153100	0.50780700	-0.24656500
C	-2.71577900	-0.64377000	-1.09938100
H	-3.21342100	-1.62224800	-1.13535900
C	-3.57181800	0.33487500	-0.29042400
C	-2.89609400	1.71351200	-0.36106300
H	-2.88179300	2.00686200	-1.41389700
H	-3.50861900	2.44378500	0.17411000
C	-1.48189400	1.70449700	0.21507100
H	-1.55367800	1.69908800	1.30592400
H	-0.98191600	2.63713500	-0.05220600
O	3.76607900	2.66229300	-0.05689200
H	3.26369900	3.45550200	0.15157000
O	3.66423500	0.52233500	-1.67829300
H	3.88717200	1.45234900	-1.81097800
H	1.36682100	-0.71940600	-1.23575100
H	-0.43048700	0.64142700	-1.31412500
O	-2.35934200	-0.23011400	-2.38958100
H	-3.04033100	-0.51615600	-3.00416900
C	-5.03501500	0.38561400	-0.66659000
H	-5.58986300	1.02392700	0.02358700
H	-5.48568400	-0.60959700	-0.64840100
H	-5.14984800	0.79581000	-1.67297200
C	0.60358800	0.35771000	1.97230900
H	0.17337500	1.29166600	2.33898800
H	1.56283500	0.23975000	2.47078600
H	-0.04446100	-0.45116500	2.30688100
O	-2.14454400	-0.86708200	1.11896700

C	3.52685900	-2.07680100	-0.85764500
H	4.61989800	-2.04435800	-0.86735600
H	3.17705900	-1.94044100	-1.88163300
H	3.23453800	-3.07316200	-0.52052700
C	3.39505400	-1.40215300	1.49958100
H	4.44848500	-1.69549700	1.49832600
H	3.28560600	-0.61014700	2.23925700
H	2.81705500	-2.26249600	1.84246000
C	-3.32814300	-0.23117500	1.09424100
O	-4.02682700	-0.16137200	2.06987800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1116.968244

119) Conformer **12aC2**

C	3.03504500	1.52916900	0.39897200
H	3.16151300	1.44125300	1.48368000
C	3.67950400	0.32769400	-0.27320500
H	4.72391000	0.26218300	0.07008200
C	2.98155400	-0.99259600	0.08505300
C	1.45097900	-0.85242200	-0.14552800
C	0.75042500	0.40187200	0.44533300
C	1.56534100	1.64020400	0.04493500
H	1.49028300	1.79044500	-1.03728100
H	1.15462600	2.53386200	0.52651700
C	0.65261200	-2.10582200	0.19513200
H	1.16450500	-3.00090400	-0.16342900
H	0.55268500	-2.22191200	1.27762200
C	-0.71697900	-2.04336700	-0.45738200
H	-1.34107400	-2.89476400	-0.16991100
H	-0.58304100	-2.10338700	-1.54402500
C	-1.48972900	-0.77273300	-0.18676400
C	-0.64237000	0.50697600	-0.24614100
C	-2.72233600	-0.64087000	-1.10235700
H	-3.22119200	-1.61842400	-1.13965600
C	-3.57097900	0.33133900	-0.29062200
C	-2.89741800	1.71290200	-0.35816400
H	-2.88864100	2.01636700	-1.40801000
H	-3.51125600	2.43691100	0.18402200
C	-1.48293500	1.70297300	0.21700700
H	-1.55490800	1.69553600	1.30786000
H	-0.98291600	2.63616900	-0.04817000
O	3.76597300	2.66292900	-0.06340100
H	3.26329900	3.45665700	0.14234200
O	3.66563900	0.51821000	-1.67844600

H	3.88882400	1.44776700	-1.81380300
H	1.36915600	-0.72072800	-1.23399700
H	-0.43586500	0.64113800	-1.31483100
O	-2.46112100	-0.17487400	-2.39729800
H	-2.32951200	-0.92773500	-2.97910800
C	-5.03496100	0.38250100	-0.66352100
H	-5.48759000	-0.61141900	-0.63451400
H	-5.14738300	0.78108200	-1.67395300
H	-5.58512500	1.02878000	0.02292900
C	0.60439600	0.36278400	1.97140700
H	0.17857300	1.29933700	2.33657100
H	1.56312700	0.24126200	2.46996000
H	-0.04732800	-0.44255500	2.30760400
O	-2.14334300	-0.87533300	1.11698800
C	3.52811600	-2.07836700	-0.85075000
H	3.23631600	-3.07390700	-0.51072400
H	4.62113400	-2.04546700	-0.86041700
H	3.17850500	-1.94530600	-1.87525800
C	3.39495000	-1.39756000	1.50455500
H	4.44765100	-1.69350700	1.50412200
H	3.28769800	-0.60287900	2.24167300
H	2.81491000	-2.25537100	1.85039000
C	-3.32417100	-0.23517300	1.09406200
O	-4.02054000	-0.15937100	2.07085500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1116.968434

120) Conformer **12aC3**

C	3.02973500	1.53275600	0.39619200
H	3.16223000	1.46061600	1.48045400
C	3.67388900	0.32492200	-0.27463400
H	4.71940000	0.25394300	0.06968000
C	2.97732300	-0.99709900	0.08021200
C	1.44738300	-0.85478600	-0.15001500
C	0.75005300	0.39956300	0.44434000
C	1.56106500	1.64157300	0.05019800
H	1.48144000	1.79880900	-1.03085300
H	1.15886700	2.53379100	0.53636400
C	0.64850100	-2.10809500	0.18949000
H	1.15761600	-3.00213400	-0.17577800
H	0.55585200	-2.22878200	1.27214300
C	-0.72488700	-2.04410300	-0.45467700
H	-1.34880100	-2.89217500	-0.15718600
H	-0.60627800	-2.10414300	-1.54226800

C	-1.49369200	-0.77065700	-0.18451800
C	-0.64253200	0.50797000	-0.24756300
C	-2.71935800	-0.64150500	-1.09744600
H	-3.21812800	-1.61947000	-1.13211300
C	-3.57317600	0.33867100	-0.28816000
C	-2.89597400	1.71645400	-0.36121400
H	-2.88286200	2.00863300	-1.41440700
H	-3.50696300	2.44806400	0.17391900
C	-1.48104700	1.70645000	0.21304800
H	-1.55171600	1.70294300	1.30398000
H	-0.97982100	2.63781200	-0.05600100
O	3.65740800	2.72509700	-0.07598700
H	4.53892600	2.77626900	0.30752300
O	3.66287000	0.51968600	-1.67866800
H	3.85877200	1.45670800	-1.80904300
H	1.36491800	-0.72102600	-1.23812800
H	-0.43173100	0.64046100	-1.31535300
O	-2.36425600	-0.22914000	-2.38850000
H	-3.04546800	-0.51660100	-3.00214300
C	-5.03685700	0.39060400	-0.66232100
H	-5.15259200	0.79986800	-1.66898600
H	-5.59007100	1.03028000	0.02791500
H	-5.48863200	-0.60408600	-0.64249100
C	0.60445900	0.35629600	1.97027200
H	-0.03365100	-0.45960800	2.30696300
H	0.16425400	1.28576300	2.33624400
H	1.56561600	0.25048300	2.46803900
O	-2.14555400	-0.86420300	1.12029700
C	3.52401500	-2.08196000	-0.85639700
H	3.23138600	-3.07802100	-0.51836000
H	4.61712000	-2.04976500	-0.86525700
H	3.17502600	-1.94693200	-1.88089700
C	3.39057400	-1.40205000	1.49984000
H	2.81034100	-2.25946700	1.84621200
H	4.44321800	-1.69833100	1.49962300
H	3.28336500	-0.60717500	2.23683400
C	-3.32814500	-0.22652700	1.09669500
O	-4.02541800	-0.15488900	2.07327100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1116.968161

121) Conformer **12aC4**

C	3.03229500	1.54991500	0.40168400
H	3.15179700	1.46475700	1.48386000

C	3.67447700	0.34149000	-0.25967700
H	4.72084700	0.28153800	0.06964500
C	2.97737100	-0.98448200	0.09918300
C	1.44838900	-0.84706900	-0.13687500
C	0.74597000	0.40978500	0.44562000
C	1.55888000	1.64886100	0.04410100
H	1.48324700	1.79727600	-1.03902700
H	1.15384400	2.54496900	0.52105200
C	0.65140400	-2.10083900	0.20558100
H	1.16467600	-2.99673200	-0.14941000
H	0.55084000	-2.21358200	1.28838000
C	-0.71776700	-2.04283100	-0.44818600
H	-1.34072000	-2.89399800	-0.15754200
H	-0.58307700	-2.10724400	-1.53450200
C	-1.49233800	-0.77201300	-0.18383300
C	-0.64623500	0.50812800	-0.24819200
C	-2.72434400	-0.64654100	-1.10108800
H	-3.22217300	-1.62478300	-1.13341100
C	-3.57466600	0.32915500	-0.29527500
C	-2.90246800	1.71102000	-0.37011800
H	-2.89283400	2.00825400	-1.42176500
H	-3.51778800	2.43757200	0.16699300
C	-1.48878900	1.70578600	0.20687000
H	-1.56248600	1.70441700	1.29762200
H	-0.98849500	2.63754000	-0.06242300
O	3.72918400	2.72853300	0.03208600
H	3.87024800	2.65476500	-0.92041500
O	3.64450800	0.62521200	-1.65706200
H	4.32233900	0.10308700	-2.09284300
H	1.37012400	-0.71915600	-1.22654800
H	-0.43790500	0.63719600	-1.31721300
O	-2.46216700	-0.18781200	-2.39851700
H	-2.33627800	-0.94407500	-2.97710200
C	-5.03843300	0.37659500	-0.66947000
H	-5.58982100	1.02592000	0.01312400
H	-5.49001100	-0.61766000	-0.63550600
H	-5.15057200	0.76968000	-1.68209500
C	0.59841100	0.37736700	1.97164800
H	1.55820200	0.27152900	2.47204700
H	-0.04303300	-0.43409200	2.31313000
H	0.16101600	1.31087800	2.33060000
O	-2.14707800	-0.86909200	1.11979500
C	3.52800100	-2.06934000	-0.83512600
H	3.24467000	-3.06725100	-0.49608100

H	4.62243100	-2.03761700	-0.84678000
H	3.16916300	-1.94797100	-1.85948400
C	3.39148800	-1.38442400	1.51963100
H	2.81783500	-2.24575200	1.86755100
H	4.44661900	-1.67230700	1.52230100
H	3.27670000	-0.58849700	2.25416300
C	-3.32828900	-0.22986900	1.09256900
O	-4.02564000	-0.14969200	2.06837200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1116.968803

122) Conformer **12aC5**

C	3.03603600	1.54757000	0.40787100
H	3.15411900	1.46187700	1.49050400
C	3.68092000	0.33969800	-0.26147400
H	4.72300700	0.27558400	0.06872200
C	2.98088400	-0.98714400	0.08608600
C	1.44920900	-0.84767100	-0.14358700
C	0.74725600	0.40725100	0.44508000
C	1.56132100	1.64907700	0.05448900
H	1.47249800	1.82099800	-1.02664600
H	1.15719700	2.54225000	0.53699700
C	0.65303200	-2.10307000	0.19642400
H	1.16498200	-2.99614400	-0.16664900
H	0.56254800	-2.21916900	1.27947600
C	-0.72090100	-2.04362800	-0.44718600
H	-1.34164200	-2.89216700	-0.14516100
H	-0.60335900	-2.10887100	-1.53461600
C	-1.49294500	-0.77094100	-0.18157900
C	-0.64467600	0.50986100	-0.24822100
C	-2.71742900	-0.64705600	-1.09685300
H	-3.21422500	-1.62604600	-1.12943500
C	-3.57419200	0.33388200	-0.29149500
C	-2.89966500	1.71290700	-0.36731000
H	-2.88540700	2.00234000	-1.42122500
H	-3.51282200	2.44468800	0.16497100
C	-1.48570300	1.70754600	0.20929200
H	-1.55775700	1.70576100	1.30007800
H	-0.98604200	2.63941900	-0.06085100
O	3.73134800	2.72617900	0.03777000
H	3.90722100	2.63568600	-0.90794300
O	3.77638900	0.59152400	-1.66200500
H	2.90360400	0.50465300	-2.05854000
H	1.35017700	-0.72858500	-1.23565300

H	-0.43506400	0.64075700	-1.31669700
O	-2.36047100	-0.23779500	-2.38830600
H	-3.04056300	-0.52694400	-3.00245100
C	-5.03744700	0.38197100	-0.66775900
H	-5.59269200	1.02234200	0.02017100
H	-5.48727500	-0.61353000	-0.64591500
H	-5.15264400	0.78845100	-1.67559300
C	0.60082800	0.36523200	1.97095400
H	1.56075500	0.25809200	2.47042100
H	-0.03963400	-0.44883200	2.30729600
H	0.16192700	1.29603000	2.33457200
O	-2.14534100	-0.86164200	1.12227400
C	3.53060400	-2.07438400	-0.84573500
H	3.24777600	-3.06960100	-0.49786000
H	4.62282500	-2.03245300	-0.86268200
H	3.17603900	-1.95943300	-1.87173800
C	3.38985200	-1.38896300	1.50817700
H	4.44200000	-1.68658500	1.50885600
H	3.28373700	-0.59064500	2.24121900
H	2.80822000	-2.24409700	1.85751300
C	-3.33000400	-0.22678900	1.09533600
O	-4.02834900	-0.15425600	2.07074300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1116.967243

123) Conformer **12aC6**

C	3.03253000	1.54787400	0.40575100
H	3.15318900	1.45912700	1.48747800
C	3.67368200	0.34152400	-0.26035900
H	4.72042800	0.28025700	0.06756100
C	2.97669900	-0.98543800	0.09526100
C	1.44749500	-0.84755300	-0.13905700
C	0.74577600	0.40805100	0.44720400
C	1.55881500	1.64838400	0.04979500
H	1.48270200	1.80093700	-1.03270100
H	1.15434700	2.54279500	0.53042900
C	0.65109100	-2.10188800	0.20238600
H	0.55650300	-2.21820500	1.28534700
H	1.16299300	-2.99648000	-0.15795600
C	-0.72107600	-2.04407200	-0.44511200
H	-1.34322000	-2.89261400	-0.14532200
H	-0.59992400	-2.10841200	-1.53216600
C	-1.49371500	-0.77145100	-0.18202000
C	-0.64529300	0.50891500	-0.24838300

C	-2.71760900	-0.64931600	-1.09830600
H	-3.21430500	-1.62849600	-1.12946100
C	-3.57538100	0.33267500	-0.29524400
C	-2.90106700	1.71163100	-0.37276800
H	-2.88590300	1.99907500	-1.42722700
H	-3.51509100	2.44417100	0.15759000
C	-1.48767700	1.70720600	0.20519000
H	-1.56125100	1.70781100	1.29591400
H	-0.98737700	2.63838500	-0.06616400
O	3.72928700	2.72768300	0.03930400
H	3.87000900	2.65653300	-0.91346500
O	3.64211000	0.63006500	-1.65661300
H	4.31755300	0.10742300	-2.09548600
H	1.36772000	-0.71743300	-1.22824200
H	-0.43221000	0.63768300	-1.31617000
O	-2.36020300	-0.24250600	-2.39041200
H	-3.04308800	-0.52776600	-3.00329900
C	-5.03839000	0.37973800	-0.67259900
H	-5.15317100	0.78539300	-1.68083400
H	-5.59447900	1.02036600	0.01443100
H	-5.48781500	-0.61596500	-0.65030500
C	0.59743900	0.37156700	1.97297500
H	-0.03913400	-0.44435300	2.31268000
H	0.15433200	1.30173700	2.33358400
H	1.55783400	0.27066200	2.47329400
O	-2.14829300	-0.86107200	1.12155000
C	3.52674900	-2.06763100	-0.84251200
H	3.16737500	-1.94306900	-1.86629200
H	3.24313500	-3.06643300	-0.50639400
H	4.62118800	-2.03615800	-0.85448100
C	3.39186000	-1.38911000	1.51426500
H	3.27416400	-0.59620800	2.25159400
H	2.82088200	-2.25351400	1.85888400
H	4.44791100	-1.67361200	1.51612200
C	-3.33226000	-0.22614300	1.09250300
O	-4.03206600	-0.15209900	2.06707900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1116.968635

124) Conformer **12aC7**

C	3.03583900	1.54959500	0.40328900
H	3.15261000	1.46757600	1.48636200
C	3.68178900	0.33954300	-0.26113300
H	4.72349400	0.27671000	0.07049700

C	2.98160200	-0.98628000	0.09012800
C	1.45009800	-0.84740400	-0.14110300
C	0.74744000	0.40904900	0.44323500
C	1.56141900	1.64945500	0.04811600
H	1.47311000	1.81689300	-1.03378100
H	1.15683200	2.54452000	0.52668200
C	0.65341000	-2.10207400	0.20072900
H	1.16660100	-2.99657600	-0.15692100
H	0.55740500	-2.21413300	1.28371200
C	-0.71784100	-2.04277900	-0.44862100
H	-1.33924300	-2.89376200	-0.15480600
H	-0.58757900	-2.10844900	-1.53537000
C	-1.49172700	-0.77172700	-0.18246500
C	-0.64553700	0.50871800	-0.24846300
C	-2.72416000	-0.64512300	-1.09888800
H	-3.22242900	-1.62287700	-1.13175200
C	-3.57342200	0.33060400	-0.29144600
C	-2.90066400	1.71215800	-0.36630200
H	-2.89167800	2.00969700	-1.41787000
H	-3.51490500	2.43893600	0.17159800
C	-1.48646700	1.70635000	0.20942300
H	-1.55869000	1.70366300	1.30021700
H	-0.98665400	2.63841900	-0.05969700
O	3.73138100	2.72701500	0.03003200
H	3.90884500	2.63321000	-0.91505400
O	3.77889400	0.58652000	-1.66241300
H	2.90626000	0.50015200	-2.05936800
H	1.35243200	-0.73103400	-1.23365200
H	-0.44065600	0.63871600	-1.31826400
O	-2.45957600	-0.18656000	-2.39595500
H	-2.36443300	-0.94242300	-2.98074200
C	-5.03739200	0.37899300	-0.66461800
H	-5.58781600	1.02912500	0.01796000
H	-5.48969000	-0.61488100	-0.62984600
H	-5.14977500	0.77166100	-1.67738000
C	0.60170100	0.37169300	1.96937500
H	-0.04345200	-0.43790100	2.30772800
H	1.56104000	0.26003700	2.46889500
H	0.16829400	1.30587400	2.33091100
O	-2.14420300	-0.86840200	1.12143600
C	3.53181800	-2.07643600	-0.83800600
H	3.17758000	-1.96496300	-1.86452000
H	3.24924400	-3.07060900	-0.48692300
H	4.62402000	-2.03426800	-0.85480100

C	3.38981700	-1.38371700	1.51370300
H	3.28646700	-0.58210600	2.24355700
H	2.80583300	-2.23573900	1.86673800
H	4.44109200	-1.68437100	1.51519800
C	-3.32607700	-0.22907400	1.09582600
O	-4.02200100	-0.14986900	2.07240300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1116.967396

125) Conformer **12aC8**

C	3.03481700	1.52607200	0.41110300
H	3.16077300	1.42948500	1.49507700
C	3.67953400	0.33018500	-0.27069700
H	4.72406800	0.26285000	0.07153900
C	2.98269700	-0.99324000	0.07793500
C	1.45219100	-0.85333000	-0.15317300
C	0.75131100	0.39680500	0.44630500
C	1.56506100	1.63937000	0.05701200
H	1.49199400	1.79920300	-1.02399900
H	1.15348900	2.52852900	0.54600000
C	0.65462500	-2.10946800	0.17905700
H	1.16624200	-3.00067200	-0.18927500
H	0.55970700	-2.23513700	1.26089500
C	-0.71753900	-2.04478300	-0.46814400
H	-1.34035400	-2.89581500	-0.17712500
H	-0.59662800	-2.09937100	-1.55591800
C	-1.48987700	-0.77553100	-0.19249900
C	-0.64097600	0.50482900	-0.24796300
C	-2.72511700	-0.64836200	-1.10417900
H	-3.22206100	-1.62455500	-1.12614300
C	-3.57428700	0.33235900	-0.29204700
C	-2.90050300	1.71326800	-0.34837100
H	-2.91306500	2.05735400	-1.38924700
H	-3.50983400	2.43143600	0.20594700
C	-1.48006200	1.70260000	0.21444300
H	-1.54708900	1.69467900	1.30497100
H	-0.98202400	2.63563000	-0.05362100
O	3.76499500	2.66343800	-0.04228300
H	3.26880900	3.45646100	0.18120900
O	3.66434400	0.53110100	-1.67442100
H	3.89101300	1.46059500	-1.80400100
H	1.37147400	-0.71474200	-1.24085700
H	-0.40890500	0.64146000	-1.31322300
O	-2.47922700	-0.32867200	-2.44124800

H	-2.14155600	0.56991200	-2.50766900
C	-5.03902600	0.38569500	-0.66134100
H	-5.58765200	1.03041100	0.02774000
H	-5.49079500	-0.60840300	-0.63322600
H	-5.15607300	0.78567100	-1.67087800
C	0.60059000	0.34631600	1.97135100
H	1.55955300	0.22661700	2.46971300
H	-0.04666200	-0.46511700	2.30082900
H	0.16988100	1.27807500	2.34291100
O	-2.14094500	-0.87413200	1.11158100
C	3.39505800	-1.40756200	1.49498100
H	4.44864000	-1.70019800	1.49376900
H	2.81725700	-2.26978000	1.83339000
H	3.28436700	-0.61886400	2.23799800
C	3.53098400	-2.07191500	-0.86503600
H	3.18213600	-1.93190000	-1.88884200
H	4.62393800	-2.03774700	-0.87340500
H	3.23981500	-3.07003000	-0.53224000
C	-3.32455600	-0.23795100	1.09123500
O	-4.02166900	-0.17025700	2.06735100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1116.966969

126) Conformer **12bC1**

C	3.02125100	1.89095100	-0.24843900
H	3.46818600	2.72630700	-0.79912100
H	3.21500300	2.08160200	0.81145300
C	3.70131800	0.60467400	-0.67108100
H	3.50956900	0.46356400	-1.74750600
C	3.14531200	-0.63821900	0.04128200
C	1.59790200	-0.63829100	-0.13795100
C	0.82773500	0.67281700	0.18175300
C	1.53121400	1.83414100	-0.53505000
H	1.38632500	1.72024200	-1.61714000
H	1.06715200	2.78395200	-0.25671700
C	0.90434100	-1.82614200	0.52066000
H	1.46729900	-2.74625400	0.35321600
H	0.85317800	-1.69103200	1.60414600
C	-0.48947600	-2.00638500	-0.05257900
H	-1.03494500	-2.80384800	0.46082100
H	-0.40384200	-2.30641800	-1.10293500
C	-1.34323600	-0.75941800	-0.03718000
C	-0.59524600	0.52241500	-0.43671000
C	-2.61098000	-0.92568000	-0.88401500

H	-3.03423400	-1.91590500	-0.66781500
C	-3.50463700	0.15624300	-0.27125900
C	-2.93937500	1.52124200	-0.69487700
H	-2.99237300	1.56210200	-1.78587200
H	-3.58252000	2.31497200	-0.30583000
C	-1.50543900	1.73716400	-0.21596300
H	-1.53113500	1.98213400	0.84911000
H	-1.08879900	2.61172400	-0.71854700
O	5.10525700	0.66333800	-0.45376200
H	5.44583200	1.41812100	-0.94235500
H	1.46437400	-0.77070000	-1.22350200
H	-0.43717700	0.41767400	-1.51688300
C	-4.98200700	0.02291600	-0.56232700
H	-5.35350500	-0.96775800	-0.28945500
H	-5.17038900	0.17833100	-1.62749300
H	-5.55494100	0.76719800	-0.00605300
O	-2.34063200	-0.79941800	-2.25315300
H	-3.02450600	-1.25998800	-2.74653500
C	3.62595900	-0.69984900	1.49397200
H	3.09473500	-1.47812900	2.04581500
H	3.50158200	0.23876500	2.03289700
H	4.68921200	-0.94418300	1.51823600
C	3.71519500	-1.86783500	-0.67824500
H	3.32284700	-1.94797400	-1.69646400
H	3.48118000	-2.79408200	-0.14999600
H	4.80203200	-1.78892900	-0.73693600
C	0.75210400	0.98411100	1.68016200
H	1.74164900	1.07167100	2.12279200
H	0.20380900	0.22705200	2.23947400
H	0.24936400	1.93904600	1.84554100
O	-1.93218500	-0.59121400	1.28998000
C	-3.16022800	-0.05566700	1.18946300
O	-3.82058900	0.19424600	2.16243100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1041.792646

127) Conformer **12bC2**

C	3.02101900	1.89105400	-0.25506000
H	3.21374700	2.08586900	0.80426900
H	3.46796700	2.72454200	-0.80856300
C	3.70220000	0.60356200	-0.67223800
H	3.51165100	0.45844900	-1.74836700
C	3.14613100	-0.63708900	0.04401400
C	1.59887300	-0.63802900	-0.13650500

C	0.82794300	0.67366500	0.17864000
C	1.53120700	1.83234900	-0.54252700
H	1.38696800	1.71390500	-1.62421800
H	1.06657800	2.78308700	-0.26840000
C	0.90476100	-1.82464400	0.52392100
H	1.46916700	-2.74484300	0.36221100
H	0.84760400	-1.68583700	1.60660800
C	-0.48647500	-2.00616900	-0.05520300
H	-1.03280000	-2.80795100	0.45056500
H	-0.38704600	-2.30604800	-1.10533300
C	-1.34194600	-0.76059900	-0.03855400
C	-0.59598900	0.52084500	-0.43722300
C	-2.61869500	-0.92478000	-0.88566000
H	-3.04350200	-1.91385600	-0.66854400
C	-3.50359400	0.15306300	-0.26995400
C	-2.94036800	1.52082400	-0.69275600
H	-3.00032300	1.57073200	-1.78281900
H	-3.58355400	2.31060500	-0.29576000
C	-1.50581300	1.73574000	-0.21571900
H	-1.53085900	1.97986700	0.84957100
H	-1.08912000	2.61065200	-0.71762200
O	5.10578600	0.66352900	-0.45354500
H	5.44639900	1.41779300	-0.94291700
H	1.46671300	-0.77327800	-1.22195700
H	-0.44293100	0.41477800	-1.51827100
C	-4.98178000	0.02138200	-0.55751500
H	-5.16718200	0.16577300	-1.62395200
H	-5.55039500	0.77255900	-0.00615400
H	-5.35514900	-0.96573200	-0.27502500
O	-2.44954600	-0.75677000	-2.26618800
H	-2.28119600	-1.61347100	-2.66652600
C	3.62584800	-0.69379200	1.49722900
H	4.68837100	-0.94112700	1.52314500
H	3.09210600	-1.46808800	2.05228600
H	3.50411700	0.24754300	2.03197700
C	3.71683200	-1.86897500	-0.67095600
H	4.80364300	-1.78968400	-0.72952800
H	3.32497800	-1.95299500	-1.68906300
H	3.48326500	-2.79349900	-0.13948500
C	0.75305100	0.98984600	1.67613100
H	0.20047200	0.23709800	2.23716000
H	0.25497900	1.94775100	1.83838000
H	1.74257500	1.07371900	2.11941500
O	-1.92986300	-0.59851200	1.29038400

C	-3.15535300	-0.05791800	1.19066900
O	-3.81317200	0.19921300	2.16341200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1041.792718

128) Conformer **12bC3**

C	-3.02114700	-1.89117400	-0.28987000
H	-3.21261100	-2.10586200	0.76799900
H	-3.46964000	-2.71237500	-0.85647900
C	-3.70809600	-0.60113200	-0.68832600
H	-3.53888100	-0.44693900	-1.76155700
C	-3.14370400	0.63746400	0.03867600
C	-1.59691100	0.64056300	-0.13974900
C	-0.82792700	-0.67351600	0.16780000
C	-1.52906600	-1.82597100	-0.56532600
H	-1.38006700	-1.69881400	-1.64529900
H	-1.06549100	-2.77896400	-0.29699700
C	-0.90384400	1.82347500	0.52842700
H	-1.46676400	2.74459900	0.36621000
H	-0.85477700	1.68059100	1.61111400
C	0.49128500	2.00773200	-0.04005400
H	1.03554200	2.80134900	0.48051400
H	0.40840100	2.31532600	-1.08842500
C	1.34441000	0.76039300	-0.03138900
C	0.59737600	-0.51762500	-0.44436100
C	2.61527000	0.93328900	-0.87224400
H	3.03796700	1.92158300	-0.64627600
C	3.50637600	-0.15393500	-0.26522500
C	2.94234000	-1.51505000	-0.70264600
H	2.99961800	-1.54668500	-1.79371000
H	3.58360900	-2.31232500	-0.31779500
C	1.50651300	-1.73458100	-0.23118000
H	1.52835900	-1.98897700	0.83174300
H	1.09157900	-2.60457400	-0.74300500
O	-5.11980400	-0.70894600	-0.56394700
H	-5.31927600	-0.97676500	0.33858500
H	-1.46440600	0.78246400	-1.22435300
H	0.44286200	-0.40334900	-1.52406000
C	4.98488000	-0.01863300	-0.54951900
H	5.17734500	-0.16515100	-1.61521800
H	5.55542300	-0.76778200	0.00265600
H	5.35565200	0.96957100	-0.26690600
O	2.34945800	0.81846800	-2.24320200
H	3.03693500	1.27990800	-2.73076100

C	-3.62620000	0.67980800	1.49196500
H	-4.68452600	0.95120400	1.52412600
H	-3.08580700	1.43721600	2.06281700
H	-3.51683900	-0.26899900	2.01874500
C	-3.71713100	1.87392700	-0.66372500
H	-3.49707200	2.79392800	-0.11866400
H	-4.80301600	1.78418600	-0.73220000
H	-3.31814300	1.97476800	-1.67745900
C	-0.75841600	-1.00102500	1.66289200
H	-0.25251800	-1.95549600	1.82076400
H	-1.74967000	-1.09829700	2.09987500
H	-0.21660900	-0.24757900	2.23338700
O	1.92813700	0.58079600	1.29643000
C	3.15650900	0.04580500	1.19594900
O	3.81317300	-0.21239900	2.16922600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1041.793018

129) Conformer **12bC4**

C	3.01804700	1.89798600	-0.26616900
H	3.21348500	2.09856200	0.79181000
H	3.46647800	2.72426400	-0.82520000
C	3.70010100	0.61486400	-0.67938800
H	3.50474900	0.46586400	-1.75372700
C	3.14729500	-0.62861500	0.04967300
C	1.59943400	-0.63822700	-0.13119200
C	0.82677100	0.67437800	0.17763200
C	1.52782300	1.83252000	-0.54636500
H	1.37957800	1.71382600	-1.62740800
H	1.06265100	2.78249600	-0.27055000
C	0.90579700	-1.82040400	0.53868500
H	1.46685700	-2.74330900	0.38142000
H	0.85480700	-1.67436500	1.62068900
C	-0.48806600	-2.00714100	-0.03258800
H	-1.03244500	-2.80002400	0.48896800
H	-0.40229300	-2.31768700	-1.07986000
C	-1.34295700	-0.76100100	-0.02958400
C	-0.59540500	0.51698200	-0.44113200
C	-2.61005800	-0.93668600	-0.87546000
H	-3.03283300	-1.92496500	-0.64952800
C	-3.50469900	0.15081500	-0.27414700
C	-2.93998800	1.51176100	-0.71125000
H	-2.99254800	1.54161600	-1.80260700
H	-3.58372300	2.30901800	-0.33050300

C	-1.50640200	1.73353600	-0.23396300
H	-1.53294800	1.99007000	0.82834100
H	-1.09003400	2.60280100	-0.74582400
O	5.09510300	0.80043800	-0.48386000
H	5.56043300	0.05032700	-0.86408700
H	1.46652500	-0.78058900	-1.21571600
H	-0.43580300	0.40158600	-1.51998700
C	-4.98186600	0.01380000	-0.56455300
H	-5.35293000	-0.97436800	-0.28218100
H	-5.16999200	0.15877600	-1.63123700
H	-5.55539100	0.76314100	-0.01573400
O	-2.33858900	-0.82414000	-2.24555200
H	-3.02363000	-1.28713000	-2.73506300
C	3.62752900	-0.67321800	1.50214700
H	3.10222900	-1.44917300	2.06286000
H	3.49698700	0.27038500	2.03046400
H	4.69283700	-0.90999900	1.53299000
C	3.71574600	-1.86647900	-0.65631500
H	3.43767200	-2.79036800	-0.14650800
H	4.80953900	-1.84555400	-0.66554500
H	3.36813600	-1.93002600	-1.69147300
C	0.74917800	0.99721300	1.67353900
H	1.73816700	1.09831900	2.11447900
H	0.20814600	0.24049900	2.24025800
H	0.23802200	1.94896400	1.83088900
O	-1.93266900	-0.58010200	1.29545500
C	-3.16102300	-0.04629500	1.18883900
O	-3.82212800	0.21284400	2.15884700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1041.792588

130) Conformer **12bC5**

C	-3.02100000	-1.89110100	-0.29636600
H	-3.21138900	-2.10975900	0.76088400
H	-3.46959900	-2.71041300	-0.86561300
C	-3.70899800	-0.59995300	-0.68945500
H	-3.54098300	-0.44185100	-1.76231300
C	-3.14448200	0.63635300	0.04139300
C	-1.59785100	0.64025300	-0.13823700
C	-0.82815300	-0.67437200	0.16477600
C	-1.52913400	-1.82407900	-0.57270000
H	-1.38080300	-1.69229700	-1.65220900
H	-1.06501200	-2.77797800	-0.30864400
C	-0.90420400	1.82192100	0.53172100

H	-1.46862000	2.74308200	0.37532300
H	-0.84896700	1.67525200	1.61357200
C	0.48830200	2.00751500	-0.04285500
H	1.03345000	2.80557500	0.46998300
H	0.39143100	2.31483900	-1.09105200
C	1.34313400	0.76156300	-0.03281600
C	0.59811400	-0.51618400	-0.44464700
C	2.62293400	0.93218300	-0.87414400
H	3.04719400	1.91938400	-0.64760500
C	3.50530500	-0.15082700	-0.26396700
C	2.94328500	-1.51485700	-0.70010500
H	3.00737100	-1.55589700	-1.79027600
H	3.58460900	-2.30810600	-0.30705300
C	1.50688600	-1.73322000	-0.23026000
H	1.52813200	-1.98628700	0.83299700
H	1.09189300	-2.60377100	-0.74104600
O	-5.12047900	-0.70872100	-0.56390600
H	-5.31885400	-0.98025700	0.33776200
H	-1.46668700	0.78498200	-1.22271300
H	0.44877100	-0.40084300	-1.52524200
C	4.98458500	-0.01729900	-0.54502500
H	5.55089200	-0.77308800	0.00238500
H	5.35720200	0.96738500	-0.25324400
H	5.17385400	-0.15318600	-1.61189500
O	2.45872800	0.77514800	-2.25648400
H	2.28942400	1.63462900	-2.65044600
C	-3.62627800	0.67379100	1.49509800
H	-3.08330700	1.42686300	2.06925500
H	-3.51991100	-0.27775700	2.01755600
H	-4.68374600	0.94826200	1.52878600
C	-3.71860500	1.87505000	-0.65651500
H	-3.49919000	2.79322000	-0.10810400
H	-4.80443400	1.78485900	-0.72521200
H	-3.31982100	1.97984200	-1.66993400
C	-0.75940400	-1.00667200	1.65894700
H	-0.25934500	-1.96474200	1.81357200
H	-1.75062500	-1.09880600	2.09697000
H	-0.21207600	-0.25813800	2.23075300
O	1.92595600	0.58842500	1.29676900
C	3.15182800	0.04835900	1.19704800
O	3.80599000	-0.21679600	2.17005400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1041.793031

131) Conformer **12bC6**

C	-3.01787200	-1.89797400	-0.27285700
H	-3.21203600	-2.10270100	0.78456700
H	-3.46646100	-2.72234200	-0.83456900
C	-3.70119400	-0.61369300	-0.68044200
H	-3.50747400	-0.46072700	-1.75452700
C	-3.14808400	0.62750400	0.05234300
C	-1.60038900	0.63790300	-0.12989400
C	-0.82699700	-0.67524000	0.17432500
C	-1.52792000	-1.83057300	-0.55415000
H	-1.38048700	-1.70704400	-1.63476400
H	-1.06213500	-2.78152300	-0.28284000
C	-0.90610400	1.81883700	0.54169100
H	-1.46866900	2.74175900	0.39032800
H	-0.84883900	1.66898800	1.62283300
C	0.48509000	2.00691000	-0.03572800
H	1.03030400	2.80435900	0.47799000
H	0.38540900	2.31694800	-1.08286300
C	1.34169800	0.76217900	-0.03112800
C	0.59619000	-0.51552600	-0.44162900
C	2.61785600	0.93555300	-0.87728600
H	3.04220600	1.92270600	-0.65076800
C	3.50367700	-0.14776900	-0.27260400
C	2.94103300	-1.51157300	-0.70865100
H	3.00055300	-1.55070100	-1.79916400
H	3.58478200	-2.30488900	-0.31971800
C	1.50679400	-1.73218500	-0.23320000
H	1.53257700	-1.98744600	0.82943600
H	1.09043900	-2.60198200	-0.74412400
O	-5.09575900	-0.80066600	-0.48347300
H	-5.56216600	-0.04973000	-0.86073500
H	-1.46893700	0.78308800	-1.21430400
H	0.44180400	-0.39900100	-1.52140500
C	4.98167600	-0.01247300	-0.55952700
H	5.35462600	0.97201400	-0.26749800
H	5.16670100	-0.14630700	-1.62740000
H	5.55087700	-0.76872600	-0.01576800
O	2.44793400	0.78099200	-2.25929600
H	2.28002900	1.64159300	-2.65135900
C	-3.62739700	0.66724300	1.50532500
H	-3.09847000	1.43809700	2.06967400
H	-3.50099500	-0.27957300	2.02888300
H	-4.69164200	0.90853100	1.53788200
C	-3.71720700	1.86766100	-0.64909100

H	-3.36973100	1.93527200	-1.68404100
H	-3.43980800	2.78985700	-0.13583800
H	-4.81097300	1.84606100	-0.65837900
C	-0.75023500	-1.00291100	1.66932900
H	-1.73923200	-1.09812200	2.11140900
H	-0.20305000	-0.25145600	2.23725200
H	-0.24558500	-1.95865600	1.82343400
O	1.93028500	0.58775300	1.29579300
C	3.15612300	0.04875900	1.19016400
O	3.81453600	-0.21734500	2.16003200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1041.792566

132) Conformer **12bC7**

C	3.02004800	1.89520500	-0.22257100
H	3.21176500	2.07218200	0.84000200
H	3.46627700	2.73854200	-0.76132600
C	3.70256200	0.61557900	-0.66134300
H	3.51256400	0.48852700	-1.73981400
C	3.14736300	-0.63762100	0.03366800
C	1.60018600	-0.63802100	-0.14752500
C	0.82864300	0.66831600	0.18792500
C	1.53064500	1.84038900	-0.51249200
H	1.38826400	1.74126900	-1.59644800
H	1.06492700	2.78565300	-0.22182800
C	0.90740500	-1.83497000	0.49537000
H	1.47107300	-2.75207300	0.31485000
H	0.85696500	-1.71481200	1.58059400
C	-0.48684600	-2.00885200	-0.07918800
H	-1.03140700	-2.81325600	0.42414800
H	-0.40194300	-2.29661600	-1.13321900
C	-1.34199200	-0.76395900	-0.04830900
C	-0.59452600	0.52219700	-0.43371200
C	-2.62012200	-0.92679600	-0.89208400
H	-3.04244500	-1.91233800	-0.66686000
C	-3.50675600	0.15534700	-0.27168300
C	-2.94294400	1.52840100	-0.67297500
H	-3.02635600	1.62749600	-1.76171900
H	-3.58119200	2.31214100	-0.25723800
C	-1.50327700	1.73704400	-0.20542500
H	-1.52427700	1.97330400	0.86109100
H	-1.08838100	2.61466000	-0.70330200
O	5.10579200	0.67341500	-0.44097400
H	5.44709100	1.43212000	-0.92294900

H	1.46885800	-0.75726200	-1.23492500
H	-0.41516200	0.42898300	-1.51409000
C	-4.98529300	0.02797400	-0.55880900
H	-5.55320300	0.77472300	-0.00082900
H	-5.35786500	-0.96133500	-0.28386400
H	-5.17376900	0.18015100	-1.62381500
O	-2.45564500	-0.90364100	-2.27889300
H	-2.18697000	-0.02447900	-2.56266200
C	3.62598900	-0.71828900	1.48605000
H	3.09641500	-1.50587700	2.02609000
H	3.49838500	0.21218700	2.03818300
H	4.68985600	-0.95993900	1.50817800
C	3.71968500	-1.85658200	-0.70185100
H	3.32877700	-1.92337600	-1.72157400
H	3.48642200	-2.79025700	-0.18657600
H	4.80643400	-1.77521100	-0.75813200
C	0.74866800	0.95972600	1.68993500
H	0.24443100	1.91156800	1.86789400
H	1.73780600	1.04362000	2.13394300
H	0.20210400	0.19395400	2.23868100
O	-1.92876100	-0.60720200	1.28063900
C	-3.15660000	-0.06949700	1.18716700
O	-3.81544400	0.17270400	2.16230500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1041.791571

133) Conformer **12bC8**

C	-3.01984000	-1.89604800	-0.26412100
H	-3.20896900	-2.09746500	0.79672500
H	-3.46763500	-2.72536000	-0.81921200
C	-3.70934300	-0.61238500	-0.67853900
H	-3.54194600	-0.47231000	-1.75398900
C	-3.14582700	0.63688900	0.03092500
C	-1.59922400	0.64041500	-0.14921900
C	-0.82884000	-0.66910400	0.17383500
C	-1.52844600	-1.83241600	-0.54326000
H	-1.38212700	-1.71968800	-1.62527400
H	-1.06307900	-2.78101600	-0.26287000
C	-0.90704500	1.83234700	0.50380800
H	-1.47059500	2.75061600	0.32862000
H	-0.85902700	1.70406100	1.58830500
C	0.48870300	2.01044500	-0.06556200
H	1.03196900	2.81080700	0.44552900
H	0.40683000	2.30635500	-1.11756300

C	1.34317900	0.76505000	-0.04194300
C	0.59662500	-0.51717900	-0.44147500
C	2.62445100	0.93502300	-0.87962900
H	3.04618600	1.91833200	-0.64382600
C	3.50840400	-0.15298600	-0.26581300
C	2.94556200	-1.52204400	-0.68179500
H	3.03275300	-1.61132900	-1.77111400
H	3.58197400	-2.30985000	-0.27097700
C	1.50421100	-1.73444600	-0.22136600
H	1.52155600	-1.98061100	0.84295200
H	1.09089900	-2.60730600	-0.72881200
O	-5.12041200	-0.72066300	-0.55055000
H	-5.31848000	-0.97728300	0.35555000
H	-1.46872800	0.76948100	-1.23571600
H	0.42104100	-0.41375700	-1.52151100
C	4.98805800	-0.02369200	-0.54621000
H	5.35999900	0.96297100	-0.26111600
H	5.18053600	-0.16652600	-1.61179300
H	5.55350500	-0.77562400	0.00728300
O	2.46485500	0.92450000	-2.26710600
H	2.19970300	0.04729900	-2.56011500
C	-3.62654500	0.69865200	1.48401700
H	-4.68579900	0.96656000	1.51337400
H	-3.08850800	1.46647600	2.04301800
H	-3.51314800	-0.24183200	2.02464500
C	-3.72163000	1.86268300	-0.68801600
H	-4.80747300	1.77063700	-0.75343800
H	-3.32449500	1.94953000	-1.70375900
H	-3.50178900	2.79056200	-0.15645600
C	-0.75490000	-0.97715700	1.67269100
H	-0.24800300	-1.92895800	1.84281300
H	-1.74569800	-1.07037400	2.11133800
H	-0.21426400	-0.21531600	2.23274800
O	1.92486400	0.59622300	1.28764500
C	3.15293700	0.05891600	1.19374600
O	3.80817800	-0.19216800	2.16903600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1041.791886

134) Conformer **12bC9**

C	3.01687900	1.90240000	-0.24017900
H	3.46458000	2.73676000	-0.78752100
H	3.21031100	2.08941300	0.82059600
C	3.70141900	0.62586700	-0.66950500

H	3.50819000	0.49112200	-1.74609700
C	3.14927300	-0.62823800	0.04190500
C	1.60168400	-0.63807800	-0.14097600
C	0.82773500	0.66981100	0.18395700
C	1.52727000	1.83884700	-0.52366400
H	1.06050400	2.78430000	-0.23540100
H	1.38141500	1.73497800	-1.60663100
C	0.90884300	-1.82968500	0.51293100
H	1.47060500	-2.74967300	0.34220400
H	0.85864200	-1.69889800	1.59686200
C	-0.48549900	-2.00984700	-0.05969200
H	-1.02895000	-2.80996200	0.45158400
H	-0.40051200	-2.30776700	-1.11088300
C	-1.34175200	-0.76561900	-0.04075700
C	-0.59471000	0.51693400	-0.43782000
C	-2.61922100	-0.93755500	-0.88374100
H	-3.04113400	-1.92107000	-0.64910900
C	-3.50679100	0.15014400	-0.27456200
C	-2.94337400	1.51944600	-0.68900300
H	-3.02593800	1.60785100	-1.77875400
H	-3.58231900	2.30692200	-0.28149600
C	-1.50418000	1.73362200	-0.22253900
H	-1.52618500	1.98087600	0.84144000
H	-1.08945200	2.60625200	-0.72919400
O	5.09547300	0.81094000	-0.46869100
H	5.56316100	0.06806900	-0.86008300
H	1.47096300	-0.76701100	-1.22749900
H	-0.41415400	0.41340500	-1.51704400
C	-4.98510800	0.01930600	-0.56127600
H	-5.17313000	0.16119400	-1.62777900
H	-5.55361800	0.77109800	-0.01073600
H	-5.35735300	-0.96749500	-0.27704400
O	-2.45369400	-0.92790000	-2.27057000
H	-2.18651000	-0.05104400	-2.56276000
C	3.62771900	-0.69205000	1.49422400
H	3.49569400	0.24405700	2.03538800
H	4.69323400	-0.92794100	1.52276800
H	3.10298800	-1.47632300	2.04373300
C	3.72001200	-1.85554800	-0.68042900
H	4.81372000	-1.83256600	-0.68830500
H	3.37354300	-1.90542800	-1.71671000
H	3.44295200	-2.78674600	-0.18359000
C	0.74602400	0.97243900	1.68370900
H	0.20581000	0.20733200	2.23954200

H	0.23438600	1.92169400	1.85385400
H	1.73464900	1.06861300	2.12631500
O	-1.92939200	-0.59658700	1.28620300
C	-3.15750900	-0.06041500	1.18664900
O	-3.81718300	0.19071000	2.15892600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1041.791502

135) Conformer **13C1**

C	-1.94598100	0.59023200	-0.04361700
H	-2.60371200	1.46729400	0.01255300
C	-2.82262100	-0.64868100	0.09871900
H	-2.19636500	-1.54523500	0.03673000
C	-0.24238700	-0.48674900	-1.55943300
H	-0.91543400	-1.31739500	-1.78864100
H	0.35870000	-0.34852400	-2.46100200
C	-1.11363900	0.72801000	-1.31792600
O	-0.28719800	1.88731500	-1.02649400
C	-0.08385100	1.95159900	0.29927000
C	-0.80540300	0.79239600	0.95674100
C	0.11165600	-0.44453200	1.01484800
C	0.66405800	-0.89259500	-0.38009600
C	1.33416500	-0.14087000	1.85101800
C	2.50913100	-0.03595500	0.99700100
C	2.07031900	-0.25086500	-0.41238300
O	3.01889900	-0.74425200	-1.34997000
C	2.61403800	0.61718400	-1.45343000
H	3.37329800	1.34837500	-1.18620300
H	2.01999900	0.86326800	-2.32632800
O	2.31616700	-1.16857200	1.84649000
O	0.57729900	2.81981900	0.80091900
C	-3.84717500	-0.71449800	-1.02811800
H	-3.37769300	-0.77975200	-2.01253000
H	-4.48719700	0.17319200	-1.02033400
H	-4.48936600	-1.59015500	-0.91006400
C	-3.51993900	-0.65875600	1.45351800
H	-4.16357700	-1.53646800	1.54602500
H	-4.14711500	0.23022200	1.57207500
H	-2.80900500	-0.67985000	2.28277900
H	-1.69334400	0.98254900	-2.20399200
H	-1.11757600	1.07505800	1.96190000
H	-0.46425100	-1.25503700	1.46989500
C	0.83013200	-2.41459400	-0.43655200
H	1.22554600	-2.70873700	-1.41113500

H	-0.14039200	-2.89951700	-0.30469600
H	1.50560900	-2.77669700	0.33646200
H	3.37037200	0.58398100	1.22101100
H	1.23515000	0.41099100	2.78057000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -883.526202

136) Conformer **16aC1**

H	0.80834000	1.79223400	-1.49052300
H	2.24422700	-0.16517500	-1.61012700
H	-0.83601900	-3.28072800	0.34229900
H	-1.18531900	-2.67693300	1.95591500
H	-3.22844400	-2.12774200	0.80486700
H	1.39110500	-2.27417100	-0.60374500
H	0.63808100	0.50801000	2.88522600
H	-0.97006000	1.24788300	2.92331800
H	-0.77654900	-0.46981600	3.29316200
H	2.13055400	0.41574300	1.36831100
H	3.24438700	-1.75099700	0.88786600
H	4.25159800	-0.96622100	-0.33457000
H	4.42251700	-0.52872600	1.36882400
H	4.07403200	1.87746400	0.87806000
H	2.63844500	2.45336100	0.03187500
H	3.88511100	1.56385500	-0.85022800
H	-2.54805600	3.51377700	-0.72352300
H	-1.48549700	2.68218500	-1.87041200
H	-0.79833500	3.71272200	-0.59442300
H	-2.38080200	-1.68243800	-0.66195300
C	-2.58314900	0.89861800	-0.03242700
N	-1.54561500	1.90213500	0.11811600
C	-0.26930000	1.23276000	0.30846100
C	-0.63686400	0.00976800	1.18196200
C	-2.15970100	-0.21680700	0.91983400
C	0.06576400	-1.33347700	0.83113500
C	-1.05868300	-2.37505000	0.91205500
C	-2.31809900	-1.65641800	0.42824200
H	0.82183200	-1.54870400	1.59116500
C	0.51380000	0.88769400	-0.95887500
C	1.67168600	-0.07020600	-0.67709600
H	-2.68828800	-0.09705100	1.86882400
C	3.69985800	-0.80182400	0.59636900
C	-0.41810300	0.34322600	2.65562900
H	0.39177700	1.90834200	0.86722100
C	2.66340500	0.30117700	0.41979200

C	0.83314500	-1.34314100	-0.50759600
C	3.34812600	1.62550500	0.10150300
O	-0.29833100	0.12796600	-1.89400800
C	-0.08834100	-1.18416300	-1.69070000
C	-1.59106500	2.99375100	-0.81803800
O	-0.58226600	-2.02121100	-2.39820500
H	-2.66118800	0.52338400	-1.06569100
H	-3.55423600	1.33227000	0.22765000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -828.963812

137) Conformer **16aC2**

H	-0.79904400	-1.42807900	-1.85894400
H	-2.38290300	0.36831000	-1.42934100
H	0.80425800	3.15358200	0.65051400
H	1.27028700	2.43644900	2.18957700
H	3.21929400	2.01202400	0.78610000
H	-1.62643900	2.24916800	0.00680800
H	1.02193200	-1.81555400	2.53168700
H	0.52914200	-0.29404000	3.28197100
H	-0.66564100	-1.32135800	2.48636900
H	-2.04075700	-0.86474500	1.31511200
H	-4.36229400	0.64410500	0.04178200
H	-4.39987900	-0.17628600	1.60639300
H	-3.36167900	1.23172400	1.37583500
H	-3.86888200	-2.36573100	0.56511300
H	-2.42717400	-2.59540000	-0.42392600
H	-3.79038900	-1.66188900	-1.05334000
H	1.87885900	-3.46871000	-0.67095200
H	2.93464700	-2.63425800	-1.83242700
H	1.20369600	-2.74008000	-2.14535200
H	2.21304600	1.49998000	-0.56503600
C	2.77726100	-1.02964900	0.29469300
N	1.76539900	-1.34687800	-0.68997200
C	0.44808500	-1.14115000	-0.10513300
C	0.66171600	-0.20918800	1.12489200
C	2.17826700	0.11125500	1.09118500
C	-0.06888200	1.16970400	1.05862500
C	1.06316600	2.21184700	1.13893000
C	2.27885500	1.52046900	0.52615300
H	-0.72187200	1.26087500	1.93039100
C	-0.53542300	-0.63069300	-1.16447700
C	-1.73814900	0.10858700	-0.57810400
H	2.57404400	0.11534500	2.11080500

C	-3.74768200	0.33153900	0.89201400
C	0.35921500	-0.95188600	2.42533800
H	0.02581500	-2.09411000	0.26025400
C	-2.62844300	-0.59670200	0.43605300
C	-0.98940500	1.38224800	-0.16612300
C	-3.20587100	-1.87819400	-0.15342200
O	0.08024700	0.40349100	-1.97264500
C	-0.18867900	1.59838400	-1.42765000
C	1.95030900	-2.60684300	-1.35906000
O	0.17242100	2.62538600	-1.93969200
H	2.98661500	-1.88624100	0.96178900
H	3.72015300	-0.76630800	-0.19616800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -828.963446

138) Conformer **16bC1**

H	-1.44208300	-1.96735300	1.06026500
C	0.11626000	-0.80021100	1.93530200
H	3.19373500	-2.27003800	-0.26602300
C	1.02506400	-2.45722200	-0.33812600
C	1.78543300	3.11706100	0.24374300
C	-3.12335500	1.95690100	-0.21401400
H	-3.56613800	2.14273200	0.76982800
H	1.13408800	-2.96603700	-1.30068600
H	1.00603800	3.80362200	-0.09751300
H	0.81345500	-0.94869200	-3.13527500
H	-2.15847900	0.38072400	-1.29838700
H	1.06931200	0.79641300	-2.98528500
C	-1.59203800	0.23673200	0.77372100
C	0.37665900	1.21359000	-0.46617600
O	0.42506500	0.50630000	1.89736300
H	0.75977300	-3.21260100	0.40655100
H	-1.34397200	-2.72549900	-1.17415000
C	-0.83482700	-1.09939200	0.80156000
C	2.30147300	-1.69652700	-0.00711100
H	-4.28760600	-0.34597300	0.76064300
C	0.47766900	-0.04665200	-2.62028300
H	-3.89385500	2.14423700	-0.96557300
H	2.79758600	0.71978300	0.95683600
H	-0.28501600	1.79237400	-1.12320600
H	1.70844000	3.02723000	1.34015400
C	2.68858100	0.87427200	-0.12905400
H	-0.58956700	2.14699900	1.23578700
H	-2.12148700	0.32656000	1.73299100

C	-2.61987700	0.52079800	-0.31790200
C	0.67924100	-0.16211200	-1.11198100
C	2.19300100	-0.39953800	-0.80923300
O	0.55497300	-1.53362200	2.77992400
H	2.70862500	-0.52479500	-1.76412500
C	-3.79105400	-0.44735500	-0.20982000
N	1.67670800	1.86193700	-0.45051300
H	3.66095300	1.20584500	-0.50718900
H	-4.53209700	-0.23902800	-0.98539100
H	-0.56751900	0.12058700	-2.88441200
O	-1.04570800	-1.85547000	-1.45730100
H	-2.32969400	2.69196700	-0.36707400
C	-0.36992500	1.14726100	0.86255400
H	-3.47181100	-1.48415800	-0.32263700
H	2.75291500	3.57366000	0.01888000
H	2.36769600	-1.48511100	1.06181200
C	-0.07811900	-1.40338500	-0.52203000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -904.135217

139) Conformer **16bC2**

H	-1.44190700	-1.96503800	1.06156700
C	0.11700800	-0.78844700	1.93793500
H	3.19898900	-2.26278100	-0.24936300
C	1.03058100	-2.45743900	-0.31295800
C	1.77905800	3.12482200	0.22449100
C	-3.13553800	1.94696000	-0.22077100
H	-2.34625200	2.68693300	-0.37333400
H	0.76505000	-3.20647500	0.43637100
H	1.70146600	3.04135000	1.32130800
H	0.83376400	-0.96308100	-3.13286100
H	-2.15907800	0.37430300	-1.30024900
H	1.04611200	0.77797800	-2.99670800
C	-1.59295500	0.23937100	0.77111600
C	0.37476300	1.21356900	-0.47425600
O	0.42275600	0.51843800	1.89314200
H	1.14842400	-2.98521900	-1.26625800
H	-0.70195900	-2.23226000	-2.15900600
C	-0.83545000	-1.09708200	0.80718900
C	2.30534300	-1.69023900	0.00644700
H	-3.45143500	-1.49645500	-0.32875300
C	0.47200800	-0.06921400	-2.61494200
H	-3.58181700	2.13176600	0.76166600
H	2.79486600	0.73426900	0.95389500

H	-0.28848300	1.78613800	-1.13524200
H	2.74574000	3.58199500	-0.00250700
C	2.68679800	0.88127200	-0.13303100
H	-0.59399200	2.15417400	1.22256800
H	-2.12123300	0.33272100	1.73063100
C	-2.62275400	0.51396700	-0.32055300
C	0.68120400	-0.16653600	-1.10696800
C	2.19395300	-0.39809300	-0.80518300
O	0.55425500	-1.51547300	2.78828000
H	2.71178200	-0.52859300	-1.75829800
C	-3.78499900	-0.46495200	-0.21146800
N	1.67337000	1.86506500	-0.46224200
H	3.65895500	1.21183100	-0.51249100
H	-4.28040400	-0.36908400	0.76025800
H	-0.57717300	0.07920800	-2.87771700
O	-1.10396200	-1.91829900	-1.34321100
H	-3.90554200	2.12786900	-0.97442100
C	-0.37273300	1.15285900	0.85459500
H	-4.52975400	-0.26097300	-0.98483300
H	0.99842600	3.80756300	-0.12146800
H	2.37309600	-1.47012200	1.07347800
C	-0.07889100	-1.41095100	-0.50468200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -904.135890

140) Conformer **16bC3**

H	-1.43252000	-1.98333000	1.04629600
C	0.11636600	-0.80435100	1.93357100
H	3.21433800	-2.24186200	-0.25188900
C	1.04945900	-2.44981700	-0.31827900
C	1.76204400	3.13178700	0.23963100
C	-3.15759800	1.93671600	-0.18330200
H	-3.92970500	2.12455300	-0.93242100
H	1.15937800	-2.97244700	-1.27261000
H	2.72441100	3.59745200	0.01172600
H	1.07602200	0.78376900	-2.99391800
H	-2.15801100	0.43971500	-1.30539800
H	-0.56109300	0.13080000	-2.89223900
C	-1.59313200	0.22538200	0.77206800
C	0.37067300	1.21450400	-0.46744400
O	0.42066800	0.50388100	1.89555400
H	0.78875000	-3.19595000	0.43563400
H	-1.69505500	-1.39966700	-1.61155700
C	-0.83128100	-1.10981200	0.79793300

C	2.31776700	-1.67332500	0.00277000
H	-3.45709400	-1.51673900	-0.33224000
C	0.48118900	-0.05263300	-2.61938500
H	-2.37644600	2.68793100	-0.31760800
H	2.80225300	0.74665500	0.95048500
H	-0.29593200	1.78877300	-1.12411500
H	0.97513500	3.81042900	-0.10016100
C	2.68642800	0.89752000	-0.13518000
H	-0.60117500	2.14029500	1.23641400
H	-2.12594100	0.30920900	1.72928700
C	-2.62552000	0.51313900	-0.31524600
C	0.68482700	-0.16001400	-1.11144600
C	2.20018000	-0.38348800	-0.80922200
O	0.55601300	-1.53547900	2.77866800
H	2.71694900	-0.51134600	-1.76317900
C	-3.78228500	-0.47826400	-0.23693900
N	1.66382400	1.87499500	-0.45337700
H	3.65358700	1.23766200	-0.51889900
H	-4.29540200	-0.38274500	0.72446000
H	0.80580300	-0.96128100	-3.12943700
O	-0.98103500	-2.01381300	-1.41923600
H	-3.60452000	2.08771000	0.80398300
C	-0.37546500	1.14232600	0.86217800
H	-4.51108600	-0.27990100	-1.02569100
H	1.68895100	3.04193900	1.33626900
H	2.38467300	-1.45142100	1.06964400
C	-0.06335300	-1.41498400	-0.51822200

No imaginary frequency.

Gibbs Free Energies (a.u.) =-904.134158

141) Conformer **17C1**

C	-3.35530700	-1.82460400	-0.92048900
H	-3.63597500	-2.42605400	-0.05077900
H	-3.98897300	-2.17373500	-1.73999500
C	-3.69437300	-0.36374400	-0.61879500
H	-4.66253500	-0.32826600	-0.10258800
C	-2.64505700	0.30096800	0.30976200
C	-1.29647800	0.23897300	-0.40563400
C	-1.00501700	-1.25159900	-0.30603300
C	-1.87971500	-2.05725700	-1.24710800
H	-1.65223000	-1.73790900	-2.26751800
H	-1.64224500	-3.12224900	-1.18027500
C	-0.10293900	0.88870400	0.28870200
H	-0.23333800	0.87005200	1.37501300

C	1.11680000	-0.01813200	-0.04767200
C	0.50043700	-1.40273000	-0.44354100
C	2.03923800	0.46452900	-1.17161400
H	1.57624900	0.41434800	-2.15992800
H	2.32492900	1.50740300	-0.99670900
C	3.28975000	-0.42308500	-1.04236600
H	3.23781500	-1.23244600	-1.77720000
C	3.18130400	-1.05275000	0.39197300
C	2.65320600	-2.49765200	0.31987900
H	3.06577000	-2.99202200	-0.56529600
H	3.02692000	-3.03812500	1.19411000
C	1.12277000	-2.56614500	0.31735700
H	0.76200600	-2.54454100	1.34716900
H	0.78783400	-3.51722100	-0.10465300
C	-3.11458100	1.65036600	0.80848100
H	-4.03110700	1.53926000	1.39134800
H	-3.31561200	2.31286200	-0.03341500
H	-2.36886100	2.12215200	1.45155000
C	-2.38803200	-0.69181100	1.43666100
O	-2.92585800	-0.75917700	2.50861200
O	-1.42740700	-1.55187900	1.06591100
O	-3.74981200	0.42831700	-1.79197300
H	-4.45135700	0.08214300	-2.35135100
H	-1.36448400	0.57466700	-1.43965100
H	0.68151500	-1.55312400	-1.51390200
C	0.10586900	2.32595800	-0.10644900
O	-0.27045400	2.83035800	-1.13572200
O	0.79174200	2.98922400	0.82527400
C	1.08769200	4.35669800	0.53523800
H	1.69010400	4.43395900	-0.37025800
H	1.64426200	4.72702000	1.39229600
H	0.16685200	4.92582400	0.40614300
C	2.13445800	-0.18466000	1.07758300
H	1.72948100	-0.63906200	1.98442800
H	2.56454900	0.78544400	1.34330300
O	4.39014400	-0.99952700	1.12894300
H	5.00665000	-1.63398300	0.74998800
C	4.57031400	0.35298000	-1.29212800
H	4.54021300	0.80910500	-2.28553500
H	5.45456200	-0.28680400	-1.24881000
H	4.69812000	1.15273400	-0.55870100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.051168

142) Conformer 17C2

C	-3.36378800	-1.81483200	-0.91889900
H	-3.64189900	-2.41880500	-0.05010900
H	-4.00174400	-2.15973800	-1.73687000
C	-3.69837200	-0.35434800	-0.61050300
H	-4.66428700	-0.31861700	-0.09013000
C	-2.64371300	0.30477900	0.31596500
C	-1.29819700	0.24263200	-0.40526200
C	-1.00974600	-1.24880800	-0.31269100
C	-1.89012800	-2.04929700	-1.25279500
H	-1.66647300	-1.72676800	-2.27304700
H	-1.65450100	-3.11499200	-1.19083700
C	-0.10084100	0.88720800	0.28746000
H	-0.22922800	0.86765500	1.37394600
C	1.11643900	-0.02352600	-0.05131200
C	0.49448000	-1.40229100	-0.45708700
C	2.04398200	0.46291100	-1.16982900
H	1.58731100	0.40862600	-2.16069400
H	2.32150000	1.50784100	-0.99503000
C	3.30312000	-0.41347200	-1.03666800
H	3.27388900	-1.21150100	-1.78455100
C	3.18321000	-1.06626300	0.37714600
C	2.64675800	-2.50720700	0.28273700
H	3.05691600	-2.98628600	-0.61086100
H	3.02182800	-3.07553100	1.14049100
C	1.11717900	-2.57314900	0.29084400
H	0.76176700	-2.55910200	1.32273900
H	0.77815400	-3.52030800	-0.13677000
C	-3.10820900	1.65346100	0.82128900
H	-3.31135800	2.31919600	-0.01755300
H	-2.35872500	2.12150800	1.46271200
H	-4.02252200	1.54246800	1.40764800
C	-2.38365300	-0.69245000	1.43825700
O	-2.91652600	-0.76231400	2.51253800
O	-1.42651200	-1.55323700	1.06016600
O	-3.75693700	0.44210100	-1.78054800
H	-4.46314300	0.10105600	-2.33718600
H	-1.36938400	0.58262000	-1.43765400
H	0.67110200	-1.54364500	-1.52947400
C	0.11090200	2.32436200	-0.10612000
O	-0.26414900	2.83054500	-1.13499400
O	0.79767900	2.98556900	0.82649100
C	1.09615500	4.35276200	0.53762700
H	0.17638000	4.92360700	0.40854700

H	1.69908400	4.42967400	-0.36755300
H	1.65301200	4.72148200	1.39519400
C	2.13277500	-0.20045000	1.07455100
H	1.72293800	-0.65999600	1.97765700
H	2.56449600	0.76682400	1.34747600
O	4.45260900	-1.05294000	1.00785500
H	4.36498700	-1.50226500	1.85396400
C	4.57602800	0.38491400	-1.25999600
H	4.67907500	1.18272300	-0.52029500
H	4.55059400	0.84787300	-2.25040300
H	5.46463600	-0.24501700	-1.20169300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.050770

143) Conformer **17C3**

C	-3.35128700	-1.82340100	-0.94033700
H	-3.63474400	-2.42893300	-0.07563100
H	-3.97939400	-2.15825300	-1.76795200
C	-3.69746800	-0.37047100	-0.63187400
H	-4.66518200	-0.34304200	-0.11559800
C	-2.64350000	0.29312900	0.31118900
C	-1.29616600	0.23632600	-0.40209400
C	-1.00264800	-1.25414700	-0.30770300
C	-1.87274700	-2.05514100	-1.25660200
H	-1.63668400	-1.73537600	-2.27490900
H	-1.63833300	-3.12083900	-1.18941400
C	-0.10314900	0.88706200	0.29206500
H	-0.23282900	0.86584200	1.37845600
C	1.11777500	-0.01715600	-0.04594500
C	0.50357800	-1.40275500	-0.44193800
C	2.03809800	0.46717900	-1.17081900
H	1.57410700	0.41628800	-2.15864300
H	2.32268000	1.51038100	-0.99603000
C	3.28978900	-0.41912500	-1.04297300
H	3.23763500	-1.22872600	-1.77750400
C	3.18396900	-1.04863400	0.39176800
C	2.65742200	-2.49427400	0.32114900
H	3.06941700	-2.98870100	-0.56426100
H	3.03296000	-3.03365100	1.19525900
C	1.12703500	-2.56451500	0.32040400
H	0.76699500	-2.54172500	1.35045900
H	0.79266300	-3.51650800	-0.09998200
C	-3.11187000	1.63968600	0.81903900
H	-4.05242000	1.53655700	1.36373800

H	-3.26147500	2.33824100	-0.00696600
H	-2.38366400	2.08728400	1.49817700
C	-2.39309600	-0.70389600	1.43201200
O	-2.93920400	-0.78075600	2.49961800
O	-1.43051500	-1.56244000	1.06038200
O	-3.79020600	0.32624300	-1.85839100
H	-4.17203600	1.19423400	-1.69760300
H	-1.36779600	0.57442300	-1.43570600
H	0.68712000	-1.55360300	-1.51177700
C	0.10232200	2.32558300	-0.10010500
O	-0.28476500	2.83358700	-1.12377400
O	0.79712900	2.98570100	0.82691500
C	1.09026600	4.35421400	0.53882600
H	1.68312900	4.43473800	-0.37265700
H	1.65584400	4.72126600	1.39136500
H	0.16822100	4.92395400	0.42153500
C	2.13682000	-0.18182400	1.07827900
H	1.73347700	-0.63648400	1.98572600
H	2.56573500	0.78901600	1.34312100
O	4.39355200	-0.99356200	1.12730500
H	5.01194500	-1.62435300	0.74531200
C	4.56919900	0.35819500	-1.29473900
H	4.53717900	0.81413300	-2.28816400
H	5.45417700	-0.28068900	-1.25280400
H	4.69730000	1.15815200	-0.56160000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.051322

144) Conformer **17C4**

C	-3.37375400	-1.80434800	-0.91336300
H	-3.65355400	-2.40570300	-0.04330700
H	-4.01423100	-2.14768400	-1.73003600
C	-3.70142300	-0.34189700	-0.60687800
H	-4.66651000	-0.30103500	-0.08534400
C	-2.64266900	0.31396900	0.31726600
C	-1.29843400	0.24468200	-0.40562400
C	-1.01645300	-1.24783000	-0.31091700
C	-1.90155900	-2.04594200	-1.24863900
H	-1.67774700	-1.72612100	-2.26970900
H	-1.67058000	-3.11256000	-1.18516900
C	-0.09742900	0.88507800	0.28461700
H	-0.22503700	0.86819400	1.37123700
C	1.11556100	-0.03205400	-0.05301200
C	0.48673100	-1.40823900	-0.45715200

C	2.04547300	0.45112900	-1.17255600
H	1.58889600	0.39219300	-2.16313900
H	2.31934300	1.49784400	-1.00268200
C	3.30636000	-0.42146300	-1.03410900
H	3.29470500	-1.21280000	-1.78909900
C	3.17489500	-1.08762200	0.37999700
C	2.63565600	-2.52158700	0.27166800
H	3.03227200	-2.98928400	-0.63389600
H	3.02516800	-3.08964200	1.12042700
C	1.10718200	-2.58029700	0.29070400
H	0.75723400	-2.56354700	1.32443800
H	0.76241000	-3.52659800	-0.13402100
C	-3.10060000	1.66544400	0.82110500
H	-4.01448700	1.55924800	1.40900300
H	-3.30215200	2.33073700	-0.01847600
H	-2.34821800	2.13134000	1.46071500
C	-2.38563800	-0.68275500	1.44078800
O	-2.91772700	-0.74861200	2.51570200
O	-1.43265700	-1.54821400	1.06294100
O	-3.75787600	0.45299500	-1.77807600
H	-4.46513500	0.11315300	-2.33411600
H	-1.36950800	0.58329800	-1.43846600
H	0.66141300	-1.55139800	-1.52966600
C	0.12003500	2.32073800	-0.11140900
O	-0.25617500	2.82781600	-1.13935800
O	0.81386400	2.97929600	0.81796000
C	1.11754100	4.34493200	0.52703800
H	1.71723400	4.41855100	-0.38057400
H	1.67935700	4.71168800	1.38221000
H	0.19991400	4.91991200	0.40115800
C	2.12691500	-0.21720700	1.07508000
H	1.71699200	-0.67892800	1.97575900
H	2.55500800	0.75128500	1.35519800
O	4.40094900	-1.18563700	1.08223700
H	4.79229700	-0.30822900	1.13803000
C	4.57958700	0.38379200	-1.23056900
H	4.57800900	0.84909800	-2.21946000
H	5.47223600	-0.24061900	-1.15724700
H	4.66378500	1.19530400	-0.49922600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.051352

145) Conformer **17C5**

C	-3.35989100	-1.81354200	-0.93857700
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H	-3.64083700	-2.42149200	-0.07473200
H	-3.99228700	-2.14425300	-1.76457900
C	-3.70157000	-0.36096300	-0.62368600
H	-4.66711800	-0.33315700	-0.10335600
C	-2.64228300	0.29712200	0.31724900
C	-1.29791500	0.24014700	-0.40172100
C	-1.00745400	-1.25119500	-0.31430900
C	-1.88323600	-2.04710300	-1.26215700
H	-1.65103500	-1.72425600	-2.28037900
H	-1.65060000	-3.11348100	-1.19976800
C	-0.10106800	0.88570100	0.29085500
H	-0.22880700	0.86367000	1.37742100
C	1.11738500	-0.02250000	-0.04947100
C	0.49755000	-1.40224500	-0.45540300
C	2.04284300	0.46557600	-1.16894000
H	1.58510100	0.41079300	-2.15929900
H	2.31942700	1.51076500	-0.99414500
C	3.30302400	-0.40969200	-1.03731400
H	3.27330700	-1.20794200	-1.78493600
C	3.18577200	-1.06228200	0.37693500
C	2.65080400	-2.50394200	0.28415600
H	3.06041800	-2.98321600	-0.60959200
H	3.02757800	-3.07108600	1.14193200
C	1.12127300	-2.57155000	0.29393800
H	0.76653900	-2.55639200	1.32607300
H	0.78278900	-3.51958200	-0.13215800
C	-3.10577500	1.64282000	0.83182400
H	-4.04402900	1.53964500	1.38046600
H	-3.25786800	2.34454200	0.00895000
H	-2.37360500	2.08675400	1.50911000
C	-2.38892600	-0.70426300	1.43357700
O	-2.93022100	-0.78353100	2.50346500
O	-1.42974700	-1.56352500	1.05472400
O	-3.79774600	0.33999600	-1.84751400
H	-4.17498200	1.20911400	-1.68204000
H	-1.37267200	0.58247400	-1.43371200
H	0.67664000	-1.54405100	-1.52729000
C	0.10758300	2.32408300	-0.09984500
O	-0.27811100	2.83390900	-1.12313400
O	0.80334500	2.98205400	0.82808300
C	1.09934400	4.35023000	0.54103900
H	1.69290200	4.43015600	-0.37004100
H	1.66514900	4.71565200	1.39413200
H	0.17848900	4.92184100	0.42355300

C	2.13515800	-0.19766900	1.07532700
H	1.72698200	-0.65750800	1.97903600
H	2.56577500	0.77031100	1.34741800
O	4.45597400	-1.04717900	1.00595300
H	4.36949300	-1.49441900	1.85329200
C	4.57491100	0.38970700	-1.26275600
H	4.54774600	0.85210700	-2.25337700
H	5.46414900	-0.23941200	-1.20530000
H	4.67822700	1.18798100	-0.52360200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.050905

146) Conformer **17C6**

C	-3.37007500	-1.80272400	-0.93318000
H	-3.65287500	-2.40787400	-0.06799600
H	-4.00488300	-2.13187600	-1.75796200
C	-3.70468100	-0.34805300	-0.62036200
H	-4.66956100	-0.31487100	-0.09914200
C	-2.64136000	0.30658900	0.31850100
C	-1.29814500	0.24228700	-0.40199500
C	-1.01441100	-1.25019300	-0.31231900
C	-1.89487400	-2.04365300	-1.25792600
H	-1.66228800	-1.72364100	-2.27694700
H	-1.66707400	-3.11096900	-1.19386500
C	-0.09753900	0.88347700	0.28808600
H	-0.22447700	0.86401300	1.37478600
C	1.11650400	-0.03123500	-0.05119600
C	0.48953500	-1.40845300	-0.45508400
C	2.04403700	0.45328300	-1.17208400
H	1.58614600	0.39317200	-2.16200100
H	2.31677300	1.50039800	-1.00289500
C	3.30625300	-0.41782700	-1.03499300
H	3.29472700	-1.20925000	-1.78987700
C	3.17743300	-1.08393900	0.37947800
C	2.63934600	-2.51856200	0.27276900
H	3.03452100	-2.98625800	-0.63342600
H	3.03113900	-3.08579100	1.12102300
C	1.11097100	-2.57872400	0.29454600
H	0.76229300	-2.56022600	1.32868500
H	0.76637200	-3.52607200	-0.12797700
C	-3.09820100	1.65518200	0.83149800
H	-4.03655100	1.55710900	1.38089300
H	-3.24756800	2.35643600	0.00773300
H	-2.36360400	2.09665700	1.50776400

C	-2.39143000	-0.69427900	1.43607400
O	-2.93213500	-0.76947100	2.50654100
O	-1.43643100	-1.55834700	1.05762100
O	-3.79872800	0.35144900	-1.84518300
H	-4.17300300	1.22206900	-1.68091400
H	-1.37268600	0.58319700	-1.43445900
H	0.66686000	-1.55253300	-1.52699500
C	0.11710000	2.32038500	-0.10484300
O	-0.26994200	2.83148700	-1.12692700
O	0.82053600	2.97522800	0.81962800
C	1.12204000	4.34181700	0.53069600
H	1.71191800	4.41851000	-0.38305400
H	1.69330500	4.70480000	1.38118400
H	0.20351200	4.91789500	0.41700900
C	2.12954200	-0.21447600	1.07560900
H	1.72146800	-0.67620900	1.97711500
H	2.55670000	0.75475700	1.35453200
O	4.40461500	-1.18048400	1.07990000
H	4.79465300	-0.30249500	1.13574200
C	4.57826400	0.38902400	-1.23288900
H	4.57505000	0.85429700	-2.22178500
H	5.47172400	-0.23432700	-1.16051400
H	4.66223000	1.20061800	-0.50161600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.051489

147) Conformer **17C7**

C	-3.35814800	-1.82064000	-0.93076000
H	-3.62951700	-2.43079000	-0.06526700
H	-3.99345800	-2.16055700	-1.75149600
C	-3.70674900	-0.36591000	-0.61322900
H	-4.66059700	-0.34316500	-0.07895100
C	-2.64248400	0.30062500	0.31608600
C	-1.29634700	0.24211200	-0.40062900
C	-1.00366500	-1.24927400	-0.31098400
C	-1.87938100	-2.04951200	-1.25674900
H	-1.64045700	-1.73738400	-2.27815900
H	-1.64567300	-3.11530800	-1.19281400
C	-0.10018800	0.89018800	0.29207700
H	-0.23111200	0.87186700	1.37812000
C	1.11856000	-0.01734700	-0.04655900
C	0.50181300	-1.39918200	-0.45149700
C	2.04492900	0.47088300	-1.16503800
H	1.58547000	0.42631000	-2.15526000

H	2.33024000	1.51266400	-0.98340900
C	3.29499700	-0.41736900	-1.03655200
H	3.24584200	-1.22229500	-1.77640500
C	3.18135300	-1.05553700	0.39353800
C	2.65316800	-2.49973300	0.31038600
H	3.06869200	-2.98862400	-0.57638800
H	3.02350400	-3.04588500	1.18248900
C	1.12279300	-2.56798900	0.30250000
H	0.75902100	-2.55370800	1.33131900
H	0.78909200	-3.51598300	-0.12727800
C	-3.11584300	1.64712000	0.81541100
H	-4.02010100	1.53026200	1.41613000
H	-3.34125800	2.29995600	-0.02833300
H	-2.36397300	2.13341200	1.44022900
C	-2.38356100	-0.69561700	1.43596500
O	-2.92214500	-0.77309000	2.50677400
O	-1.42466900	-1.55712100	1.05747800
O	-3.91953300	0.41539600	-1.77183500
H	-3.24853400	0.20636900	-2.42833600
H	-1.34784200	0.59222400	-1.43283000
H	0.68279100	-1.54256500	-1.52283800
C	0.10690100	2.32705500	-0.10604100
O	-0.27260100	2.82702800	-1.13645600
O	0.79323700	2.99294500	0.82225300
C	1.08711700	4.36040700	0.52853500
H	1.68767800	4.43600500	-0.37828500
H	1.64486700	4.73307700	1.38373700
H	0.16520500	4.92784800	0.40003500
C	2.13245100	-0.19119800	1.08093800
H	1.72427000	-0.65080100	1.98368900
H	2.56209900	0.77711500	1.35379100
O	4.38729700	-1.00705000	1.13521800
H	5.00485800	-1.64007200	0.75558100
C	4.57635700	0.36037500	-1.27685600
H	4.54960800	0.82309000	-2.26729900
H	5.46034900	-0.27981400	-1.23486200
H	4.70180200	1.15513500	-0.53762000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.049766

148) Conformer **17C8**

C	-3.19383700	-1.80072900	-1.21047300
H	-3.43975000	-2.57892700	-0.48188600
H	-3.80605700	-2.01360400	-2.09077300

C	-3.61641900	-0.45131800	-0.62692200
H	-4.58494300	-0.57436500	-0.12514400
C	-2.60702900	0.07232700	0.42706700
C	-1.25724600	0.23185400	-0.27060300
C	-0.87996100	-1.23078400	-0.46627300
C	-1.70713800	-1.87973200	-1.55928500
H	-1.49806000	-1.35063700	-2.49269400
H	-1.40860200	-2.92141800	-1.70347900
C	-0.10277000	0.78732500	0.56296000
H	-0.23576500	0.51154500	1.61343300
C	1.16760900	0.04314800	0.05679700
C	0.63110400	-1.26415600	-0.61700500
C	2.05812000	0.79994900	-0.93612500
H	1.60572400	0.90212700	-1.92507200
H	2.25687100	1.80980400	-0.56155700
C	3.37903000	0.00784800	-0.95488400
H	3.42670000	-0.61460100	-1.85299400
C	3.29443200	-0.93485800	0.29570500
C	2.85001400	-2.35120900	-0.10103400
H	3.26949100	-2.60039900	-1.07987500
H	3.28338600	-3.05034300	0.61868400
C	1.32916400	-2.51558500	-0.10406900
H	0.98406100	-2.72219000	0.91069800
H	1.04657500	-3.38278800	-0.70645600
C	-3.15231300	1.26698300	1.17921600
H	-4.06028600	0.99153400	1.71939600
H	-3.39321400	2.07059200	0.48297000
H	-2.43352500	1.64315700	1.91008500
C	-2.29313800	-1.11015000	1.33602200
O	-2.82730800	-1.42124000	2.36578400
O	-1.28341600	-1.82252100	0.81287400
O	-3.71737900	0.55516600	-1.61884900
H	-4.40088400	0.29074300	-2.24160900
H	-1.34545100	0.75446600	-1.22118500
H	0.81747900	-1.18335300	-1.69405500
C	0.06960000	2.28213700	0.57723800
O	0.59287900	2.88525000	1.48422500
O	-0.38373500	2.87458500	-0.52470500
C	-0.21012900	4.29077500	-0.59464300
H	0.84902500	4.54722400	-0.55981200
H	-0.72710300	4.77847800	0.23192900
H	-0.64242200	4.59492600	-1.54440600
C	2.19273400	-0.28985200	1.13712700
H	1.81820300	-0.94462900	1.92665900

H	2.55382000	0.63285300	1.60443000
O	4.52578600	-1.09148100	0.97779100
H	4.86065900	-0.21926300	1.20860000
C	4.59039600	0.92479700	-0.96394100
H	4.55544000	1.58121500	-1.83703800
H	5.52619800	0.36380500	-1.00595900
H	4.61446600	1.57336100	-0.08110600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.049827

149) Conformer **17C9**

C	-3.37586400	-1.80133600	-0.92341400
H	-3.64671000	-2.41096500	-0.05739400
H	-4.01748300	-2.13606700	-1.74136300
C	-3.71345400	-0.34487100	-0.60213900
H	-4.66446600	-0.31667400	-0.06307600
C	-2.64030200	0.31351700	0.32274300
C	-1.29811000	0.24750700	-0.40072900
C	-1.01477300	-1.24571200	-0.31494600
C	-1.90027000	-2.03913600	-1.25724400
H	-1.66455900	-1.72736100	-2.27952000
H	-1.67293700	-3.10645000	-1.19576600
C	-0.09484200	0.88670600	0.28804100
H	-0.22322300	0.87023600	1.37437000
C	1.11735900	-0.03091400	-0.05147600
C	0.48851100	-1.40479600	-0.46341800
C	2.05061600	0.45699100	-1.16633200
H	1.59699500	0.40333100	-2.15856200
H	2.32468500	1.50261500	-0.99041600
C	3.31063000	-0.41685400	-1.02876800
H	3.30024200	-1.20477600	-1.78731900
C	3.17528200	-1.08936200	0.38188600
C	2.63616500	-2.52260300	0.26487200
H	3.03575200	-2.98609600	-0.64149700
H	3.02253200	-3.09481100	1.11224100
C	1.10765700	-2.58127400	0.27886000
H	0.75478100	-2.57060000	1.31161300
H	0.76410800	-3.52501000	-0.15244000
C	-3.10258800	1.66238900	0.82602400
H	-4.00440900	1.55060100	1.43134300
H	-3.32833500	2.31748400	-0.01589500
H	-2.34445000	2.14339300	1.44736200
C	-2.38186600	-0.68589700	1.43998500
O	-2.91533000	-0.76131500	2.51350100

O	-1.43031300	-1.55287300	1.05541000
O	-3.92682200	0.43945800	-1.75860900
H	-3.26114600	0.22613000	-2.41913100
H	-1.35224700	0.59983500	-1.43202100
H	0.66353800	-1.54203800	-1.53665200
C	0.12088100	2.32198300	-0.11095700
O	-0.25817800	2.82461400	-1.14017400
O	0.81483200	2.98317800	0.81525400
C	1.11662900	4.34881800	0.52072500
H	1.71494900	4.42066200	-0.38788200
H	1.67920200	4.71788600	1.37433100
H	0.19800300	4.92212500	0.39495200
C	2.12548900	-0.22212200	1.07845000
H	1.71285900	-0.68821300	1.97561000
H	2.55301600	0.74485000	1.36456100
O	4.39914200	-1.19091000	1.08711000
H	4.79083400	-0.31398800	1.14809600
C	4.58475900	0.38845700	-1.21880000
H	4.58594600	0.85763100	-2.20585300
H	5.47677500	-0.23686400	-1.14574900
H	4.66764300	1.19697300	-0.48404800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.049940

150) Conformer **17C10**

C	-3.18784600	-1.79869600	-1.22836900
H	-3.43530100	-2.57986000	-0.50498000
H	-3.79530200	-1.99710300	-2.11332900
C	-3.61867300	-0.45909800	-0.64038600
H	-4.58559700	-0.59153800	-0.13926000
C	-2.60468100	0.06305700	0.42675500
C	-1.25666300	0.22784000	-0.26834900
C	-0.87606700	-1.23343400	-0.46785000
C	-1.69834500	-1.87748800	-1.56705700
H	-1.48141700	-1.34827900	-2.49859400
H	-1.40185100	-2.91991500	-1.71046500
C	-0.10286600	0.78602000	0.56442100
H	-0.23484300	0.50927400	1.61476000
C	1.16902000	0.04475300	0.05823600
C	0.63560500	-1.26420400	-0.61479900
C	2.05747300	0.80262600	-0.93563500
H	1.60435600	0.90324000	-1.92442100
H	2.25484200	1.81304000	-0.56183400
C	3.37952300	0.01235600	-0.95454800

H	3.42705100	-0.61141200	-1.85174100
C	3.29766200	-0.92868400	0.29765300
C	2.85567500	-2.34658100	-0.09632100
H	3.27535800	-2.59686600	-1.07479400
H	3.29045400	-3.04350400	0.62469200
C	1.33507600	-2.51354500	-0.09884600
H	0.99009800	-2.71846700	0.91631100
H	1.05386700	-3.38246500	-0.69939800
C	-3.14972200	1.25311900	1.18675200
H	-4.08348800	0.99193100	1.68856100
H	-3.33925700	2.09278000	0.51425700
H	-2.44854400	1.59626000	1.95006200
C	-2.29584700	-1.12162700	1.32981000
O	-2.83714500	-1.44114400	2.35377100
O	-1.28386000	-1.83183300	0.80642000
O	-3.75400600	0.46280700	-1.70370300
H	-4.19226000	1.25439000	-1.37752700
H	-1.34942600	0.75159200	-1.21854000
H	0.82459700	-1.18461400	-1.69143400
C	0.06684900	2.28113300	0.57905200
O	0.59364900	2.88459500	1.48366900
O	-0.39385900	2.87368300	-0.52003400
C	-0.22175500	4.29008000	-0.59050800
H	-0.65898600	4.59411300	-1.53805600
H	0.83735500	4.54730800	-0.56103600
H	-0.73479900	4.77726400	0.23882200
C	2.19512200	-0.28475900	1.13866000
H	1.82222400	-0.93923300	1.92922100
H	2.55440800	0.63935300	1.60454700
O	4.52975100	-1.08176600	0.97913000
H	4.86249000	-0.20857200	1.20934400
C	4.58962500	0.93091900	-0.96631700
H	4.55300800	1.58576200	-1.84052600
H	5.52611100	0.37106700	-1.00816200
H	4.61362900	1.58101700	-0.08461400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1229.050036

151) Conformer **18C1**

C	-1.90564900	-1.09438600	1.35593000
C	-3.60537100	-0.56864700	-0.32457000
H	-4.04710100	-1.39940600	0.24269200
C	-2.50521000	0.07465700	0.58252000
C	-1.31862400	0.46375600	-0.29948200

C	-0.77766700	-0.92815700	-0.63419100
C	-1.63928700	-1.64774000	-1.65867000
H	-1.20749100	-1.54173900	-2.65701100
H	-1.63470200	-2.71404200	-1.42210600
C	-3.05983500	-1.07128000	-1.67011000
H	-3.76168900	-1.79595900	-2.09208400
H	-3.07789400	-0.20446500	-2.33649400
C	-0.14202900	1.23011600	0.33573900
H	-0.27365400	1.36512500	1.40986300
C	1.14008200	0.36124400	0.09552000
C	0.68109100	-0.68728600	-0.93855100
C	1.67985600	-0.26091900	1.39521800
H	1.12135700	-1.11082300	1.78598600
H	1.70645100	0.50129200	2.18297400
C	3.11468700	-0.63114000	1.08664400
C	3.43794300	-0.12660000	-0.31401500
C	3.06883400	-1.28564200	-1.26996000
H	3.16039600	-0.90359700	-2.29332500
H	3.80746100	-2.08355100	-1.15635200
C	1.65808300	-1.84048600	-1.05190100
H	1.62350000	-2.45397700	-0.14670600
H	1.38833400	-2.50012600	-1.88118400
O	-0.91998400	-1.64572100	0.62727300
O	-4.60146600	0.40811800	-0.55902900
H	-5.30369300	-0.00069500	-1.07296800
C	-3.07386400	1.12261200	1.51621200
H	-3.87837300	0.69639300	2.11658300
H	-3.47639000	1.96309900	0.95304400
H	-2.30851700	1.48728200	2.20330100
H	-1.63294600	0.98894500	-1.20194600
C	0.01714900	2.59928800	-0.26983500
C	2.41517200	1.01064900	-0.45886200
H	2.72606700	1.86601500	0.15082300
H	2.30493300	1.35003100	-1.49192200
H	0.66308200	-0.16593000	-1.90628700
C	4.88377700	0.28352600	-0.48624500
H	5.54927500	-0.54048400	-0.22166800
H	5.13032800	1.13316800	0.15516500
H	5.08417200	0.56957000	-1.52199800
O	3.86546300	-1.22376600	1.81709300
O	0.52228000	3.47653700	0.60818000
H	0.63899800	4.31780000	0.14222000
O	-0.23329700	2.89578900	-1.40942100
O	-2.22258800	-1.51662000	2.42978500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.622735

152) Conformer **18C2**

C	-1.90610000	-1.07935700	1.36559900
C	-3.61212900	-0.58169700	-0.32888000
H	-4.03720100	-1.41425800	0.23948100
C	-2.50447400	0.07917100	0.58183700
C	-1.31587300	0.46264100	-0.29840200
C	-0.77796900	-0.93195800	-0.62517800
C	-1.64002500	-1.65472300	-1.64802500
H	-1.20321800	-1.55979700	-2.64532500
H	-1.64285500	-2.71907800	-1.40281000
C	-3.05958900	-1.07814500	-1.67042300
H	-3.76526000	-1.79283200	-2.09775000
H	-3.06227600	-0.21657900	-2.34873800
C	-0.13969400	1.23013700	0.33455200
H	-0.26978400	1.36232000	1.40950500
C	1.14304100	0.36118000	0.09362600
C	0.68069400	-0.69390100	-0.93258500
C	1.68732800	-0.25360800	1.39485100
H	1.12974000	-1.10135200	1.79170700
H	1.71658100	0.51275000	2.17843700
C	3.12112900	-0.62544200	1.08322100
C	3.43900200	-0.13017800	-0.32214500
C	3.06634900	-1.29579500	-1.26850600
H	3.15425500	-0.92130100	-2.29499100
H	3.80518500	-2.09301900	-1.15185300
C	1.65636700	-1.84856600	-1.04108800
H	1.62459900	-2.45563000	-0.13152300
H	1.38291200	-2.51383500	-1.86461900
O	-0.92199800	-1.64079800	0.63962200
O	-4.70759800	0.27288700	-0.55584200
H	-4.46059400	0.92526800	-1.21900200
C	-3.08471000	1.13293200	1.49929400
H	-3.89547000	0.71130100	2.09420300
H	-3.48585100	1.97041600	0.92863900
H	-2.32890900	1.51033300	2.19023400
H	-1.61839600	0.98511900	-1.20753500
C	0.01259000	2.60326800	-0.26386100
C	2.41601800	1.00679800	-0.46978700
H	2.72998100	1.86538000	0.13330600
H	2.30199400	1.33991300	-1.50471200
H	0.66172000	-0.17941300	-1.90408700

C	4.88422600	0.27857700	-0.50246800
H	5.55041400	-0.54384000	-0.23475100
H	5.13337100	1.13240600	0.13232000
H	5.08100200	0.55741400	-1.54087200
O	3.87487900	-1.21281300	1.81465100
O	0.57426300	3.46099900	0.59797600
H	0.68370500	4.30616200	0.13734900
O	-0.29250100	2.91956300	-1.38517400
O	-2.22488700	-1.49432100	2.44171700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.622839

153) Conformer **18C3**

C	-1.90625000	-1.09445600	1.35029800
C	-3.60849000	-0.57487000	-0.33793800
H	-4.04913100	-1.40569600	0.22873900
C	-2.50072000	0.07302300	0.57920200
C	-1.31650300	0.46730100	-0.30018600
C	-0.77676400	-0.92399700	-0.63777600
C	-1.63833000	-1.63760200	-1.66586400
H	-1.20608200	-1.52335400	-2.66304500
H	-1.62943800	-2.70569900	-1.43701700
C	-3.06157700	-1.07103400	-1.67784800
H	-3.76372100	-1.79356500	-2.09748700
H	-3.09020900	-0.20391900	-2.34341700
C	-0.13938200	1.23310700	0.33607000
H	-0.27099800	1.36785400	1.41034500
C	1.14167200	0.36210600	0.09712600
C	0.68274500	-0.68421800	-0.93909000
C	1.67777600	-0.26281800	1.39696600
H	1.11746300	-1.11281300	1.78494300
H	1.70409900	0.49791900	2.18615500
C	3.11278700	-0.63469300	1.09066000
C	3.43949900	-0.12886200	-0.30863000
C	3.07024600	-1.28577600	-1.26712900
H	3.16435000	-0.90216900	-2.28964900
H	3.80731300	-2.08509900	-1.15343400
C	1.65820600	-1.83867000	-1.05266200
H	1.62093800	-2.45379800	-0.14868900
H	1.38881300	-2.49622800	-1.88365600
O	-0.92199800	-1.64661200	0.62185400
O	-4.62307200	0.34529600	-0.67781700
H	-5.18333400	0.49160200	0.08916100
C	-3.07914100	1.11968700	1.50610600

H	-3.86594800	0.68661000	2.12876400
H	-3.49345200	1.95245900	0.93725400
H	-2.32021200	1.50902500	2.18620300
H	-1.63202700	0.99271400	-1.20244900
C	0.02276700	2.60195900	-0.26907200
C	2.41886900	1.01030200	-0.45380800
H	2.73007600	1.86431200	0.15765900
H	2.31112400	1.35116500	-1.48661400
H	0.66680500	-0.16141900	-1.90602500
C	4.88633100	0.27915500	-0.47752100
H	5.54993800	-0.54645700	-0.21322700
H	5.13316400	1.12726800	0.16580500
H	5.08902100	0.56661500	-1.51242100
O	3.86112800	-1.22904600	1.82217500
O	0.52484700	3.47946000	0.61091600
H	0.64530800	4.32000800	0.14456700
O	-0.22376200	2.89849900	-1.40935500
O	-2.23292900	-1.52199700	2.42024100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.624284

154) Conformer **18C4**

C	-1.90018600	-1.16751700	1.30222400
C	-3.59936700	-0.57003100	-0.36354600
H	-4.04526600	-1.42402300	0.16290300
C	-2.49768000	0.03468400	0.58869000
C	-1.31351800	0.47848000	-0.26716700
C	-0.76269700	-0.89275200	-0.66934300
C	-1.61744200	-1.56257200	-1.73216300
H	-1.18398900	-1.39864800	-2.72191400
H	-1.60069100	-2.64011400	-1.55395900
C	-3.04540300	-1.00741900	-1.72154300
H	-3.74113300	-1.71721500	-2.17235100
H	-3.08077200	-0.11410500	-2.35131900
C	-0.13941000	1.21568600	0.41896200
H	-0.28196500	1.27211400	1.49804400
C	1.14555900	0.36741000	0.13093900
C	0.69629400	-0.63066800	-0.95502800
C	1.68372000	-0.31594700	1.40133700
H	1.12754000	-1.18608600	1.74847000
H	1.70363300	0.40781000	2.22473900
C	3.12139900	-0.66387000	1.08239800
C	3.44851700	-0.08660100	-0.28841100
C	3.08916900	-1.19871000	-1.30272900

H	3.18390500	-0.76594700	-2.30541500
H	3.83133300	-1.99763600	-1.22527100
C	1.68021800	-1.77176400	-1.12039400
H	1.64462900	-2.42963700	-0.24700200
H	1.41893300	-2.39101900	-1.98282800
O	-0.90669000	-1.67451700	0.55335200
O	-4.60988300	0.36668600	-0.66951900
H	-5.17440600	0.48113300	0.09983600
C	-3.08314800	1.03040600	1.56614400
H	-3.86799400	0.56136800	2.16468500
H	-3.50144300	1.88900900	1.04026500
H	-2.32750600	1.39078400	2.26530100
H	-1.64047200	1.03507800	-1.14484500
C	0.02759900	2.64472000	-0.01991800
C	2.41992600	1.05070900	-0.38249600
H	2.72052100	1.87886900	0.26919200
H	2.31477900	1.43758200	-1.39878600
H	0.68028400	-0.06298400	-1.89642600
C	4.89288400	0.33849000	-0.43373900
H	5.56116500	-0.49389600	-0.20491800
H	5.13166900	1.15812100	0.24824600
H	5.09704900	0.67408800	-1.45383100
O	3.87088000	-1.29117200	1.78461000
O	-0.09152300	2.80696200	-1.34799500
H	0.06486700	3.74387500	-1.53573600
O	0.28008800	3.56122200	0.71758600
O	-2.23203100	-1.65229600	2.34542000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.622399

155) Conformer **19C1**

C	-0.22496600	0.34410700	1.14812300
C	0.56078300	-0.84942800	0.59359000
C	-0.17749600	-1.40918700	-0.65209000
H	-1.87312400	-0.61849300	2.11597100
H	-2.18905500	1.03482300	1.64524800
H	-2.76496600	-1.38744100	0.11467600
H	-3.15557200	0.26889700	-0.31979900
H	0.79204200	-1.62774800	1.31857000
H	-1.69405700	-0.74204900	-2.03878400
H	-0.02560600	1.08379500	-2.09293800
H	0.02237000	2.38404600	0.32213700
O	2.93231200	-0.61407100	0.01276000
H	0.21845000	0.68043700	2.08890700

H	-0.63942200	-2.36672400	-0.40120300
H	0.53217100	-1.60530000	-1.46090900
H	-1.49499900	1.70855500	-1.35713800
C	-1.71771400	0.10577900	1.31300400
C	-2.33961900	-0.38788200	-0.00759100
O	1.53139500	1.10417400	-0.19244800
C	1.82226700	-0.16659400	0.13022900
C	-1.26149000	-0.41995300	-1.08858000
C	-0.68153700	0.99048000	-1.22346900
C	0.11345700	1.33707500	0.03724700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -500.108043

156) Conformer **20aC1**

C	-0.22125800	1.42041700	-0.11023300
C	0.23814200	0.02690900	-0.56614600
C	-1.64464200	1.58242200	-0.69328000
C	-2.49665100	0.52765200	0.06264600
C	-1.51048600	-0.00600300	1.11987000
C	-0.71988000	-0.93196800	0.16725900
C	-0.55596800	1.15768400	1.36024200
C	0.67811200	2.58651500	-0.43808200
I	2.29628400	-0.43269800	-0.06976600
O	-1.68351100	-1.48554200	-0.74422800
C	-2.75199300	-0.66327500	-0.81583000
O	-3.69589200	-0.91575300	-1.51154300
C	-2.12675800	-0.68869000	2.31617600
H	0.21173900	-0.11472100	-1.64478400
H	-2.00812800	2.58395400	-0.45592000
H	-1.67628300	1.47137600	-1.77975500
H	-3.42810500	0.93406500	0.45180800
H	-0.22533400	-1.77165900	0.64962600
H	0.31635400	0.87633800	1.95552000
H	-1.04803200	2.00913300	1.83636800
H	0.83792400	2.67007500	-1.51640500
H	0.22465300	3.51831900	-0.09171400
H	1.65373900	2.48527500	0.04076600
H	-2.77040400	-1.52030100	2.01700800
H	-1.35256200	-1.08433600	2.97760100
H	-2.73509600	0.01587100	2.88791200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -836.501668

157) Conformer **20bC1**

C	1.58015900	-0.28444300	-0.04938000
C	0.96733300	-0.36098100	1.35830200
C	0.63364700	-1.00853300	-1.01997200
C	-0.66112300	-0.14786000	-0.98473100
C	-0.23343400	1.08961500	-0.16751200
C	-0.34092200	0.42916400	1.22496000
C	1.27145600	1.17588500	-0.39647100
C	3.01947400	-0.73080900	-0.13709900
O	-1.49282600	-0.44111800	1.15717400
C	-1.70558700	-0.79619900	-0.12088800
O	-2.60179300	-1.53481200	-0.43315800
C	-1.06664300	2.33149900	-0.36896100
H	1.63051200	0.12822700	2.07655900
H	0.78985100	-1.38072500	1.70796700
H	0.46264800	-2.05332000	-0.74822300
H	1.05241100	-0.99565800	-2.02886600
H	-1.05640600	0.06243100	-1.97724400
H	-0.52892500	1.11937900	2.04606000
H	1.52330800	1.43412400	-1.42887200
H	1.76139200	1.88633800	0.27569100
H	3.40890400	-0.60223300	-1.15079200
H	3.65072900	-0.15394900	0.54423600
H	3.12085200	-1.78702500	0.12803900
H	-0.72766600	3.13627200	0.28805900
H	-0.99414900	2.68328300	-1.40098400
H	-2.12267800	2.14626200	-0.15325200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -539.366038

158) Conformer **21aC1**

C	0.38018300	1.32708800	-0.64535400
C	-0.09535900	-0.11129200	-0.45542400
C	1.84823300	1.25326600	-1.09849900
C	2.58117700	0.66771100	0.14728800
C	1.47038600	0.66849800	1.20790600
C	0.74793700	-0.60755700	0.74012000
C	0.54026500	1.80128500	0.79965200
I	-2.21321300	-0.22663500	-0.05394300
H	0.02982400	-0.74615800	-1.32947500
O	1.77697000	-1.50408800	0.28704300
C	2.87215300	-0.79280000	-0.05535400
O	3.86564400	-1.32513500	-0.46508100
H	1.81287800	0.63443300	2.24033600
H	-0.24735700	1.92957400	-1.29917300

H	1.99390200	0.65681300	-2.00126400
H	2.21889400	2.25873600	-1.30286700
H	3.48642400	1.21413700	0.40008300
H	0.17901200	-1.13541600	1.50051400
H	1.01234600	2.78237400	0.87347700
H	-0.39638600	1.81377400	1.35965700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -757.991133

159) Conformer **21bC1**

C	1.59553700	-0.39493800	-0.70786100
C	1.08432100	1.02818400	-0.95756000
C	0.41115700	-1.36641600	-0.74143100
H	-0.15043600	-1.33038500	-1.67757700
H	0.75205200	-2.39351300	-0.59965500
C	-0.43938200	-0.92689100	0.49154800
H	-0.76567400	-1.76760100	1.09971100
C	0.48098000	0.09148400	1.18314100
C	0.18290200	1.28754200	0.26297500
H	0.31528200	2.27007200	0.71064500
C	1.89009200	-0.33359500	0.79309200
H	2.64819700	0.40861400	1.05392200
H	2.17334500	-1.29800500	1.22039500
H	0.53288800	1.14846600	-1.89224400
H	1.91726600	1.73461700	-0.96541400
O	-1.21949900	1.18124200	-0.07380400
C	-1.61278700	-0.09688000	0.05214600
O	-2.73981100	-0.44035900	-0.18794300
H	0.27014800	0.26230600	2.23773200
H	2.42449800	-0.69257900	-1.34983300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -460.853918

160) Conformer **22aC1**

H	-1.27161400	2.24387700	-2.16312800
H	-2.66822700	2.64082400	-1.15208700
H	-2.69181800	1.19206600	-2.16193900
H	0.36597300	2.16547900	0.07185300
H	-1.01535500	2.55510600	1.12013200
H	-0.14929100	-0.15688200	-1.75913900
H	-3.39637800	0.84232800	0.70995100
O	-3.64082300	-1.73616600	-0.08507300
H	-1.68765900	-0.91741200	2.22210900
H	-2.00893500	0.76786500	2.62209100

H	0.45414600	0.67605500	2.28175400
I	2.34915300	-0.17998700	-0.11230000
C	-2.05596300	1.81978200	-1.53196100
C	-2.69942100	-0.99603000	-0.15313100
O	-1.62410900	-1.28604000	-0.91640200
H	0.24140700	-1.51081000	0.73129400
C	-0.51537700	1.75550700	0.56970700
C	-0.66027800	-0.22556600	-0.80161200
C	-1.45743300	1.03488900	-0.39073200
C	-2.45932000	0.31677300	0.53714200
C	-1.63537000	0.10436400	1.84078500
C	0.27259700	-0.47507900	0.40088000
C	-0.21575700	0.53511000	1.43572800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -797.246994

161) Conformer **22bC1**

C	-1.50816100	-1.15600400	-0.21031600
C	-0.99571700	-1.07285700	1.23123800
H	-0.38753300	-1.92525000	1.54085200
H	-1.83342200	-0.98807200	1.92700800
C	-0.31526400	-1.31288800	-1.15836000
H	0.30396500	-2.18447700	-0.93441800
H	-0.65548900	-1.40631700	-2.19124600
C	0.44790000	0.03478100	-0.98472700
H	0.74229600	0.47925800	-1.93405800
C	-0.52222000	0.87985900	-0.13154900
C	-0.17977200	0.22946000	1.22770400
H	-0.35209500	0.86407200	2.09565800
C	-1.89649700	0.30045100	-0.45937300
H	-2.67690500	0.66248900	0.21521000
H	-2.19695700	0.50258400	-1.49055300
O	1.24260100	-0.02674400	1.19088700
C	1.63952300	-0.14403400	-0.08706500
O	2.78376500	-0.37351400	-0.37712100
C	-0.33574500	2.37531700	-0.20848900
H	0.68104800	2.66867800	0.06713200
H	-1.02585300	2.88687900	0.46703600
H	-0.52370500	2.73674500	-1.22245800
H	-2.29056600	-1.89903900	-0.36467100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -500.109857

162) Conformer **23aC1**

C	0.24138100	-0.58609500	0.23410700
C	-0.22701900	0.11643400	1.51692800
C	-1.68809900	-0.29281100	1.78378000
C	-2.46108900	0.33732800	0.58969600
C	-1.38625500	1.21285700	-0.08795700
C	-0.66994900	0.06822900	-0.84404200
C	-0.43444200	1.55570800	1.05328700
I	2.31565300	0.02219200	-0.17989900
C	0.26075700	-2.09804900	0.25178600
O	-1.70877900	-0.83230400	-1.26423500
C	-2.77638900	-0.69938400	-0.44994700
H	-3.36301100	0.86149900	0.89984300
O	-3.76814900	-1.35745900	-0.60009800
C	-1.89826700	2.33560900	-0.95613000
H	-2.01800900	0.17202500	2.71386000
H	0.47765600	2.05038400	0.71794200
H	-1.84606600	-1.36651500	1.88673000
H	-0.13964800	0.36691700	-1.74493700
H	-0.91409400	2.17625600	1.81328400
H	0.42863800	-0.04230700	2.37190300
H	0.92327900	-2.46012200	1.03883500
H	-0.73742100	-2.49837800	0.44053400
H	0.60120600	-2.50147800	-0.70216800
H	-2.55970300	1.96532000	-1.74397300
H	-2.46113700	3.05581000	-0.35789700
H	-1.06966400	2.86357000	-1.43368400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -836.496460

163) Conformer **23bC1**

C	1.59799500	0.07694100	-0.56678000
C	1.40892900	0.78015200	0.78939000
C	0.46255800	-0.02829700	1.68246100
C	-0.88952100	0.04241400	0.91279300
C	-0.60092700	1.06353500	-0.20888300
C	0.16340700	0.09772000	-1.14169400
C	0.50380500	1.93901800	0.37874900
C	2.28709900	-1.27271900	-0.55889200
O	-0.50812800	-1.17547100	-1.01772200
C	-1.13702900	-1.23701200	0.16690000
O	-1.76154600	-2.20796200	0.50414200
C	-1.80960100	1.73797900	-0.81005400
H	2.18852200	0.75463100	-1.19275000
H	2.34750400	1.04752400	1.27664900

H	0.35306100	0.45773400	2.65348700
H	0.79372600	-1.05175500	1.86906800
H	-1.73242000	0.28459200	1.55808000
H	0.12654100	0.35311800	-2.20017900
H	0.14995800	2.53877300	1.22117000
H	0.95761000	2.60182600	-0.36269800
H	2.36312800	-1.67894000	-1.57044000
H	3.29969900	-1.17535800	-0.16068700
H	1.75837700	-2.00885600	0.04944700
H	-2.33199900	2.33632200	-0.05945800
H	-1.51648900	2.40085700	-1.62794700
H	-2.52011400	1.00861400	-1.20905100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -539.361229

164) Conformer **24C1**

C	-4.54341700	1.91859300	-0.17658600
H	-4.90675500	2.00109200	0.85249200
H	-4.92727800	2.79826500	-0.70627300
C	-5.12343300	0.67034700	-0.81062800
H	-4.80156300	0.64341400	-1.86445000
C	-4.61290500	-0.62832500	-0.16604200
C	-3.05914600	-0.56407700	-0.18589200
C	-2.38590400	0.69032900	0.43625200
C	-3.02302800	1.92683500	-0.22826100
H	-2.70421100	1.96749400	-1.27787500
H	-2.66034000	2.84339900	0.24429300
C	-2.37046700	-1.83554200	0.29454800
H	-2.87566400	-2.71667600	-0.10727300
H	-2.43048900	-1.92604300	1.38336000
C	-0.92226000	-1.86279400	-0.17474900
H	-0.93958900	-1.88028400	-1.26806400
H	-0.44924800	-2.79608600	0.14645400
C	-0.08835900	-0.66714600	0.31357200
C	-0.87654900	0.64667200	0.01044100
C	1.30727200	-0.61829500	-0.45275500
C	2.07710700	0.66248700	-0.01467300
C	1.27391100	1.93108000	-0.25690100
H	1.83894000	2.79964400	0.09769300
H	1.13001300	2.07690500	-1.33449000
C	-0.07799700	1.87760100	0.43916700
H	-0.63221300	2.78943800	0.20707800
H	0.07908800	1.88189300	1.52273300
C	2.18020100	-1.84197200	-0.09465100

H	2.33227700	-1.87992600	0.98630300
H	1.65708500	-2.76154800	-0.37008000
C	3.56306100	-1.84324800	-0.75148000
H	3.48623700	-1.96845300	-1.83517300
H	4.14428800	-2.69147100	-0.37712200
C	4.28055500	-0.55300300	-0.45372400
C	3.45254400	0.72426000	-0.65962500
C	-5.07866100	-1.78860300	-1.05616900
H	-4.57296500	-1.76993500	-2.02693300
H	-6.15358800	-1.71102500	-1.22991800
H	-4.88932100	-2.75888600	-0.59287200
H	-2.81820100	-0.48709800	-1.25895800
H	-0.93935100	0.70021100	-1.08325100
C	1.11001000	-0.63316100	-1.97830500
H	0.79881400	-1.62192200	-2.32070300
H	2.03901600	-0.40596000	-2.50199000
H	0.36988000	0.08611600	-2.32792600
O	-6.54838700	0.68171000	-0.76236800
H	-6.84702200	1.48561500	-1.19717300
C	-5.21839000	-0.84043900	1.22293100
H	-5.08302300	0.01312000	1.88579400
H	-4.77011300	-1.71301800	1.70456300
H	-6.29104100	-1.02371100	1.13481100
C	-2.57662500	0.82348900	1.95685300
H	-3.48918000	1.37171600	2.19453700
H	-1.75249800	1.38081700	2.40549400
H	-2.64527600	-0.13521000	2.47073600
C	0.14360700	-0.85928800	1.82002400
H	-0.79815900	-0.87142500	2.36202500
H	0.75722900	-0.07823600	2.26998000
H	0.62781300	-1.81696800	2.01734800
C	5.57907600	-0.19250500	-1.22031000
H	6.43479200	-0.78838100	-0.89829800
H	5.41983800	-0.38269200	-2.28375700
C	5.74383200	1.32173100	-0.92617800
H	5.70327500	1.92419900	-1.83504300
H	6.67161900	1.55846600	-0.40408900
C	4.53134200	1.60821300	-0.03985500
H	4.31110700	2.65172500	0.16820200
H	2.23361400	0.57856400	1.06763200
C	4.67407900	-0.37361600	1.00467100
O	4.90275800	-1.19748000	1.85138100
O	4.79754700	0.94974200	1.23518000
H	3.37009600	0.96333900	-1.72341800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1278.194737

165) Conformer **24C2**

C	-4.54084400	1.92724800	-0.18518500
H	-4.92652900	2.80037900	-0.71995000
H	-4.90465100	2.01466700	0.84351400
C	-5.12374400	0.68297200	-0.81351500
H	-4.80213400	0.65250000	-1.86710600
C	-4.61472000	-0.62107100	-0.16066100
C	-3.06024900	-0.56328400	-0.18403200
C	-2.38550800	0.69263300	0.43377600
C	-3.02109800	1.92829900	-0.23328900
H	-2.65743000	2.84431300	0.23950500
H	-2.69987700	1.96784100	-1.28219400
C	-2.37085700	-1.83291600	0.30183200
H	-2.43094900	-1.91767200	1.39107400
H	-2.87375800	-2.71755700	-0.09476400
C	-0.92266700	-1.86267900	-0.16736200
H	-0.94004500	-1.88439100	-1.26059900
H	-0.45061500	-2.79519300	0.15744500
C	-0.08817500	-0.66587700	0.31638700
C	-0.87621600	0.64652500	0.00761200
C	1.30746000	-0.62104200	-0.45002200
C	2.07755200	0.66162500	-0.01805400
C	1.27449000	1.92911700	-0.26625900
H	1.83966900	2.79932500	0.08401100
H	1.13035600	2.06977100	-1.34450100
C	-0.07729700	1.87930700	0.43036800
H	0.08000900	1.88870800	1.51387400
H	-0.63112500	2.79020300	0.19393800
C	2.18004200	-1.84321400	-0.08594600
H	2.33214000	-1.87590800	0.99517000
H	1.65671100	-2.76402000	-0.35686000
C	3.56291000	-1.84798700	-0.74269700
H	3.48614400	-1.97838900	-1.82578600
H	4.14388100	-2.69452900	-0.36416400
C	4.28066400	-0.55649000	-0.45111900
C	3.45297100	0.71995100	-0.66337400
C	-5.07838500	-1.78712500	-1.04440700
H	-6.16438400	-1.77127100	-1.18128700
H	-4.84832900	-2.75472300	-0.59536400
H	-4.61115000	-1.74889200	-2.03322900
H	-2.82022000	-0.49016000	-1.25772000

H	-0.93941800	0.69516900	-1.08631000
C	1.11020800	-0.64320000	-1.97548100
H	0.79926600	-1.63366500	-2.31317900
H	2.03916700	-0.41829700	-2.50022800
H	0.36991800	0.07425500	-2.32852000
O	-6.54089900	0.82222700	-0.76707600
H	-6.93345100	0.09422600	-1.25681600
C	-5.22055800	-0.82674200	1.22810100
H	-4.78026600	-1.70212500	1.71194400
H	-6.29553700	-1.00193800	1.14424900
H	-5.07863000	0.02748300	1.88839600
C	-2.57570800	0.83092200	1.95405200
H	-3.48663700	1.38274100	2.18973700
H	-1.75004800	1.38772100	2.40045500
H	-2.64670100	-0.12562400	2.47163700
C	0.14354500	-0.85192700	1.82363100
H	0.62724100	-1.80901000	2.02499900
H	-0.79818400	-0.86127500	2.36572200
H	0.75755500	-0.06928200	2.27027400
C	5.57931800	-0.20010800	-1.21944800
H	6.43486600	-0.79456700	-0.89438200
H	5.42007400	-0.39561900	-2.28192700
C	5.74439400	1.31552700	-0.93290200
H	5.70396700	1.91345200	-1.84476800
H	6.67222800	1.55467900	-0.41200400
C	4.53198300	1.60670400	-0.04802000
H	4.31201000	2.65128600	0.15487000
H	2.23409900	0.58284200	1.06463800
C	4.67416900	-0.36998500	1.00634700
O	4.90261500	-1.18972700	1.85712600
O	4.79805400	0.95446000	1.23026600
H	3.37054400	0.95376300	-1.72833200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1278.194743

166) Conformer **25C1**

C	5.00803100	-0.93294500	-0.98808900
C	5.26188900	-0.04965400	0.21930300
C	4.11308300	0.99188700	0.19817600
C	-3.06921500	0.38660100	2.08792600
O	-7.02661400	1.29213100	-0.50691500
C	-0.56152800	-1.45077100	1.55705000
H	1.60788400	-0.22041500	1.15762900
O	4.97150800	-0.95329100	1.31124400

C	3.93165400	-1.71127400	0.90150800
O	3.45083500	-2.55360000	1.60923000
C	3.87468000	1.53656500	1.61598500
C	4.49782400	2.18403500	-0.68323300
C	5.78151900	2.90123700	-0.36755100
O	3.80244600	2.54915500	-1.60330700
C	-5.82828600	-1.18056600	-1.39636400
C	-5.88402200	-0.78194300	1.04110400
H	-3.44102700	-0.12607900	-1.33377600
H	-1.47138400	0.76299300	-0.94687900
C	0.45076800	-0.42420900	-2.10824100
H	2.90888900	0.47971200	-1.48046400
H	-5.26578300	2.01933700	1.33566000
H	-5.19670200	3.15453400	0.00479300
H	-5.29027900	1.32780100	-1.62248500
H	-2.93887700	2.74101300	0.89191300
H	-3.07299900	2.25399100	-0.78982000
H	-3.25835500	-2.15320700	0.91485400
H	-3.74522300	-2.53499700	-0.71378600
H	-1.34807100	-2.94324100	-0.43875200
H	-1.69872900	-1.73582300	-1.66152100
H	1.53784700	2.22368000	0.68098000
H	0.85874700	1.90069000	-0.89035400
H	-0.90422200	2.50863800	0.66910500
H	-0.37849300	1.31752000	1.83214000
H	1.35873100	-2.69261700	0.29584400
H	0.68347800	-2.92866500	-1.30382100
C	-0.76249900	-0.93726300	0.12206200
C	-1.70943700	-1.92048200	-0.58359600
C	-3.15783600	-1.82736800	-0.12460700
C	-3.39742500	2.00339800	0.22836200
C	-2.89754100	0.58865200	0.57429500
C	-3.69746700	-0.41437100	-0.30119700
H	-5.53239800	-1.78312700	1.30098800
C	-1.40568500	0.48226300	0.10996000
C	1.30008000	-2.25742700	-0.70075000
H	-5.66936300	-0.12407500	1.88203700
C	2.96967300	0.13839100	-0.44429600
H	-7.23652100	2.20312600	-0.73154400
C	-0.47742000	1.50732800	0.75864800
C	0.63258600	-0.86806200	-0.64537300
C	3.59201900	-1.28665000	-0.51784100
H	-3.93757800	0.92833400	2.46372900
C	0.91137600	1.51783100	0.13370400

C	-5.24836300	-0.31624900	-0.26991700
H	-3.19928400	-0.65578000	2.37506900
H	3.13433100	-3.26526300	-1.21320800
H	2.71760400	-1.97778400	-2.32931500
C	1.55248600	0.13484400	0.12217100
H	5.69385500	-1.78093300	-1.03205200
H	0.05162100	-2.35166200	1.57535800
H	-0.09478000	-0.72356900	2.22064900
H	4.82083100	1.68002000	2.14010800
C	2.71771300	-2.25525800	-1.27141200
H	5.01554500	-0.39735800	-1.93843400
H	-1.51473300	-1.72077900	2.00606700
H	3.27782200	0.84195400	2.20588500
H	3.35567700	2.49542400	1.60197300
H	5.72755000	3.92496800	-0.73466200
H	6.02884400	2.89199800	0.69320400
H	-2.20421100	0.77094500	2.63081800
H	1.41315800	-0.25686900	-2.59215400
H	6.26167800	0.34543400	0.37996000
H	-0.05122200	-1.20101600	-2.68728300
H	-5.74628700	-2.24641900	-1.17592400
H	-6.88745700	-0.95228100	-1.52774700
H	6.59426900	2.39532400	-0.89939500
H	-0.11837100	0.49515500	-2.22831000
H	-5.31743900	-0.98872600	-2.34502400
C	-4.90888300	2.14132600	0.30840500
C	-5.61399700	1.14248300	-0.58505800
H	-6.96862900	-0.83117700	0.92913400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1469.977512

167) Conformer **25C2**

C	4.99766200	-0.92821500	-1.01375700
C	5.26994900	-0.03018100	0.17811500
C	4.09718900	0.99998600	0.18737200
C	-3.06651400	0.43651600	2.07866500
O	-7.02811800	1.28108300	-0.52977100
C	-0.56736800	-1.41918500	1.59109000
H	1.60014100	-0.18066800	1.16315700
O	5.02427200	-0.92832400	1.28318300
C	3.97649800	-1.69646800	0.91097700
O	3.51942200	-2.53100200	1.64314300
C	3.86699800	1.50646300	1.61409800
C	4.50638800	2.16153200	-0.72765300

C	5.42794200	3.20319600	-0.15899100
O	4.12503000	2.23959100	-1.87387600
C	-5.83368500	-1.21280900	-1.36154500
C	-5.88276600	-0.75532300	1.06583000
H	-3.44559900	-0.15663300	-1.32985200
H	-1.47504500	0.73354000	-0.96762500
C	0.45155600	-0.49993100	-2.09882200
H	2.91615200	0.45089700	-1.48882800
H	-5.26279300	2.05192100	1.29084800
H	-5.19531500	3.15427300	-0.06739100
H	-5.29423700	1.28872700	-1.64958500
H	-2.93662300	2.76054100	0.82533000
H	-3.07382300	2.23291900	-0.84392200
H	-3.25997200	-2.13433000	0.96206500
H	-3.74818800	-2.55031000	-0.65783400
H	-1.35184200	-2.95429200	-0.37850600
H	-1.70043900	-1.76852800	-1.62327100
H	1.53411300	2.25053000	0.58442700
H	0.83982000	1.85605800	-0.96630900
H	-0.90643700	2.52343300	0.59667200
H	-0.36778500	1.36589300	1.78842400
H	1.38936800	-2.66776500	0.38787400
H	0.68862800	-2.97990600	-1.18830700
C	-0.76418100	-0.93837900	0.14454300
C	-1.71196900	-1.93394900	-0.54209100
C	-3.16005500	-1.83067200	-0.08416900
C	-3.39662900	2.00730400	0.18061200
C	-2.89730200	0.60089300	0.56010200
C	-3.69958300	-0.42168400	-0.29045600
H	-6.96795100	-0.80289200	0.95903200
C	-1.40631600	0.48142300	0.09620700
C	1.30915800	-2.27774000	-0.62594400
H	-5.53383600	-1.75157700	1.34739400
C	2.96635900	0.12658600	-0.44659600
H	-7.23833900	2.18589200	-0.77788700
C	-0.47671700	1.52601800	0.71095200
C	0.63288800	-0.89190900	-0.62052500
C	3.59812100	-1.29499300	-0.50505100
H	-2.19764700	0.82859400	2.60982900
C	0.90618200	1.51846000	0.07366900
C	-5.25027700	-0.32206900	-0.25773700
H	-3.93058800	0.99263200	2.44325400
H	3.13881100	-3.29265800	-1.14248400
H	2.69740600	-2.03687700	-2.28529600

C	1.54912700	0.13688600	0.11551700
H	5.69519700	-1.76637200	-1.06202000
H	-1.52239100	-1.66746700	2.04836200
H	0.03514700	-2.32663100	1.62924600
H	4.81350000	1.74928600	2.10029300
C	2.71689700	-2.28627400	-1.22071400
H	4.97489500	-0.40171600	-1.96784200
H	-0.09085700	-0.68148400	2.23609000
H	3.37579400	0.74996000	2.22429600
H	3.24674900	2.40182800	1.63298000
H	5.85601000	3.79013000	-0.96937000
H	4.85887600	3.86896700	0.49599700
H	-3.20244900	-0.59773100	2.39142100
H	1.40953200	-0.28599600	-2.57297400
H	6.26775200	0.38342200	0.30557700
H	0.00723100	-1.32224400	-2.66238500
H	-5.75254100	-2.27308900	-1.11546400
H	-6.89281600	-0.98623000	-1.49611100
H	6.22074100	2.76446800	0.44901800
H	-0.17159000	0.37821000	-2.25433100
H	-5.32468900	-1.04471200	-2.31570000
C	-4.90790400	2.14844900	0.26017100
C	-5.61573000	1.12880100	-0.60725600
H	-5.66241500	-0.07921200	1.89059800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1469.977627

168) Conformer **25C3**

C	5.01036800	-0.93613200	-0.98140200
C	5.26277000	-0.04955900	0.22390100
C	4.11381200	0.99178500	0.19881800
C	-3.07235700	0.39725900	2.07859900
O	-7.02684600	1.36969700	-0.58050200
C	-0.56491700	-1.44781200	1.55610200
H	1.60697500	-0.21745700	1.15774700
O	4.97128900	-0.95032300	1.31791400
C	3.93187300	-1.70937800	0.90909700
O	3.45021600	-2.54972400	1.61861800
C	3.87343900	1.53978000	1.61500400
C	4.49963700	2.18177300	-0.68504300
C	5.78214500	2.90077700	-0.36855800
O	3.80612500	2.54379900	-1.60773600
C	-5.83164200	-1.18348200	-1.39299300
C	-5.88322100	-0.77250600	1.04067400

H	-3.44356400	-0.12730700	-1.34062800
H	-1.46809800	0.76107000	-0.95428100
C	0.45548000	-0.43106300	-2.10959500
H	2.91231900	0.47509400	-1.48019800
H	-5.25706500	2.04628300	1.31701100
H	-5.19598100	3.15822700	-0.03302900
H	-5.32600900	1.32842300	-1.63478600
H	-2.93609200	2.74630900	0.86858600
H	-3.06902700	2.24856900	-0.80994600
H	-3.25882500	-2.15164400	0.91074300
H	-3.74480500	-2.53399000	-0.71829200
H	-1.34764300	-2.94323900	-0.44065700
H	-1.69655900	-1.73623100	-1.66435100
H	1.53836800	2.22536200	0.67344400
H	0.86073900	1.89756300	-0.89760300
H	-0.90319400	2.51024900	0.65982900
H	-0.37891900	1.32072100	1.82520700
H	1.35994600	-2.69098900	0.30401200
H	0.68628100	-2.93346000	-1.29544800
C	-0.76226800	-0.93691800	0.11975700
C	-1.70847700	-1.92043900	-0.58636300
C	-3.15724700	-1.82652100	-0.12896300
C	-3.39516600	2.00509900	0.20935400
C	-2.89724200	0.59206600	0.56451900
C	-3.69720100	-0.41369900	-0.30662700
H	-5.52387700	-1.76598300	1.31748900
C	-1.40456500	0.48293100	0.10337300
C	1.30213300	-2.25976700	-0.69435900
H	-5.68119700	-0.10468300	1.87803700
C	2.97140400	0.13654800	-0.44303000
H	-7.31853700	1.36489600	0.33658200
C	-0.47684900	1.50894600	0.75133300
C	0.63451000	-0.87026400	-0.64493900
C	3.59383200	-1.28867400	-0.51182100
H	-3.94142600	0.94087100	2.45035600
C	0.91244600	1.51785200	0.12768500
C	-5.24725700	-0.31512400	-0.27349800
H	-3.20285200	-0.64386300	2.37032900
H	3.13680900	-3.26924000	-1.20208500
H	2.72127700	-1.98493800	-2.32232400
C	1.55331500	0.13477400	0.12115000
H	5.69633400	-1.78416000	-1.02225500
H	0.04359400	-2.35180100	1.57698700
H	-0.09492700	-0.72129700	2.21817900

H	4.81881900	1.68443700	2.14018800
C	2.72032200	-2.25938300	-1.26363000
H	5.01892600	-0.40313600	-1.93318800
H	-1.51971700	-1.71189800	2.00527000
H	3.27570400	0.84658400	2.20568300
H	3.35447600	2.49861600	1.59801000
H	5.72729000	3.92415100	-0.73656100
H	6.02857900	2.89271100	0.69239600
H	-2.20883500	0.78424800	2.62190100
H	1.41861500	-0.26181000	-2.59133200
H	6.26233200	0.34611400	0.38456300
H	-0.04231400	-1.21115300	-2.68786200
H	-5.76554100	-2.24848900	-1.16289100
H	-6.88730500	-0.94069000	-1.53034300
H	6.59592600	2.39548500	-0.89942100
H	-0.11638000	0.48606900	-2.23386300
H	-5.31488700	-1.00725200	-2.34143200
C	-4.90632900	2.15169900	0.28344800
C	-5.62241800	1.14661100	-0.59393900
H	-6.96798800	-0.84799800	0.92555300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1469.977970

169) Conformer **25C4**

C	5.00772200	-0.93432400	-0.98887600
C	5.26209700	-0.05003100	0.21768200
C	4.11326300	0.99145300	0.19623300
C	-3.06786500	0.38575400	2.08989900
O	-7.00293400	1.42777000	-0.48476300
C	-0.56111000	-1.45057100	1.55875500
H	1.60854900	-0.21990200	1.15761400
O	4.97224400	-0.95279900	1.31046700
C	3.93224000	-1.71112900	0.90183100
O	3.45182400	-2.55295100	1.61043100
C	3.87530200	1.53720300	1.61371500
C	4.49762300	2.18297200	-0.68620200
C	5.78146400	2.90039800	-0.37164000
O	3.80181200	2.54745000	-1.60619800
C	-5.82868200	-1.17802500	-1.38746800
C	-5.88581300	-0.76903400	1.04714100
H	-3.44248800	-0.12583400	-1.33258300
H	-1.47191700	0.76183100	-0.94610500
C	0.45006600	-0.42692100	-2.10764400
H	2.90852100	0.47793600	-1.48154900

H	-5.26437100	2.02835700	1.33677800
H	-5.19526900	3.15924200	0.00371900
H	-5.28220200	1.34275000	-1.61923600
H	-2.93699200	2.73842300	0.89987800
H	-3.06827400	2.25746900	-0.78371300
H	-3.25843900	-2.15069600	0.91835900
H	-3.74323800	-2.53735000	-0.70921700
H	-1.34918700	-2.94343700	-0.43621800
H	-1.69957500	-1.73619200	-1.65922100
H	1.53813200	2.22379300	0.67864600
H	0.85814200	1.89917900	-0.89196000
H	-0.90368200	2.50865100	0.66795600
H	-0.37747000	1.31854200	1.83183200
H	1.35933300	-2.69259600	0.29857500
H	0.68305000	-2.93064700	-1.30039300
C	-0.76230200	-0.93757300	0.12364300
C	-1.70983200	-1.92045800	-0.58121500
C	-3.15806700	-1.82678800	-0.12170300
C	-3.39568900	2.00412200	0.23280300
C	-2.89723400	0.58845600	0.57603000
C	-3.69856200	-0.41376200	-0.29961900
H	-5.55288800	-1.77791500	1.30199800
C	-1.40558500	0.48173700	0.11087100
C	1.29996700	-2.25862900	-0.69850500
H	-5.65443900	-0.11832000	1.88885900
C	2.96963400	0.13745200	-0.44512400
H	-7.46439100	0.90286000	-1.14437800
C	-0.47700700	1.50740000	0.75822200
C	0.63247200	-0.86923100	-0.64435700
C	3.59193300	-1.28766600	-0.51771500
H	-3.93129300	0.93416500	2.46753600
C	0.91143400	1.51732100	0.13243700
C	-5.24946100	-0.30928100	-0.26444500
H	-3.20510500	-0.65581100	2.37677500
H	3.13394900	-3.26685000	-1.21129500
H	2.71647900	-1.98026600	-2.32817100
C	1.55266300	0.13440500	0.12186100
H	5.69354800	-1.78233200	-1.03244300
H	0.05008900	-2.35278700	1.57696100
H	-0.09211200	-0.72397000	2.22140900
H	4.82162200	1.68130100	2.13734900
C	2.71725200	-2.25691100	-1.27004800
H	5.01480100	-0.39951600	-1.93966200
H	-1.51442700	-1.71820700	2.00894600

H	3.27885400	0.84291100	2.20440400
H	3.35605200	2.49591400	1.59914100
H	5.72712600	3.92401500	-0.73901000
H	6.02960100	2.89150400	0.68892300
H	-2.19915300	0.76326400	2.63155400
H	1.41219000	-0.25850500	-2.59168600
H	6.26196000	0.34520200	0.37754200
H	-0.05068700	-1.20502900	-2.68603300
H	-5.69810200	-2.24271800	-1.18813900
H	-6.90686600	-1.02141300	-1.48916500
H	6.59384400	2.39441500	-0.90398600
H	-0.12047500	0.49145600	-2.22856900
H	-5.36010900	-0.95073600	-2.34965200
C	-4.90588300	2.14950400	0.30971200
C	-5.61099500	1.15704800	-0.58381400
H	-6.97251300	-0.79723400	0.94335700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1469.977970

170) Conformer **25C5**

C	5.00012000	-0.93073300	-1.00732200
C	5.27123300	-0.02906800	0.18211700
C	4.09768000	1.00052400	0.18787900
C	-3.07085400	0.44621800	2.06845600
O	-7.02880700	1.35763400	-0.60212200
C	-0.57193500	-1.41772100	1.58972200
H	1.59945800	-0.17761300	1.16360800
O	5.02546300	-0.92412500	1.28955400
C	3.97824200	-1.69373300	0.91905100
O	3.52079700	-2.52596700	1.65364400
C	3.86590100	1.51002300	1.61317500
C	4.50732000	2.15973300	-0.72984700
C	5.42569500	3.20471500	-0.16230400
O	4.12905600	2.23313300	-1.87742000
C	-5.83709000	-1.21456400	-1.35953700
C	-5.88212900	-0.74719200	1.06412200
H	-3.44841900	-0.15724800	-1.33741100
H	-1.47133000	0.73118800	-0.97477800
C	0.45706700	-0.50843100	-2.09959700
H	2.91935300	0.44601300	-1.48817600
H	-5.25304900	2.07944500	1.27172100
H	-5.19380000	3.15744100	-0.10556700
H	-5.33196700	1.29009300	-1.66140500
H	-2.93316500	2.76495600	0.80145900

H	-3.06947200	2.22660600	-0.86431000
H	-3.26093400	-2.13362300	0.95594700
H	-3.74791700	-2.54889600	-0.66481100
H	-1.35179500	-2.95443200	-0.38250000
H	-1.69800900	-1.76785100	-1.62722100
H	1.53430900	2.25183300	0.57654600
H	0.84088100	1.85188200	-0.97331800
H	-0.90554900	2.52403700	0.58861900
H	-0.36804500	1.36737100	1.78193300
H	1.39183200	-2.66492700	0.39839500
H	0.69220600	-2.98569300	-1.17672000
C	-0.76411300	-0.93873700	0.14210700
C	-1.71113200	-1.93384300	-0.54617400
C	-3.15973200	-1.82990900	-0.09024200
C	-3.39398700	2.00836600	0.16120000
C	-2.89714900	0.60374500	0.54986600
C	-3.69948600	-0.42094900	-0.29680000
H	-6.96711000	-0.82565200	0.95314600
C	-1.40521400	0.48142700	0.08975600
C	1.31191700	-2.28030400	-0.61749300
H	-5.52192200	-1.73371000	1.36371900
C	2.96808200	0.12480400	-0.44498500
H	-7.31686500	1.37535700	0.31594600
C	-0.47621400	1.52663900	0.70426400
C	0.63505600	-0.89477300	-0.61937700
C	3.60044600	-1.29673100	-0.49843800
H	-2.20394400	0.84095300	2.60077800
C	0.90694500	1.51786700	0.06783300
C	-5.24933300	-0.32086000	-0.26193800
H	-3.93612200	1.00375100	2.42830000
H	3.14213000	-3.29671500	-1.12926800
H	2.70106500	-2.04503000	-2.27676600
C	1.54998500	0.13658000	0.11492800
H	5.69809800	-1.76870000	-1.05251800
H	-1.52900600	-1.65755800	2.04713000
H	0.02346200	-2.32977000	1.62995400
H	4.81175500	1.75515300	2.09946300
C	2.72002800	-2.29071400	-1.21133500
H	4.97780600	-0.40703100	-1.96292800
H	-0.09001200	-0.68219800	2.23323700
H	3.37518300	0.75436500	2.22480400
H	3.24452200	2.40465700	1.62949200
H	5.85357300	3.79087000	-0.97334800
H	4.85444100	3.87053400	0.49071900

H	-3.20726200	-0.58681600	2.38522200
H	1.41547800	-0.29135900	-2.57137900
H	6.26866100	0.38560800	0.30890500
H	0.01847200	-1.33467500	-2.66193000
H	-5.77176000	-2.27396000	-1.10464000
H	-6.89274500	-0.97372800	-1.50040200
H	6.21864000	2.76881000	0.44757700
H	-0.16981700	0.36619700	-2.25993500
H	-5.32210900	-1.06130300	-2.31292600
C	-4.90478300	2.15860000	0.23498500
C	-5.62471000	1.13328500	-0.61548900
H	-5.67839700	-0.05960700	1.88489400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1469.978054

171) Conformer **25C6**

C	4.99724400	-0.92926200	-1.01498600
C	5.27023200	-0.03025600	0.17600900
C	4.09727700	0.99971900	0.18535100
C	-3.06558600	0.43529000	2.08067700
O	-7.00402600	1.41797600	-0.51118900
C	-0.56711400	-1.41965000	1.59285500
H	1.60099500	-0.18048600	1.16345900
O	5.02552600	-0.92761000	1.28193300
C	3.97760600	-1.69618300	0.91108000
O	3.52122300	-2.53028000	1.64418100
C	3.86787900	1.50709100	1.61187400
C	4.50574500	2.16062800	-0.73082000
C	5.42692000	3.20324400	-0.16331800
O	4.12419000	2.23735100	-1.87706900
C	-5.83422100	-1.21011900	-1.35270400
C	-5.88486000	-0.74232000	1.07136000
H	-3.44709900	-0.15642400	-1.32868900
H	-1.47530200	0.73227500	-0.96641700
C	0.45092700	-0.50264700	-2.09776400
H	2.91541200	0.44918100	-1.48973300
H	-5.26125400	2.06169500	1.29138900
H	-5.19320300	3.15905500	-0.06943100
H	-5.28586400	1.30379000	-1.64687200
H	-2.93441400	2.75784300	0.83354400
H	-3.06847800	2.23630500	-0.83776000
H	-3.26019000	-2.13200000	0.96537100
H	-3.74618300	-2.55272700	-0.65345300
H	-1.35308400	-2.95464300	-0.37619500

H	-1.70131200	-1.76882200	-1.62098600
H	1.53421200	2.25025400	0.58293900
H	0.83894800	1.85450400	-0.96703900
H	-0.90601300	2.52291000	0.59676300
H	-0.36681200	1.36588900	1.78881900
H	1.39032300	-2.66750600	0.39104200
H	0.68838500	-2.98201400	-1.18419200
C	-0.76402100	-0.93899200	0.14632300
C	-1.71242000	-1.93402800	-0.53976600
C	-3.16037600	-1.83019800	-0.08139500
C	-3.39457900	2.00795300	0.18509600
C	-2.89706200	0.60044700	0.56193400
C	-3.70076500	-0.42117400	-0.28895000
H	-6.97189700	-0.77104100	0.97140700
C	-1.40620600	0.48058400	0.09750300
C	1.30922600	-2.27895100	-0.62327300
H	-5.55291500	-1.74542500	1.34926500
C	2.96620700	0.12568000	-0.44728300
H	-7.46685700	0.88143400	-1.16038200
C	-0.47638300	1.52554200	0.71133500
C	0.63280900	-0.89321000	-0.61915100
C	3.59812100	-1.29587000	-0.50499300
H	-2.19342300	0.82096200	2.61102400
C	0.90610100	1.51767800	0.07314300
C	-5.25151600	-0.31494000	-0.25253600
H	-3.92515400	0.99754900	2.44665600
H	3.13859900	-3.29418800	-1.14022200
H	2.69618400	-2.03956400	-2.28393000
C	1.54929000	0.13627000	0.11561900
H	5.69489100	-1.76733600	-1.06307700
H	-1.52238500	-1.66422500	2.05158300
H	0.03217300	-2.32925700	1.63055100
H	4.81461900	1.75056200	2.09727900
C	2.71651100	-2.28793100	-1.21912500
H	4.97372400	-0.40350000	-1.96945500
H	-0.08707600	-0.68332900	2.23681100
H	3.37733500	0.75084900	2.22292900
H	3.24734000	2.40225800	1.63055700
H	5.85438500	3.78977300	-0.97430600
H	4.85774800	3.86921300	0.49137600
H	-3.20821000	-0.59820300	2.39307600
H	1.40859000	-0.28802900	-2.57221900
H	6.26805300	0.38363400	0.30241700
H	0.00746300	-1.32591200	-2.66063200

H	-5.70392100	-2.26976300	-1.12799700
H	-6.91250800	-1.05502800	-1.45526100
H	6.22016600	2.76538600	0.44474300
H	-0.17319200	0.37469800	-2.25390400
H	-5.36791400	-1.00659600	-2.32131000
C	-4.90453500	2.15683200	0.26094800
C	-5.61252200	1.14356100	-0.60654900
H	-5.64977400	-0.07224100	1.89664500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1469.977765

172) Conformer **26C1**

C	3.63762600	1.11773200	1.27616000
H	2.77097400	1.25957500	1.93301000
H	4.37881300	1.86298700	1.58220000
C	4.19255700	-0.28799200	1.45436000
H	4.43947300	-0.47819900	2.50370500
H	5.12970100	-0.37509900	0.88952100
C	3.20175900	-1.32681600	0.95021200
H	2.32948500	-1.33418600	1.61268300
H	3.63894600	-2.32931700	1.01758800
C	2.77264600	-1.08483900	-0.50101100
C	2.22759200	0.34776500	-0.74276500
C	3.25076700	1.35026200	-0.17651100
H	4.15830600	1.26206200	-0.78830500
H	2.89217600	2.37295500	-0.32448500
C	1.78711400	-2.15544300	-0.96943200
H	1.68081300	-2.11062000	-2.05827800
H	2.19395100	-3.14683600	-0.74274800
C	0.41619400	-1.99827500	-0.32618600
H	0.48459700	-2.19234700	0.74942500
H	-0.27695000	-2.74175200	-0.73058400
C	-0.14387800	-0.59798500	-0.55361900
C	0.83824800	0.49218400	-0.05733700
C	-1.48102900	-0.37541800	0.10693300
C	-2.08908100	1.01754500	-0.13253100
C	-1.14700500	2.05843700	0.46074100
H	-1.52858300	3.06526600	0.26579100
H	-1.08059000	1.95676500	1.54639300
C	0.25161000	1.90949000	-0.15209600
H	0.91979700	2.60796700	0.35691800
H	0.22373600	2.22961700	-1.19696900
C	-1.57643700	-0.57731500	1.63094500
H	-1.62449600	-1.64323200	1.85533800

H	-0.71355700	-0.16894500	2.15513600
C	-2.88149500	0.16201500	1.99523300
H	-2.70060100	1.02027100	2.64332900
H	-3.61008100	-0.47750900	2.49551700
C	-3.38236800	0.63989200	0.61708500
H	-4.21061200	1.34516700	0.62539400
H	3.68086500	-1.17213200	-1.11396400
O	-2.53617600	-1.24862600	-0.42626100
C	2.14463600	0.61606500	-2.24937000
H	1.91047500	1.66426600	-2.45201400
H	1.39812400	0.00568800	-2.75927900
H	3.11273600	0.40514200	-2.71332500
C	-2.38445900	1.35508200	-1.59278100
H	-1.47409100	1.47470500	-2.18053000
H	-2.93196500	2.30034100	-1.63588200
H	-2.99388900	0.59756900	-2.08901800
C	-3.70714400	-0.64919600	-0.11214400
O	-4.77169500	-1.14738000	-0.37119700
H	1.00096900	0.29315300	1.00804200
H	-0.30267600	-0.46441300	-1.63026800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -929.473966

173) Conformer **27C1**

C	-3.04685500	0.98949500	0.08521800
C	-2.48499100	-0.34534600	-0.44654700
C	-2.30128900	2.20044600	-0.39381600
H	-2.40222100	2.27414100	-1.48107200
H	-2.72344900	3.11529400	0.03211600
C	-0.82835200	2.05315700	0.00405700
H	-0.73655500	2.19203200	1.08542200
H	-0.24810100	2.86203800	-0.45104600
C	-0.20092500	0.70939600	-0.39074500
C	-1.04010400	-0.50686000	0.05030600
C	1.25122700	0.61108000	0.09471800
C	1.95880500	-0.71342700	-0.27219700
C	1.05543600	-1.89007800	0.14959700
H	1.52593600	-2.82496100	-0.17508900
H	1.01549700	-1.93763700	1.24413900
C	-0.36560800	-1.80197200	-0.38984400
H	-0.94632700	-2.66283300	-0.04007700
H	-0.35341400	-1.86546300	-1.48190100
H	-1.05675200	-0.51638100	1.14482200
H	1.80328600	1.42833000	-0.38818900

C	-2.57989600	-0.50020000	-1.96486200
H	-2.44839100	-1.54772900	-2.24333300
H	-1.81882200	0.07890600	-2.48897000
H	-3.54930500	-0.18201000	-2.35066800
H	-0.15763600	0.68791900	-1.48703700
C	2.25987900	-0.82440000	-1.76265000
H	2.78110400	-1.75908500	-1.98967600
H	2.88044600	-0.00006200	-2.11905000
H	1.34245600	-0.81712600	-2.35554900
C	1.47362400	0.73600700	1.60362400
H	1.37993100	1.76556000	1.95612100
H	0.73042500	0.14870200	2.15059400
C	2.88155000	0.17786600	1.84210400
H	2.94925200	-0.34966600	2.79594400
H	3.59802200	1.00052900	1.89886000
C	3.22445500	-0.74315900	0.64390300
H	3.32198700	-1.77420900	1.00366800
C	-3.61183300	-1.14012800	0.24915600
H	-3.69720800	-2.20886500	0.06542000
C	-3.51431800	-0.71013600	1.72723500
H	-2.73849300	-1.28359000	2.23716700
H	-4.45012200	-0.88160800	2.26118800
C	-3.14989100	0.78551400	1.60775000
H	-2.22113800	1.02595600	2.12360800
H	-3.92713200	1.44276000	2.00075100
O	-4.43102400	0.94030800	-0.37022600
C	-4.81010500	-0.36122500	-0.26955900
O	-5.91971800	-0.73252400	-0.52578500
C	4.58847400	-0.42576200	0.00089200
H	4.66957100	-1.04887800	-0.89823900
C	5.70872000	-0.85620300	0.94655800
H	6.69523900	-0.67914500	0.51188900
H	5.63843000	-1.92155300	1.18289600
H	5.65978200	-0.30213500	1.88935600
C	4.78800600	1.03064200	-0.43960600
H	3.85796800	1.43097400	-0.85187800
H	5.01822900	1.65009400	0.43450100
C	5.89093700	1.20150700	-1.47558500
H	6.85747600	0.85205200	-1.10425000
H	6.00984300	2.25081500	-1.75718600
H	5.66444500	0.63729800	-2.38540200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1047.208958

174) Conformer **27C2**

C	3.22917200	0.84787400	0.19363500
C	2.55390100	-0.53824700	0.20020000
C	2.68273000	1.79571100	1.22039200
H	3.17844900	2.76893800	1.16027700
H	2.88129400	1.39313300	2.21844600
C	1.17604300	1.94703400	0.98503400
H	1.01900900	2.53672000	0.07740500
H	0.73836400	2.53227500	1.80004900
C	0.41886800	0.61726100	0.86520300
C	1.06229000	-0.36958700	-0.12733400
C	-1.07228200	0.85761500	0.58756200
C	-1.92555400	-0.42176900	0.34011400
C	-1.16235100	-1.41062900	-0.56016100
H	-1.72547000	-2.34895700	-0.61466000
H	-1.14202300	-1.01349300	-1.58191000
C	0.27253000	-1.67317200	-0.13389600
H	0.73449400	-2.39143300	-0.82028200
H	0.29781800	-2.13392300	0.85851900
H	0.97287900	0.05952800	-1.13164800
H	-1.47473400	1.32416600	1.49845800
C	2.75747500	-1.32297700	1.49682500
H	3.78869500	-1.27471800	1.84907700
H	2.51742400	-2.37621000	1.33809600
H	2.12334000	-0.95824300	2.30566700
H	0.46570700	0.13742300	1.85136100
C	-2.23341500	-1.06606300	1.69061300
H	-1.30772700	-1.28748600	2.22832900
H	-2.78226900	-2.00490700	1.59860200
H	-2.81719000	-0.39517500	2.32566400
C	-1.46279300	1.79579200	-0.54913100
H	-1.16393300	2.83195200	-0.37645400
H	-1.02270600	1.47838900	-1.50204800
C	-2.97320700	1.62084000	-0.57292800
H	-3.44575700	2.04298500	-1.46224200
H	-3.40115700	2.13543500	0.29659200
C	-3.18779700	0.10485400	-0.45684300
H	-3.09842700	-0.29757500	-1.47476200
C	3.50994700	-1.05190900	-0.89856500
H	3.47694300	-2.10185600	-1.18104000
C	3.34223500	-0.03369600	-2.04509500
H	4.20258600	-0.03475200	-2.71592800
H	2.46285400	-0.27864700	-2.64289800
C	3.17336400	1.29567300	-1.27808500

H	2.23785600	1.79610400	-1.52448200
H	3.98593100	1.99915200	-1.46605300
O	4.63049300	0.50570200	0.40519800
C	4.83518900	-0.65862700	-0.26610600
O	5.90780800	-1.18801100	-0.32928800
C	-4.57984900	-0.32562500	0.03213000
H	-4.63111900	-0.18389400	1.11961400
C	-4.83399200	-1.79911200	-0.28267100
H	-4.00811900	-2.43869300	0.03003800
H	-4.95959100	-1.93455700	-1.36266200
H	-5.73691200	-2.17092600	0.20600400
C	-5.68570300	0.53905000	-0.58432100
H	-5.49203400	1.58997900	-0.35399900
H	-5.63585000	0.45134200	-1.67765700
C	-7.09105700	0.19499700	-0.11074300
H	-7.81882200	0.90946700	-0.50359100
H	-7.15553200	0.22504200	0.98156800
H	-7.40515200	-0.79982500	-0.43370300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1047.207640

175) Conformer **27C3**

C	3.22917200	0.84787400	0.19363500
C	2.55390100	-0.53824700	0.20020000
C	2.68273000	1.79571100	1.22039200
H	3.17844900	2.76893800	1.16027700
H	2.88129400	1.39313300	2.21844600
C	1.17604300	1.94703400	0.98503400
H	1.01900900	2.53672000	0.07740500
H	0.73836400	2.53227500	1.80004900
C	0.41886800	0.61726100	0.86520300
C	1.06229000	-0.36958700	-0.12733400
C	-1.07228200	0.85761500	0.58756200
C	-1.92555400	-0.42176900	0.34011400
C	-1.16235100	-1.41062900	-0.56016100
H	-1.72547000	-2.34895700	-0.61466000
H	-1.14202300	-1.01349300	-1.58191000
C	0.27253000	-1.67317200	-0.13389600
H	0.73449400	-2.39143300	-0.82028200
H	0.29781800	-2.13392300	0.85851900
H	0.97287900	0.05952800	-1.13164800
H	-1.47473400	1.32416600	1.49845800
C	2.75747500	-1.32297700	1.49682500
H	3.78869500	-1.27471800	1.84907700

H	2.51742400	-2.37621000	1.33809600
H	2.12334000	-0.95824300	2.30566700
H	0.46570700	0.13742300	1.85136100
C	-2.23341500	-1.06606300	1.69061300
H	-1.30772700	-1.28748600	2.22832900
H	-2.78226900	-2.00490700	1.59860200
H	-2.81719000	-0.39517500	2.32566400
C	-1.46279300	1.79579200	-0.54913100
H	-1.16393300	2.83195200	-0.37645400
H	-1.02270600	1.47838900	-1.50204800
C	-2.97320700	1.62084000	-0.57292800
H	-3.44575700	2.04298500	-1.46224200
H	-3.40115700	2.13543500	0.29659200
C	-3.18779700	0.10485400	-0.45684300
H	-3.09842700	-0.29757500	-1.47476200
C	3.50994700	-1.05190900	-0.89856500
H	3.47694300	-2.10185600	-1.18104000
C	3.34223500	-0.03369600	-2.04509500
H	4.20258600	-0.03475200	-2.71592800
H	2.46285400	-0.27864700	-2.64289800
C	3.17336400	1.29567300	-1.27808500
H	2.23785600	1.79610400	-1.52448200
H	3.98593100	1.99915200	-1.46605300
O	4.63049300	0.50570200	0.40519800
C	4.83518900	-0.65862700	-0.26610600
O	5.90780800	-1.18801100	-0.32928800
C	-4.57984900	-0.32562500	0.03213000
H	-4.63111900	-0.18389400	1.11961400
C	-4.83399200	-1.79911200	-0.28267100
H	-4.00811900	-2.43869300	0.03003800
H	-4.95959100	-1.93455700	-1.36266200
H	-5.73691200	-2.17092600	0.20600400
C	-5.68570300	0.53905000	-0.58432100
H	-5.49203400	1.58997900	-0.35399900
H	-5.63585000	0.45134200	-1.67765700
C	-7.09105700	0.19499700	-0.11074300
H	-7.81882200	0.90946700	-0.50359100
H	-7.15553200	0.22504200	0.98156800
H	-7.40515200	-0.79982500	-0.43370300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1047.206457

176) Conformer **28C1**

C	-0.55861200	-0.98552300	0.65945700
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H	-1.15040900	-1.87551200	0.87396300
C	0.91221500	-1.34005400	0.44699900
H	1.00826400	-1.85625200	-0.51117300
C	1.73498700	-0.04337300	0.43156400
H	2.28440100	-0.02575500	1.37883100
C	0.74636700	1.14451000	0.47707100
H	1.26882600	2.09936200	0.50320800
C	-0.29983300	1.10487500	-0.65018900
C	-1.14494200	-0.20082100	-0.51978700
C	-1.29436700	2.27592400	-0.61696600
H	-1.33766200	2.71568100	0.38532100
H	-1.00865100	3.07618800	-1.30229100
C	-2.64264000	1.65013100	-0.94952400
H	-2.74033500	1.49884800	-2.03050200
H	-3.48871900	2.26193800	-0.62885100
C	-2.58610600	0.30512600	-0.23182300
H	-2.66881900	0.50186900	0.84255300
O	1.40377500	-2.16326900	1.49197000
H	0.97492900	-3.02262900	1.42864400
C	0.02064300	0.97731800	1.78395500
O	-0.64940500	-0.17963800	1.85913600
C	-1.09745900	-1.02871500	-1.80106100
H	-0.07185500	-1.18440200	-2.13465500
H	-1.61892400	-0.50544400	-2.60616900
H	-1.57815400	-2.00091800	-1.66620900
H	0.23676400	1.09367200	-1.59827200
C	-3.72302100	-0.61887000	-0.59918700
H	-3.69700800	-0.85758200	-1.66932200
H	-4.67126600	-0.10134800	-0.40306400
C	2.82796800	0.00205700	-0.65363300
C	3.83850400	-1.11232800	-0.40281500
H	3.35293000	-2.08888800	-0.38180600
H	4.35779300	-0.96596300	0.54662500
H	4.58811800	-1.11524200	-1.19926400
C	3.54210400	1.34794100	-0.66497000
H	4.37965900	1.31510300	-1.36683500
H	3.94160500	1.59308500	0.32201300
H	2.87157600	2.14854600	-0.98003000
O	2.19627300	-0.21442000	-1.91679800
H	2.88659200	-0.27769400	-2.58459100
O	-3.63603000	-1.80366900	0.17871800
H	-4.35749500	-2.38481400	-0.07643300
O	0.00826200	1.74711600	2.71244500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.136025

177) Conformer **28C2**

C	-0.40739000	-0.31054400	1.25450900
H	-0.92221000	-0.81899900	2.07246100
C	1.08375000	-0.64655500	1.26868600
H	1.20857200	-1.68188400	0.94283000
C	1.80903800	0.30135700	0.30176200
H	2.36422700	1.00423800	0.93194900
C	0.73720100	1.13151100	-0.44195000
H	1.18885700	1.85160300	-1.12224100
C	-0.31258100	0.26338100	-1.15688300
C	-1.05855300	-0.60922300	-0.10061900
C	-1.39143600	1.07032600	-1.89678400
H	-1.45903600	2.08500100	-1.48938300
H	-1.16994000	1.17037300	-2.96106300
C	-2.69175300	0.32752500	-1.61712400
H	-2.78317800	-0.54980200	-2.26776400
H	-3.57925500	0.94288200	-1.77179800
C	-2.52687900	-0.11239500	-0.16620500
H	-2.61010500	0.78339100	0.45910900
O	1.64183300	-0.47333900	2.56006800
H	1.29545400	-1.16167900	3.13673400
C	0.03683000	1.89851700	0.64602400
O	-0.54587200	1.09834400	1.55010100
C	-0.96271700	-2.09716400	-0.43457100
H	-1.53070900	-2.31588400	-1.34146500
H	-1.36418200	-2.72037000	0.36943800
H	0.06818600	-2.39588500	-0.62301500
H	0.21540300	-0.38691400	-1.85341500
C	-3.56817400	-1.08525400	0.33862500
H	-3.28595200	-1.46015900	1.33219300
H	-3.64719800	-1.94882200	-0.33259100
C	2.88531700	-0.38074000	-0.56470300
C	3.97458300	-0.95388000	0.33570700
H	3.55972700	-1.65578600	1.06033000
H	4.49145800	-0.16153700	0.88116800
H	4.71466300	-1.48160900	-0.27258900
C	3.50191000	0.59889200	-1.55527300
H	4.33157600	0.11861700	-2.08081400
H	3.89434400	1.48299700	-1.04711200
H	2.77259400	0.91821500	-2.30081000
O	2.25650600	-1.44796000	-1.27659000
H	2.94158700	-1.93153800	-1.74908900

O	-4.81075700	-0.40194200	0.40731900
H	-5.48253300	-1.03096500	0.68375000
O	-0.02511300	3.09614700	0.76860100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.135773

178) Conformer **28C3**

C	-0.39808000	0.02791600	1.33482400
H	-0.91132500	-0.28758700	2.24590600
C	1.05644800	-0.44224500	1.34813300
H	1.07293200	-1.52377700	1.19657400
C	1.80817700	0.26160100	0.20825900
H	2.45440100	1.00349400	0.68945600
C	0.77392800	1.05595300	-0.62309900
H	1.24962600	1.60750500	-1.43233700
C	-0.38652200	0.18720300	-1.13893500
C	-1.14750500	-0.42566400	0.07680400
C	-1.42783400	0.96599200	-1.96041900
H	-1.37433000	2.03581600	-1.73074400
H	-1.25974100	0.86352900	-3.03428700
C	-2.77439100	0.41818600	-1.50535800
H	-2.99228200	-0.53470800	-1.99469500
H	-3.60585400	1.09417800	-1.71919000
C	-2.56504500	0.20424700	-0.00983400
H	-2.50123300	1.19800600	0.44682000
O	1.69713900	-0.11377800	2.56951200
H	1.32148900	-0.66013600	3.26709400
C	0.20596200	2.05497300	0.34701000
O	-0.39310900	1.47388900	1.39573000
C	-1.19819500	-1.94890100	-0.00130500
H	-1.81979200	-2.25803100	-0.84172500
H	-1.63551500	-2.38190800	0.90214200
H	-0.20423300	-2.37051300	-0.14991200
H	0.04278700	-0.61524100	-1.73764900
C	-3.69969400	-0.48594200	0.72381900
H	-4.51747100	0.23632200	0.84455700
H	-3.37010100	-0.77035700	1.73317600
C	2.77464400	-0.65012300	-0.57208300
C	3.85928300	-1.16469300	0.36857900
H	3.42702900	-1.69675300	1.21707900
H	4.46932500	-0.34410300	0.75198700
H	4.51884400	-1.85043000	-0.17106200
C	3.41762100	0.09265100	-1.73674700
H	4.17619500	-0.54085900	-2.20409200

H	3.90793500	1.00935300	-1.40038200
H	2.67940700	0.34944800	-2.49758700
O	2.02071300	-1.75738000	-1.06833300
H	2.63589900	-2.37321100	-1.47898400
O	-4.16436600	-1.62182000	0.01336700
H	-4.89383900	-2.00115000	0.51029500
O	0.25675700	3.25711200	0.26843500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.133323

179) Conformer **28C4**

C	-0.56190200	-1.01388400	0.59638400
H	-1.12267700	-1.91622000	0.83374100
C	0.89083700	-1.33856700	0.27895500
H	0.93381600	-1.72881200	-0.74162700
C	1.70517900	-0.04059300	0.38870700
H	2.14053600	-0.06779700	1.39533800
C	0.71249500	1.14146900	0.37906000
H	1.21946900	2.10597900	0.37914600
C	-0.34985600	1.06588700	-0.73484300
C	-1.21477500	-0.21921300	-0.54188300
C	-1.32342400	2.25752200	-0.72180500
H	-1.29106700	2.76225000	0.24922200
H	-1.06671800	3.00413100	-1.47526200
C	-2.70369500	1.64607500	-0.92727600
H	-2.88927800	1.45954700	-1.99072700
H	-3.51016800	2.28734600	-0.56546600
C	-2.62038600	0.32635600	-0.16613600
H	-2.62121300	0.56051300	0.90340100
O	1.35269000	-2.33211700	1.17137700
H	2.29115800	-2.43990900	0.96991700
C	0.00011100	0.97639800	1.69641900
O	-0.60472000	-0.21525900	1.80575000
C	-1.28870800	-1.04822400	-1.82120900
H	-1.85545200	-0.51397700	-2.58677400
H	-1.78086300	-2.00743700	-1.64508600
H	-0.30301400	-1.24544000	-2.24315000
H	0.15767700	1.01768200	-1.69806000
C	-3.79912900	-0.58440400	-0.41824800
H	-3.86638000	-0.84434800	-1.48166400
H	-4.71841700	-0.04458400	-0.15611800
C	2.93608300	0.01900000	-0.53112000
C	3.85883300	1.15604400	-0.11508800
H	4.11216400	1.07620500	0.94396300

H	3.40111300	2.13111400	-0.29286100
H	4.78402200	1.11643600	-0.69619800
C	2.64300700	0.10839200	-2.02056200
H	3.57930700	0.01384500	-2.57803000
H	2.20711800	1.07295100	-2.28487600
H	1.97529400	-0.68702600	-2.35471400
O	3.57854900	-1.23568800	-0.25144100
H	4.36482700	-1.30943500	-0.80143300
O	-3.66760200	-1.75407000	0.37489100
H	-4.42037900	-2.32444800	0.19769200
O	-0.03753000	1.76311900	2.60836100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.134897

180) Conformer **29C1**

C	35.40501900	-6.31244300	-0.61113900
H	34.47957100	-5.73971300	-0.67542300
C	35.14127700	-7.74478000	-0.15089900
H	34.81458300	-7.71157200	0.89304500
C	36.44064400	-8.55759500	-0.28111100
H	36.26501600	-9.29594700	-1.06933500
C	37.54568300	-7.60474200	-0.78630000
H	38.47371500	-8.14155200	-0.97769900
C	37.75789700	-6.42266200	0.17215100
C	36.43587200	-5.59934800	0.27317400
C	38.85483400	-5.44108200	-0.26743300
H	39.81031700	-5.64889400	0.21750600
H	39.02233500	-5.51487500	-1.34723300
C	38.29587800	-4.06365100	0.06276800
H	38.78507000	-3.25988900	-0.49161500
H	38.41683400	-3.84524900	1.12981100
C	36.81633900	-4.19894100	-0.28379400
H	36.73580600	-4.23784500	-1.37543800
O	34.14337100	-8.36977800	-0.93805800
H	33.30986000	-7.90959400	-0.79535600
C	37.04652200	-7.05790400	-2.09354800
O	35.90171100	-6.37396900	-1.96774500
C	35.94685700	-5.50124300	1.71561400
H	35.88944300	-6.47937500	2.19487300
H	34.96051200	-5.03514000	1.77364300
H	36.63979400	-4.90037700	2.30890200
H	38.00738100	-6.82671600	1.15622100
C	35.98191100	-3.02810600	0.17938000
H	36.40314800	-2.10880900	-0.24799600

H	36.02544300	-2.92950500	1.27089300
C	36.79380700	-9.33759200	0.99401500
H	36.83992000	-8.63720900	1.83668400
C	38.16690700	-9.98507800	0.92421400
H	38.33313600	-10.55375600	1.84816100
H	38.94856000	-9.21726600	0.87011200
C	35.72113700	-10.37708400	1.30053000
H	35.93244600	-10.87695000	2.24890500
H	35.68618300	-11.13630100	0.51615100
H	34.72954800	-9.92648400	1.37338500
O	34.64150200	-3.20671100	-0.25282400
H	34.12317200	-2.45913800	0.05672200
O	37.56022000	-7.18477100	-3.17723100
O	38.22972300	-10.83767400	-0.20624500
H	39.09909300	-11.24569000	-0.22844000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.130124

181) Conformer **29C2**

C	35.31375100	-6.38328200	-0.59027400
H	34.38087200	-5.81978200	-0.65928900
C	35.04798600	-7.81323400	-0.12104800
H	34.72549800	-7.77436400	0.92388400
C	36.34695600	-8.62687100	-0.25267300
H	36.16922000	-9.36533400	-1.04026900
C	37.45309400	-7.67590800	-0.75967800
H	38.38078400	-8.21381700	-0.94906400
C	37.66565200	-6.49225400	0.19671800
C	36.34517300	-5.66714700	0.29042200
C	38.76522400	-5.51138400	-0.23929200
H	39.71757100	-5.71850100	0.25208500
H	38.93931900	-5.58984900	-1.31778800
C	38.20358700	-4.13274100	0.08322100
H	38.69520700	-3.32999700	-0.46799600
H	38.31150800	-3.91174500	1.15131800
C	36.72804500	-4.27437100	-0.27571700
H	36.65986500	-4.32490600	-1.36800300
O	34.04727700	-8.44017300	-0.90164700
H	33.20938700	-7.99403600	-0.74116700
C	36.95460000	-7.13359500	-2.06901300
O	35.80689600	-6.45121200	-1.94579400
C	35.85426500	-5.55851200	1.73323700
H	35.79615500	-6.53304700	2.21966100
H	34.86550200	-5.09614500	1.79403100

H	36.54528400	-4.95202700	2.32217600
H	37.90984300	-6.89501100	1.18254200
C	35.84214600	-3.12774600	0.15655400
H	35.97280300	-2.92019700	1.22546100
H	34.78584700	-3.38265500	-0.00703100
C	36.70029900	-9.40663400	1.02262900
H	36.74901000	-8.70591100	1.86485600
C	38.07210200	-10.05675900	0.95068400
H	38.23817000	-10.62648100	1.87398300
H	38.85528000	-9.29051200	0.89642900
C	35.62617200	-10.44398100	1.33131200
H	35.58834200	-11.20330900	0.54719800
H	34.63551000	-9.99168700	1.40608200
H	35.83853800	-10.94388700	2.27939800
O	36.19621400	-1.98801700	-0.61148500
H	35.66988200	-1.24514600	-0.30415100
O	37.46751300	-7.26269200	-3.15207700
O	38.13151400	-10.90831300	-0.18060000
H	39.00013400	-11.31783000	-0.20482600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.129498

182) Conformer **29C3**

C	35.39453900	-6.31930600	-0.73163300
H	34.46576900	-5.75040200	-0.78007700
C	35.14012500	-7.76124100	-0.29799300
H	34.81057400	-7.74853600	0.74524800
C	36.44578900	-8.56503800	-0.43587100
H	36.26981800	-9.29921200	-1.23060500
C	37.54038500	-7.59703400	-0.93971900
H	38.47359200	-8.11666800	-1.15170300
C	37.75281500	-6.43004600	0.03665100
C	36.42603500	-5.61758400	0.16102400
C	38.83988100	-5.43413100	-0.39457600
H	39.80084100	-5.64543900	0.07777900
H	38.99792900	-5.48631300	-1.47707500
C	38.27556900	-4.06678800	-0.03311100
H	38.75572600	-3.24953100	-0.57547100
H	38.40378100	-3.86869900	1.03703400
C	36.79422300	-4.20412200	-0.37089000
H	36.70546200	-4.22173600	-1.46248200
O	34.15112100	-8.38037100	-1.09997600
H	33.31486700	-7.92432000	-0.95994800
C	37.02839100	-7.03249500	-2.23547000

O	35.88398600	-6.35322300	-2.09184400
C	35.94412700	-5.55150800	1.60763500
H	35.89583100	-6.53940500	2.06742400
H	34.95514900	-5.09315500	1.67999100
H	36.63639000	-4.95806300	2.20907300
H	38.01223300	-6.84988200	1.01160300
C	35.95606500	-3.04807800	0.12174400
H	36.36820900	-2.11782400	-0.29044100
H	36.00711000	-2.97085700	1.21463500
C	36.79530800	-9.35344300	0.83499500
H	36.84507700	-8.66008800	1.68373100
C	38.15579700	-10.02035600	0.72301900
H	38.93807500	-9.26947300	0.56633200
H	38.15993800	-10.69627500	-0.14494400
C	35.71514500	-10.38868700	1.12575100
H	35.93204200	-10.92069600	2.05189100
H	35.66235700	-11.12292100	0.31575000
H	34.73023300	-9.92803500	1.22122400
O	34.61369200	-3.22706100	-0.30416600
H	34.09268400	-2.48924600	0.02375700
O	37.53672500	-7.14256500	-3.32333900
O	38.41406700	-10.73710900	1.91784900
H	39.29452800	-11.11603600	1.85319200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.129677

183) Conformer **29C4**

C	35.42308000	-6.19891500	-0.57576900
H	34.61045700	-5.47206500	-0.58517000
C	34.97590400	-7.52427700	0.03704100
H	34.80430900	-7.36335000	1.10588800
C	36.08203100	-8.57327600	-0.17500800
H	35.67288300	-9.30445300	-0.88277600
C	37.26542100	-7.87299100	-0.87799000
H	38.06103500	-8.57799200	-1.10804000
C	37.79683000	-6.69003900	-0.05461300
C	36.66538900	-5.63153000	0.12164600
C	38.98550200	-5.95959600	-0.69735900
H	39.94212700	-6.30881500	-0.30450700
H	39.00260300	-6.13346800	-1.77870100
C	38.72406600	-4.48359600	-0.42883200
H	39.27312200	-3.82212400	-1.10253600
H	39.01511100	-4.22148900	0.59472800
C	37.21190100	-4.36437300	-0.59351000

H	36.98789000	-4.45771700	-1.66171400
O	33.78716200	-8.00472800	-0.56565100
H	33.07279700	-7.39216400	-0.36259400
C	36.70905800	-7.32976400	-2.16271600
O	35.72527100	-6.44041400	-1.96921500
C	36.38747900	-5.35175100	1.59612400
H	36.22379700	-6.26998400	2.16176000
H	35.51249900	-4.71030300	1.72546200
H	37.24410800	-4.85048700	2.05237700
H	38.09359300	-7.07760900	0.92129400
C	36.66264800	-3.03178800	-0.14186200
H	37.18282700	-2.23571000	-0.69044100
H	36.85928500	-2.87388300	0.92557800
C	36.43284400	-9.35356000	1.10140900
H	36.74626000	-8.65100800	1.88286200
C	37.57487100	-10.34015400	0.90954000
H	37.44195400	-10.87642700	-0.04103200
H	37.53608400	-11.08464500	1.71438700
C	35.20898600	-10.11540900	1.60036300
H	34.93175100	-10.90491400	0.89494500
H	34.34248000	-9.46319200	1.71738100
H	35.41252400	-10.58222300	2.56642700
O	35.26809800	-2.98447900	-0.40467100
H	34.93357000	-2.13576200	-0.10273400
O	37.05151800	-7.61698900	-3.28323500
O	38.82172400	-9.66463500	0.93801800
H	39.51514600	-10.30895400	0.77144300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.129223

184) Conformer **29C5**

C	35.39335800	-6.17968100	-0.68056300
H	34.57157600	-5.46177100	-0.72283900
C	34.90398300	-7.53063500	-0.16063800
H	34.63991700	-7.41341900	0.89455900
C	36.03475500	-8.56404200	-0.31678600
H	35.68932800	-9.28231500	-1.06927500
C	37.26119800	-7.83287300	-0.90939500
H	38.07435600	-8.52191200	-1.13213300
C	37.72662300	-6.68638200	0.00119900
C	36.57716900	-5.63998700	0.13209100
C	38.95730800	-5.92407700	-0.51374700
H	39.88227200	-6.28677800	-0.06192400
H	39.05975400	-6.05240400	-1.59665400

C	38.66324300	-4.46222800	-0.20325900
H	39.25976400	-3.76915200	-0.79803200
H	38.86204700	-4.24423900	0.85232600
C	37.16948700	-4.34755100	-0.48931700
H	37.03812100	-4.40564500	-1.57548100
O	33.77793000	-7.99142800	-0.88341600
H	33.03663000	-7.40351500	-0.70512700
C	36.79778100	-7.23925600	-2.21015000
O	35.79840400	-6.36028600	-2.05489600
C	36.18576200	-5.41945700	1.59250000
H	37.00148000	-4.93401800	2.13205900
H	35.98248200	-6.35928000	2.10727900
H	35.29794600	-4.78864300	1.68673900
H	37.94590000	-7.10682300	0.98562600
C	36.52151100	-3.05471700	-0.04770300
H	36.74296600	-2.85208300	1.00706200
H	35.42989400	-3.12341700	-0.15196200
C	36.29743500	-9.35524500	0.97306600
H	36.51746200	-8.65179600	1.78559100
C	37.50456200	-10.26714300	0.83322800
H	38.40218400	-9.68093200	0.60782900
H	37.34011600	-10.96438900	-0.00167800
C	35.06184300	-10.15988600	1.35855600
H	34.83028400	-10.89854300	0.58478700
H	34.18556400	-9.52064400	1.48023000
H	35.22691300	-10.69107500	2.29576200
O	37.02741400	-2.01046400	-0.86491200
H	36.65518700	-1.18080300	-0.55425400
O	37.22471600	-7.48303000	-3.31049700
O	37.68786500	-10.97337900	2.04781700
H	38.48050900	-11.50966000	1.96333600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.129212

185) Conformer **29C6**

C	35.26838900	-6.45058900	-0.64332500
H	34.34088700	-5.87754600	-0.70742400
C	34.99303900	-7.87010600	-0.15071300
H	34.69549600	-7.81361000	0.90082700
C	36.27620800	-8.70692200	-0.29939300
H	36.06876100	-9.43895700	-1.08931900
C	37.38931800	-7.77345500	-0.82486300
H	38.31250800	-8.32040900	-1.00190700
C	37.62482900	-6.58332300	0.11717000

C	36.31930600	-5.73745800	0.21574300
C	38.73409300	-5.62375600	-0.34105100
H	39.68762800	-5.83922200	0.14450900
H	38.89799800	-5.71727300	-1.42008800
C	38.19612300	-4.23279900	-0.03055300
H	38.69336500	-3.44399200	-0.59686000
H	38.31838100	-3.99989300	1.03350700
C	36.71480500	-4.35732700	-0.37194800
H	36.63412600	-4.42049900	-1.46277900
O	33.96623100	-8.49302700	-0.90070900
H	33.13866000	-8.03225700	-0.72857800
C	36.88182100	-7.23894000	-2.13339600
O	35.74268500	-6.54186900	-2.00434100
C	35.84778000	-5.60448100	1.66308700
H	36.55339300	-4.99844900	2.23498000
H	35.78639200	-6.57207900	2.16296600
H	34.86508600	-5.13007600	1.73127700
H	37.87690500	-6.98775800	1.09875000
C	35.84941500	-3.19347000	0.05545500
H	35.99437600	-2.97485100	1.12031600
H	34.78801300	-3.43596200	-0.09366900
C	36.62350700	-9.51435600	0.96110000
H	36.73307400	-8.83162000	1.81218100
C	37.93038900	-10.28369400	0.84139300
H	37.98882300	-10.75912800	-0.14824600
H	37.93764600	-11.08458700	1.59105200
C	35.50241000	-10.50002100	1.27518000
H	34.53094100	-10.00732800	1.33344800
H	35.68472700	-10.99997900	2.22878500
H	35.43412300	-11.26784200	0.49831100
O	36.20993600	-2.06743500	-0.72991500
H	35.69763300	-1.31389500	-0.42484400
O	37.37908300	-7.38410200	-3.22213600
O	39.03318700	-9.41687700	1.05124500
H	39.84050800	-9.92378400	0.92876900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -961.128840

186) Conformer **30C1**

O	-1.73998200	2.71480200	-0.60385800
C	2.82740000	2.42584400	-0.07763700
C	-1.63437100	1.61354800	-0.14977700
C	-0.78228200	0.74750200	-2.33887900
H	2.74869100	2.64226900	-1.14596600

H	2.22865900	3.15978400	0.46400000
H	3.86806000	2.54205500	0.22844700
H	0.43859500	1.29209100	2.43635000
H	1.37776400	-0.20567500	2.62700600
H	-0.14416700	-0.00317400	3.48566800
H	-1.59940500	1.32531700	-2.76919600
H	-0.65824100	-0.14677800	-2.94857700
H	0.11956600	1.35579200	-2.37658000
H	5.06949300	0.72105400	-0.54051500
H	4.66668100	-0.25381800	0.86644800
H	4.96933100	-1.02889600	-0.69802600
H	3.30067900	-2.05625600	1.19405600
H	0.71949400	-3.33275100	-1.32005300
H	-0.85366600	-2.61883200	-1.03386000
H	0.19611500	-3.04641300	0.33074400
H	-4.47361100	0.41810300	0.58638300
H	-4.56376200	-0.93125800	1.72660100
H	2.47742100	0.82277900	1.28764100
O	-2.79708200	-1.07256600	-1.81557200
C	2.32844100	1.03009800	0.22292600
C	-1.11412700	0.38660100	-0.90875800
C	0.37494500	0.20912900	2.54739900
H	-0.35382900	-1.51093100	1.53885200
C	0.85148200	-1.27161400	-0.75434000
O	0.93319300	1.06513200	-0.06712100
C	3.03857200	-0.05922000	-0.56501200
O	-2.00587900	1.34823300	1.11149200
H	-4.78582800	-1.21799500	-0.00839800
H	0.89282200	-0.98335300	-1.80857800
H	2.77245800	-2.13895600	-1.00631800
C	0.12775600	-0.10213800	-0.04265000
C	4.51522700	-0.15942400	-0.21345500
O	2.38797400	-1.83162500	0.99604000
H	2.94598500	0.17825500	-1.63267000
H	-2.21834200	-0.08249600	2.51538000
H	-2.52729300	-1.93965200	0.77920700
C	0.17627500	-2.63405500	-0.67849000
C	-2.73672300	-0.88358900	0.57423400
C	-4.23188500	-0.63687100	0.72903100
C	2.31521500	-1.38370900	-0.34944400
C	-2.27000200	-0.60839800	-0.83720600
C	-0.39405000	-0.42914600	1.39967200
C	-1.86511700	-0.03657000	1.48473800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1038.440690

187) Conformer **30C2**

O	-1.73577300	2.70942700	-0.63114300
C	2.81857500	2.42945900	-0.06829300
C	-1.63159300	1.61276400	-0.16626000
C	-0.77512800	0.72657000	-2.34491300
H	2.74619900	2.64358000	-1.13763600
H	2.21191400	3.16080900	0.46806100
H	3.85625900	2.55117600	0.24488300
H	0.43629800	1.29255000	2.43981600
H	1.37245800	-0.20610200	2.62996700
H	-0.14988800	-0.00050000	3.48956100
H	-1.58761300	1.30671000	-2.78094700
H	-0.65496300	-0.17245800	-2.94828300
H	0.13041100	1.32932700	-2.38458800
H	5.05389600	0.75551500	-0.54137400
H	4.67495900	-0.28793900	0.83792800
H	4.97224000	-0.99266900	-0.75113500
H	2.28113600	-2.69130500	1.10417700
H	0.74675400	-3.35310400	-1.26807100
H	-0.83522100	-2.64157400	-1.03376100
H	0.16203000	-3.03928800	0.36333500
H	-4.46939700	0.44679800	0.55677400
H	-4.57964500	-0.88343100	1.71715900
H	2.47534100	0.82454300	1.29565100
O	-2.78018000	-1.10511300	-1.80960200
C	2.32571800	1.03166800	0.23151900
C	-1.11225300	0.37799300	-0.91299500
C	0.36983900	0.20986600	2.55112100
H	-0.37651400	-1.50583800	1.54754200
C	0.85573300	-1.27727000	-0.74217600
O	0.92899900	1.06238400	-0.06156300
C	3.03718400	-0.05307200	-0.56212100
O	-2.00376700	1.36060100	1.09776000
H	-4.79305700	-1.19552900	-0.01456500
H	0.89007500	-1.00496800	-1.80133200
H	2.79215100	-2.12968600	-0.99388600
C	0.12699400	-0.10552500	-0.03874700
C	4.51870300	-0.14365900	-0.23290800
O	2.50926100	-1.76305800	1.01576500
H	2.92136200	0.18536000	-1.62704600
H	-2.22680000	-0.05676900	2.51283500
H	-2.54803500	-1.92692600	0.79615200

C	0.18636500	-2.64215200	-0.65461400
C	-2.74457800	-0.87125400	0.57653100
C	-4.23851300	-0.60797800	0.71729600
C	2.32729900	-1.37777400	-0.33917300
C	-2.26589700	-0.61838600	-0.83525600
C	-0.40228900	-0.42408300	1.40327700
C	-1.87126900	-0.02086600	1.48255400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1038.440170

188) Conformer **31C1**

C	-0.89977200	0.34485600	0.60093800
C	-0.08141800	1.12107200	-0.44069200
H	-0.57532700	2.03374700	-0.75777500
C	1.28407200	1.41899000	0.16957600
C	2.08125300	0.15417600	0.41434200
H	2.25273300	0.08786300	1.49514800
C	1.16291400	-1.01147900	0.00621000
H	1.65954500	-1.97385000	0.11564200
C	-0.14755500	-1.02357600	0.83898300
C	-1.07358700	-2.16111200	0.33851900
H	-0.65429200	-2.67989900	-0.52661600
H	-1.22116100	-2.90629700	1.12322100
C	-2.37482300	-1.52661500	-0.03321600
H	-3.06003500	-2.00609000	-0.72439400
C	-2.27698800	-0.06541100	0.09141700
O	1.62937900	2.54033700	0.43867800
O	-2.98288700	-0.84327200	1.05920400
C	-3.17505800	0.84107300	-0.70410300
O	-4.46887000	0.65990800	-0.46709600
H	-4.55399100	0.00359800	0.24844600
O	-2.78281400	1.65054000	-1.50086600
O	0.12422900	0.34066700	-1.63087400
C	0.79303700	-0.81056900	-1.43592800
O	1.03006000	-1.53875800	-2.36034100
O	0.15310400	-1.13922100	2.20619300
H	0.58054800	-1.98861800	2.35999800
C	-1.06116700	1.20264100	1.85376100
H	-0.10656400	1.40471300	2.33702300
H	-1.51900600	2.15898000	1.58914300
H	-1.69872300	0.69613000	2.57538200
C	3.45867000	0.16454600	-0.29263100
H	3.30004700	0.45196600	-1.33998200
C	4.11235900	-1.21249400	-0.27728600

H	3.56705900	-1.94654500	-0.87252200
H	4.20011400	-1.59299000	0.74509600
H	5.12017200	-1.14109900	-0.69211700
C	4.39345400	1.18548100	0.34367200
H	4.60262600	0.91343900	1.38311200
H	3.97255800	2.18975100	0.33542100
H	5.34373200	1.20411900	-0.19477200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.936844

189) Conformer **31C2**

C	-0.89929900	0.34646400	0.57113900
C	-0.08252300	1.10927600	-0.47972900
H	-0.57854900	2.01387600	-0.81707600
C	1.27769300	1.42466900	0.13603800
C	2.07481100	0.16737000	0.42115100
H	2.22563100	0.12048800	1.50580600
C	1.17125500	-1.01217300	0.01358800
H	1.67058800	-1.96850900	0.14764400
C	-0.14663900	-1.03120100	0.81601600
C	-1.06993200	-2.16075700	0.29123300
H	-0.65711100	-2.65043600	-0.59385600
H	-1.19231500	-2.93426200	1.05222900
C	-2.37900400	-1.52614400	-0.04466800
H	-3.08359200	-2.00132300	-0.71876800
C	-2.28224400	-0.06549700	0.08771800
O	1.61856300	2.55325100	0.37872200
O	-2.95671300	-0.85267900	1.07278300
C	-3.20119000	0.84296500	-0.67949800
O	-4.48867800	0.66815700	-0.40658500
H	-4.55999800	0.01069400	0.30887200
O	-2.82619500	1.65003200	-1.48691100
O	0.13814900	0.31022800	-1.65480200
C	0.82332200	-0.82734700	-1.43730100
O	1.09370800	-1.55670700	-2.35097400
O	0.23100000	-1.22952300	2.15299000
H	-0.56135100	-1.31922100	2.69320500
C	-1.03575100	1.21258900	1.82110700
H	-0.07857800	1.36812500	2.31697000
H	-1.44529800	2.19016700	1.55567000
H	-1.71197700	0.74706400	2.53766600
C	3.46658600	0.17063500	-0.25734700
H	3.32918800	0.43997600	-1.31247400
C	4.12457500	-1.20351900	-0.20486100

H	5.14170200	-1.13448700	-0.59675100
H	3.59617400	-1.94890200	-0.80115300
H	4.18897100	-1.56768700	0.82511500
C	4.38467100	1.20526600	0.38134600
H	4.57221700	0.95133600	1.42946400
H	3.96137600	2.20791400	0.34689100
H	5.34624900	1.21752500	-0.13683700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.937666

190) Conformer **31C3**

C	-0.89547500	-0.05976100	-0.65321800
C	-0.10686600	-1.23337000	-0.06117100
H	-0.64885500	-2.17219500	-0.11739800
C	1.24472700	-1.32705000	-0.76453800
C	2.02291600	-0.03874300	-0.64259600
H	1.92647100	0.43937200	-1.62613800
C	1.24864000	0.85548000	0.34437700
H	1.80619800	1.75045900	0.61567000
C	-0.10386700	1.26992900	-0.28223400
C	-0.96888100	2.04925800	0.73988400
H	-0.53599700	2.03829800	1.74274800
H	-1.05241000	3.09656200	0.44265300
C	-2.30543500	1.38458100	0.76232400
H	-2.99696000	1.53089800	1.58519800
C	-2.26355800	0.14053800	-0.01830700
O	1.61767600	-2.31660600	-1.33809100
O	-2.89875400	1.31373500	-0.53416200
C	-3.22099000	-0.98286100	0.26339000
O	-4.49821500	-0.66392100	0.09382300
H	-4.53986200	0.24662000	-0.25015900
O	-2.88128400	-2.07622300	0.62869100
O	0.18191000	-1.01951100	1.33282300
C	0.91885600	0.07807700	1.59095100
O	1.21016500	0.35550000	2.72117900
O	0.21941700	2.05166400	-1.40171900
H	-0.59411300	2.38225600	-1.79760200
C	-1.06506500	-0.29157800	-2.15306600
H	-0.11409300	-0.26315400	-2.68399000
H	-1.52411700	-1.26754400	-2.32899100
H	-1.71255100	0.46801200	-2.59019100
C	3.52609400	-0.24920400	-0.40431300
H	3.82985200	-0.95491900	-1.18487900
C	3.85555900	-0.87796500	0.94287300

H	4.91894400	-1.12333500	0.98595200
H	3.29893900	-1.80365600	1.11228300
H	3.64438900	-0.19551000	1.76941400
C	4.30462600	1.04171900	-0.61415100
H	4.05837800	1.79047200	0.14392600
H	4.10312900	1.47612800	-1.59645700
H	5.37765500	0.84984500	-0.54362400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.937831

191) Conformer **31C4**

C	-0.89428500	-0.02717900	-0.67946100
C	-0.11133500	-1.22429800	-0.12485800
H	-0.65637300	-2.15737000	-0.22423900
C	1.24878000	-1.29867200	-0.81160300
C	2.03018600	-0.02061000	-0.62867400
H	1.94500900	0.49543000	-1.59479600
C	1.24358300	0.83854100	0.37627500
H	1.80210500	1.71949500	0.69218500
C	-0.10243400	1.28028900	-0.27175000
C	-0.97094900	2.05263200	0.75107600
H	-0.53235300	2.04921500	1.75139400
H	-1.07948500	3.09654400	0.44954300
C	-2.30166000	1.37291800	0.78333200
H	-2.97528700	1.49347200	1.62534700
C	-2.25950500	0.14593500	-0.02369600
O	1.62596000	-2.26808000	-1.41626400
O	-2.92309100	1.31826500	-0.49812100
C	-3.20041500	-0.99412500	0.25258400
O	-4.48297700	-0.67807700	0.12143300
H	-4.53395200	0.24084400	-0.19957200
O	-2.84802000	-2.09509000	0.58141600
O	0.15871300	-1.06524500	1.28016300
C	0.88796500	0.02431000	1.58979500
O	1.14886500	0.26856200	2.73555800
O	0.14505600	2.03380900	-1.43041500
H	0.56995600	2.86092100	-1.17831000
C	-1.07706900	-0.21326400	-2.18405500
H	-0.12619000	-0.21554200	-2.71608200
H	-1.57783200	-1.16480600	-2.37918900
H	-1.68337900	0.59225300	-2.59296800
C	3.52896700	-0.24528400	-0.37848300
H	3.84014500	-0.92875800	-1.17575800
C	3.83597600	-0.91551900	0.95390700

H	4.89788300	-1.16538700	1.00680600
H	3.27407000	-1.84399200	1.08649000
H	3.61306600	-0.25752700	1.79719500
C	4.31638100	1.04730500	-0.53876800
H	4.06156700	1.77539300	0.23651100
H	4.13254500	1.51020700	-1.51153400
H	5.38734600	0.84858200	-0.45689900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.937522

192) Conformer **31C5**

C	-0.89402300	0.35048300	0.59748100
C	-0.08572900	1.11027200	-0.46285100
H	-0.58176000	2.01769400	-0.79000400
C	1.28449700	1.41868600	0.13179100
C	2.08348000	0.15951400	0.39932700
H	2.25639100	0.11059700	1.48053400
C	1.16677300	-1.01509700	0.00886600
H	1.66337200	-1.97407000	0.13472400
C	-0.13770300	-1.02711000	0.83342400
C	-1.06660600	-2.15982800	0.32803400
H	-0.67198600	-2.64447100	-0.56822200
H	-1.16343300	-2.93563100	1.09060300
C	-2.38768500	-1.53030800	0.03108400
H	-3.11179700	-2.00392500	-0.62316600
C	-2.28839900	-0.06573200	0.14390900
O	1.63215300	2.54577300	0.37394300
O	-2.92607800	-0.84843700	1.14870500
C	-3.19639100	0.83982100	-0.62784800
O	-4.44204400	0.37789400	-0.67262500
H	-4.96589700	0.99048200	-1.21067500
O	-2.84407900	1.86095700	-1.16150500
O	0.11148100	0.31056300	-1.64314800
C	0.79409300	-0.83037800	-1.43603800
O	1.04489500	-1.56217100	-2.35366800
O	0.26166100	-1.22167000	2.16572200
H	-0.52452900	-1.30239600	2.71632700
C	-1.00814100	1.22017500	1.84748700
H	-0.04345400	1.37784200	2.32808000
H	-1.42281500	2.19593600	1.58370400
H	-1.67348600	0.75646900	2.57526200
C	3.46047600	0.15932000	-0.30848200
H	3.30097300	0.42836000	-1.36063400
C	4.11618700	-1.21634000	-0.26961600

H	5.12417000	-1.15053900	-0.68506500
H	3.57197300	-1.96106800	-0.85232300
H	4.20344700	-1.57928200	0.75910400
C	4.39465200	1.19222600	0.30929700
H	4.60497100	0.93821100	1.35306600
H	3.97247900	2.19564500	0.28416300
H	5.34457400	1.20264100	-0.23005100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.937111

193) Conformer **31C6**

C	-0.86138800	-0.22931600	-0.61364100
C	0.01640900	-1.09076200	0.30174700
H	-0.41598600	-2.06695500	0.49759900
C	1.40302400	-1.21871800	-0.32775900
C	2.04905300	0.13378700	-0.52154400
H	1.99720300	0.32584400	-1.60039800
C	1.11461500	1.16713300	0.13801500
H	1.56632000	2.15833900	0.15627200
C	-0.23087000	1.23098900	-0.62038700
C	-1.22730900	2.16623400	0.10965000
H	-0.84834300	2.49810400	1.07891000
H	-1.40651300	3.06470800	-0.48424900
C	-2.48476700	1.38472500	0.30173800
H	-3.22735700	1.67705900	1.03653900
C	-2.27268500	-0.01673400	-0.08591500
O	1.87876800	-2.28294100	-0.62662600
O	-3.00339000	0.87907700	-0.92816000
C	-3.11899800	-1.11453900	0.49437100
O	-4.41428200	-1.00008100	0.22753700
H	-4.53514400	-0.23626000	-0.36512100
O	-2.68379100	-2.01521500	1.16030600
O	0.20094200	-0.46917500	1.58678400
C	0.79844800	0.73629500	1.54381500
O	1.00124300	1.34702000	2.55690600
O	0.08065700	1.69439500	-1.90784400
H	-0.73578900	1.80564400	-2.40673000
C	-0.93004800	-0.88764300	-1.98981700
H	0.03749800	-0.89433900	-2.49048500
H	-1.26961600	-1.92158600	-1.89219500
H	-1.63446500	-0.36179400	-2.63372800
C	3.53585800	0.23231900	-0.12145800
H	3.75750200	1.30589000	-0.10642600
C	4.42986800	-0.40582400	-1.17780800

H	5.48092000	-0.24344800	-0.92752700
H	4.24785100	0.02544400	-2.16558800
H	4.25757000	-1.48182900	-1.23938600
C	3.84778100	-0.32992900	1.26037000
H	3.64440500	-1.40296900	1.30645800
H	3.28150000	0.16284700	2.05243800
H	4.90732600	-0.18743600	1.48413000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.936714

194) Conformer **31C7**

C	-0.86027000	-0.16992400	-0.65990200
C	0.01416500	-1.11359400	0.17631700
H	-0.41879800	-2.10417900	0.27064300
C	1.40886800	-1.17996800	-0.44233600
C	2.05568200	0.18421700	-0.49208600
H	2.01679400	0.47987900	-1.54854600
C	1.10739000	1.14667600	0.24551400
H	1.55770300	2.13203000	0.36977300
C	-0.22901100	1.27524400	-0.54120300
C	-1.23113300	2.16226600	0.23771700
H	-0.85038600	2.44904100	1.22042900
H	-1.43358800	3.08349100	-0.31271900
C	-2.48142200	1.35895900	0.39658800
H	-3.20617400	1.59087700	1.16997200
C	-2.26807600	-0.00818100	-0.09760100
O	1.89028400	-2.21010500	-0.83687100
O	-3.02723200	0.93859600	-0.85085500
C	-3.09692000	-1.15184100	0.41824500
O	-4.39855800	-1.01765000	0.19402000
H	-4.53020900	-0.20962700	-0.33497200
O	-2.64757900	-2.10213400	1.00076600
O	0.17937200	-0.61934900	1.51793200
C	0.76508300	0.59006900	1.59837800
O	0.93425900	1.11018900	2.66731200
O	0.01839600	1.76415500	-1.83420500
H	0.35027900	2.66610400	-1.76741600
C	-0.94383300	-0.70717600	-2.08683800
H	0.02876700	-0.71939900	-2.57758100
H	-1.33131800	-1.72887700	-2.07474200
H	-1.60884200	-0.08728300	-2.68449500
C	3.53547900	0.24487200	-0.06144500
H	3.75606800	1.31242100	0.05579200
C	4.44776000	-0.29431500	-1.15655100

H	5.49430600	-0.15589500	-0.87488300
H	4.28171200	0.22550800	-2.10369000
H	4.27744300	-1.36000300	-1.31933000
C	3.82355000	-0.44159200	1.26841700
H	3.61933900	-1.51406300	1.21273400
H	3.24263200	-0.02225800	2.09169200
H	4.87886200	-0.32165600	1.52325200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.935759

195) Conformer **31C8**

C	-0.89402400	0.35048800	0.59749100
C	-0.08572200	1.11027800	-0.46283500
H	-0.58174800	2.01770300	-0.78998500
C	1.28450100	1.41868100	0.13181900
C	2.08348400	0.15950600	0.39933100
H	2.25641800	0.11058100	1.48053400
C	1.16676800	-1.01510000	0.00887600
H	1.66336100	-1.97407600	0.13473100
C	-0.13770300	-1.02710400	0.83344200
C	-1.06660900	-2.15982700	0.32806400
H	-0.67197800	-2.64449300	-0.56817500
H	-1.16345000	-2.93561200	1.09065000
C	-2.38768100	-1.53030600	0.03108800
H	-3.11178200	-2.00392800	-0.62317200
C	-2.28839400	-0.06573000	0.14390300
O	1.63215200	2.54576200	0.37400500
O	-2.92609000	-0.84842600	1.14869400
C	-3.19637500	0.83981900	-0.62787500
O	-4.44202700	0.37789100	-0.67266600
H	-4.96587500	0.99047900	-1.21072200
O	-2.84405600	1.86095200	-1.16153200
O	0.11148600	0.31057200	-1.64313400
C	0.79408200	-0.83037800	-1.43602600
O	1.04486900	-1.56217600	-2.35365600
O	0.26166800	-1.22165300	2.16573800
H	-0.52451700	-1.30239100	2.71634800
C	-1.00815500	1.22017700	1.84749600
H	-0.04347200	1.37784600	2.32809700
H	-1.42283000	2.19593700	1.58371300
H	-1.67350400	0.75646600	2.57526500
C	3.46046500	0.15931100	-0.30850900
H	3.30093800	0.42833800	-1.36066000
C	4.11618100	-1.21634700	-0.26964100

H	5.12415800	-1.15054600	-0.68510700
H	3.57196100	-1.96108300	-0.85233200
H	4.20345900	-1.57927800	0.75908200
C	4.39465200	1.19222600	0.30923700
H	4.60499300	0.93822700	1.35300500
H	3.97247800	2.19564500	0.28409900
H	5.34456200	1.20263500	-0.23013100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.937110

196) Conformer **31C9**

C	-0.88812000	-0.05252200	-0.70793800
C	-0.11655800	-1.22251100	-0.08219600
H	-0.66283600	-2.15694500	-0.14811000
C	1.25569000	-1.33667900	-0.73698500
C	2.04319700	-0.05752800	-0.60013800
H	1.98304400	0.41076700	-1.59217400
C	1.23950800	0.85460300	0.34185100
H	1.79510800	1.74893800	0.62410300
C	-0.08997000	1.26850300	-0.35812300
C	-0.96463300	2.10723000	0.60388900
H	-0.54220100	2.15354100	1.61012900
H	-1.05065100	3.13433600	0.24219400
C	-2.30656200	1.44956200	0.64346600
H	-2.99675300	1.61750400	1.46353500
C	-2.26405000	0.17148500	-0.08495300
O	1.63738100	-2.33625000	-1.28831200
O	-2.89402200	1.32208300	-0.63576100
C	-3.19609000	-0.95109900	0.25181500
O	-4.41215500	-0.51136200	0.56063600
H	-4.95431900	-1.28033000	0.79245000
O	-2.89001500	-2.11663900	0.25617500
O	0.12511100	-0.99465800	1.31990600
C	0.85318100	0.10641400	1.58807500
O	1.09144100	0.40858500	2.72525800
O	0.19013600	1.95387600	-1.55202000
H	0.60327600	2.79646100	-1.33506300
C	-1.04665700	-0.31647600	-2.20356400
H	-0.08745200	-0.35288700	-2.71957800
H	-1.55223100	-1.27329700	-2.35446900
H	-1.64052000	0.47086500	-2.66300000
C	3.53425600	-0.27898500	-0.30524600
H	3.86030700	-0.99662800	-1.06575600
C	3.80624000	-0.89469000	1.06067300

H	4.86559800	-1.14520300	1.14997300
H	3.23764800	-1.81531900	1.21719800
H	3.56530500	-0.20195600	1.87050900
C	4.33292900	1.00194600	-0.50016300
H	4.06683400	1.76136900	0.24051200
H	4.17187000	1.42723600	-1.49392900
H	5.40078500	0.80096300	-0.38836100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.936767

197) Conformer **31C10**

C	0.88952200	0.09031800	-0.66759800
C	0.11337200	1.22928400	0.00458000
H	0.65886200	2.16691700	-0.00550000
C	-1.24759100	1.37149100	-0.67110900
C	-2.03169900	0.08251100	-0.61718500
H	-1.94822800	-0.33704800	-1.62826700
C	-1.24930100	-0.87109400	0.30513000
H	-1.80744200	-1.77846000	0.53055900
C	0.09401500	-1.25317500	-0.36055600
C	0.96360600	-2.09339700	0.60679400
H	0.55412200	-2.11645200	1.61928800
H	1.01427400	-3.12823300	0.26179200
C	2.31483800	-1.45879100	0.61954100
H	3.03126500	-1.65588700	1.40981000
C	2.27185900	-0.16484700	-0.08033100
O	-1.62377800	2.39662200	-1.17684300
O	2.85980500	-1.31642500	-0.67980900
C	3.22726900	0.93671200	0.25639000
O	4.45687500	0.48280300	0.47617700
H	5.01233300	1.23849000	0.72031600
O	2.92076600	2.09927000	0.33651200
O	-0.15702400	0.93485700	1.38898000
C	-0.90037500	-0.16994600	1.59114700
O	-1.18308100	-0.50958300	2.70674800
O	-0.24456300	-1.97153700	-1.51862700
H	0.56675800	-2.26971600	-1.94399300
C	1.02857100	0.41232700	-2.15437500
H	0.06813600	0.41655800	-2.66891500
H	1.48637000	1.39678200	-2.27715700
H	1.66734200	-0.31938600	-2.64818000
C	-3.53092900	0.28430000	-0.34974000
H	-3.84073200	1.03591000	-1.08375000
C	-3.84285700	0.83366200	1.03578200

H	-4.90484900	1.07904000	1.10568200
H	-3.28103400	1.74615700	1.25286400
H	-3.62450600	0.10308200	1.81811500
C	-4.31729500	-0.98926200	-0.62602300
H	-4.06535100	-1.78205900	0.08391400
H	-4.12862500	-1.36590700	-1.63439100
H	-5.38872400	-0.79841500	-0.53197900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1107.937247

198) Conformer **32C1**

C	0.73809600	0.10794800	0.87518100
C	0.15093600	-0.72673300	-0.27301600
H	0.85605400	-1.46303300	-0.65251600
C	-1.12086200	-1.38873600	0.22948600
C	-2.21583900	-0.37339300	0.50162300
H	-2.50158600	-0.48184900	1.55562700
C	-1.56714800	1.01417300	0.31642500
H	-2.28047900	1.81437500	0.49867600
C	-0.35020800	1.15997300	1.25372100
C	0.33295500	2.52935900	1.16328400
H	-0.36363900	3.32602900	0.89155900
H	0.74821000	2.78637500	2.14164400
C	1.46803200	2.34951900	0.16280300
H	2.24953400	3.10371600	0.27752900
H	1.10465700	2.42480300	-0.86682600
C	1.98709200	0.94132800	0.44964300
O	-1.19879400	-2.57611600	0.42500800
O	-0.20756200	0.11257300	-1.39117400
C	-1.09792300	1.08036600	-1.10569700
O	-1.43748600	1.85773300	-1.95841100
H	-0.71872800	0.97845000	2.26693500
C	1.08360000	-0.81229400	2.04327200
H	0.21657300	-1.36463900	2.41192100
H	1.47160400	-0.21834300	2.87370500
H	1.84975600	-1.53290700	1.74985900
C	-3.47913100	-0.61635300	-0.35922500
H	-3.16400700	-0.70685300	-1.40692600
C	-4.45539600	0.55044600	-0.26139500
H	-4.72386700	0.74730500	0.78121700
H	-5.37348500	0.30575300	-0.80038300
H	-4.05763000	1.46989900	-0.69312500
C	-4.18036500	-1.90934500	0.03722200
H	-3.52234400	-2.77425300	-0.03447100

H	-5.04371300	-2.07702800	-0.61089200
H	-4.54335800	-1.84518200	1.06796500
C	2.84710600	0.39402600	-0.67951400
H	3.62939000	1.14373600	-0.90643500
H	2.23791700	0.31173500	-1.58327900
N	3.44079800	-0.90795100	-0.42353200
C	4.50600900	-0.84465700	0.55453900
H	4.90204200	-1.84688400	0.73164900
H	4.14026700	-0.45816500	1.50661400
H	5.34032600	-0.20062100	0.22273900
C	3.92659100	-1.49920300	-1.65251200
H	4.72255100	-0.89795400	-2.12758100
H	3.10856300	-1.60278400	-2.36899100
H	4.33270800	-2.49275500	-1.45018200
H	2.60655300	1.01466300	1.35028500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -943.385523

199) Conformer **32C2**

C	-0.71664800	0.20841600	-0.84698800
C	-0.17530700	-0.76718300	0.20560900
H	-0.92085500	-1.49285800	0.52361500
C	1.07025200	-1.45742200	-0.32522500
C	2.15604300	-0.46030200	-0.66699100
H	2.18900400	-0.45473100	-1.76559800
C	1.64119800	0.92810800	-0.24035300
H	2.40582100	1.69601000	-0.34663400
C	0.40274300	1.26914900	-1.10224200
C	-0.21968500	2.63741200	-0.79652900
H	0.50817700	3.34379700	-0.39033900
H	-0.60055900	3.06963000	-1.72569700
C	-1.38223300	2.35956100	0.14842200
H	-2.13461800	3.15085800	0.12783900
H	-1.03914000	2.27497000	1.18404600
C	-1.94388200	1.02561100	-0.34064800
O	1.16396900	-2.65139400	-0.45943400
O	0.24363600	-0.06178200	1.39492900
C	1.18328100	0.88116300	1.18751500
O	1.53598700	1.58583500	2.09585800
H	0.73500500	1.22518200	-2.14245500
C	-1.07153300	-0.57708600	-2.10738900
H	-0.21458000	-1.11665400	-2.51887000
H	-1.42751800	0.10756000	-2.88023400
H	-1.86205800	-1.30044200	-1.89783600

C	3.55130800	-0.90480800	-0.19835600
H	3.66127300	-1.92105400	-0.59248200
C	3.70321400	-0.97738400	1.31532800
H	3.67504800	0.01473400	1.77165700
H	4.66640500	-1.42570900	1.56916900
H	2.92447300	-1.58913400	1.77846300
C	4.64286300	-0.04364500	-0.81782900
H	4.56258200	-0.01763200	-1.90754800
H	5.62791300	-0.44065500	-0.56177100
H	4.60190900	0.98564600	-0.45066600
C	-2.84701800	0.36824500	0.69206100
H	-3.60636000	1.11132500	1.00293600
H	-2.25975000	0.14766200	1.58775400
N	-3.48112900	-0.86617500	0.26049600
C	-4.51914100	-0.63684000	-0.72210300
H	-4.94745700	-1.59193400	-1.03353300
H	-4.11602800	-0.14747300	-1.60956600
H	-5.33688900	-0.00749200	-0.32707700
C	-4.01794500	-1.58875800	1.39438100
H	-4.80132900	-1.02100000	1.92786700
H	-3.22128500	-1.81586900	2.10643100
H	-4.45643200	-2.53123500	1.05907300
H	-2.53863600	1.24303800	-1.23481700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -943.385580

200) Conformer **32C3**

C	-0.53373200	0.60446500	0.82089900
C	0.15034500	0.89231100	-0.52618600
H	-0.39013100	1.61183600	-1.13799100
C	1.55898400	1.38909500	-0.24137600
C	2.43322300	0.29912200	0.34832800
H	2.79614800	0.66539300	1.31698000
C	1.50020800	-0.90252200	0.60265800
H	2.03985300	-1.74046300	1.03722400
C	0.33364300	-0.48647100	1.52305700
C	-0.62150400	-1.64061400	1.85173900
H	-0.11815700	-2.61033500	1.84787100
H	-1.02591700	-1.49386300	2.85708700
C	-1.75023400	-1.53769500	0.83216500
H	-2.65979900	-2.03964200	1.16517800
H	-1.47112800	-1.99150000	-0.12348100
C	-1.95044200	-0.03380600	0.67685300
O	1.88919000	2.53338800	-0.42871500

O	0.25860300	-0.30761600	-1.31738300
C	0.94691600	-1.30597700	-0.73120400
O	1.06980500	-2.36248100	-1.29164800
H	0.78609500	-0.08548700	2.43386000
C	-0.62612100	1.89620500	1.62903600
H	0.34317700	2.37805500	1.77117700
H	-1.03560300	1.67863700	2.61744400
H	-1.28890300	2.61623800	1.14100500
C	3.66687300	-0.01525200	-0.53227500
H	3.31563900	-0.19416900	-1.55679800
C	4.38706200	-1.27152600	-0.05585800
H	4.67307300	-1.18127800	0.99673200
H	5.30083900	-1.41214000	-0.63761800
H	3.78338800	-2.17268300	-0.17183100
C	4.63988500	1.15642700	-0.56391800
H	4.17144200	2.07222500	-0.92179600
H	5.48234800	0.92082100	-1.21830300
H	5.03766100	1.34910700	0.43752400
C	-2.73734200	0.39303400	-0.55131700
H	-2.22998800	0.02187100	-1.44599800
H	-2.74643600	1.49879400	-0.62242900
N	-4.09283100	-0.12972600	-0.58183800
C	-4.67415400	0.04543800	-1.89561800
H	-5.67324000	-0.39542700	-1.92040000
H	-4.05969700	-0.45554800	-2.64679900
H	-4.76599500	1.10874500	-2.18276300
C	-4.94354000	0.46530300	0.42622500
H	-5.02726400	1.56166700	0.31293800
H	-4.56857500	0.25641900	1.42908600
H	-5.94711200	0.04126300	0.35273300
H	-2.49312400	0.30799700	1.56495300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -943.385190

201) Conformer **32C4**

C	-0.71554200	0.16026900	-0.87132100
C	-0.07004200	-0.64222700	0.26619200
H	-0.73026000	-1.41361100	0.65671600
C	1.24049400	-1.24127200	-0.22118600
C	2.22692500	-0.16431300	-0.62229300
H	2.31896600	-0.25045400	-1.71318400
C	1.54273300	1.19034700	-0.35035400
H	2.22579000	2.01848900	-0.53688200
C	0.28479600	1.30194700	-1.24080700

C	-0.48406400	2.61907400	-1.07718800
H	0.16157100	3.44108300	-0.75892300
H	-0.91147000	2.90327000	-2.04250100
C	-1.60802000	2.31871900	-0.09316400
H	-2.44134800	3.01847500	-0.18581400
H	-1.25610600	2.38007200	0.94114500
C	-2.02329000	0.88855800	-0.43426100
O	1.43220400	-2.42945200	-0.29119300
O	0.26042600	0.21638100	1.37976200
C	1.08861100	1.23390200	1.07702300
O	1.36780900	2.05189700	1.91376100
H	0.62907700	1.18481900	-2.27152200
C	-0.98588300	-0.77679300	-2.04610200
H	-0.07623900	-1.25574800	-2.41679700
H	-1.41852200	-0.21207100	-2.87479600
H	-1.69106100	-1.55892600	-1.75773600
C	3.64960500	-0.32685500	-0.04399700
H	4.14106400	0.63815200	-0.21581400
C	4.43358600	-1.38577700	-0.80973600
H	3.98729400	-2.37340200	-0.67899600
H	5.46371200	-1.42690000	-0.44757300
H	4.46038300	-1.16407700	-1.87980400
C	3.68848100	-0.61169300	1.45318700
H	3.20358300	0.16736100	2.04353100
H	4.72646500	-0.67224900	1.78815200
H	3.21264900	-1.56790400	1.68671500
C	-2.84812400	0.24721000	0.67160100
H	-3.68334300	0.93192800	0.91451200
H	-2.23904300	0.18417900	1.57750900
N	-3.34505900	-1.08620300	0.37582300
C	-4.40320200	-1.07253100	-0.61189800
H	-4.72594100	-2.09519800	-0.81836900
H	-4.05701100	-0.63677100	-1.54987800
H	-5.28376600	-0.49751500	-0.27300700
C	-3.79890100	-1.74233700	1.58398200
H	-4.63902000	-1.21084900	2.06606200
H	-2.98188800	-1.80770000	2.30610500
H	-4.13262600	-2.75607200	1.35177400
H	-2.63999300	0.94705700	-1.33808800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -943.384383

202) Conformer **32C5**

C	-0.52269300	0.57533100	0.82654800
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C	0.12309600	0.91983500	-0.52344300
H	-0.46810700	1.61148600	-1.12034700
C	1.52073300	1.47552900	-0.29729200
C	2.40517400	0.48132500	0.42145500
H	2.52221200	0.89595800	1.43259900
C	1.58754300	-0.81531900	0.57476200
H	2.18598400	-1.62753000	0.98403500
C	0.37542600	-0.51897500	1.48905700
C	-0.53244500	-1.73183400	1.73476200
H	0.00597300	-2.67792800	1.64092500
H	-0.91893200	-1.68476200	2.75638000
C	-1.68661400	-1.59269800	0.74837500
H	-2.57641900	-2.13653300	1.06852700
H	-1.41823600	-1.97782800	-0.23971400
C	-1.92631000	-0.08801500	0.68917200
O	1.86184100	2.57657900	-0.64810600
O	0.29308100	-0.26359900	-1.33110600
C	1.03890200	-1.23038800	-0.75886500
O	1.17109700	-2.28983900	-1.31091200
H	0.78678800	-0.14993800	2.43179300
C	-0.62177000	1.84860900	1.66315500
H	0.34271700	2.34519000	1.79375400
H	-1.00443100	1.60702300	2.65660900
H	-1.30595700	2.56712200	1.20348200
C	3.82040900	0.39429100	-0.17342600
H	4.16536900	1.43333600	-0.21185200
C	3.86415000	-0.15979900	-1.59143300
H	3.60042200	-1.21950300	-1.61903700
H	4.87512900	-0.06498700	-1.99395200
H	3.19147400	0.37796600	-2.26485900
C	4.75918400	-0.37535900	0.74482800
H	4.76237400	0.04140800	1.75520300
H	5.78081900	-0.33435900	0.36009300
H	4.48033900	-1.43047800	0.81455800
C	-2.75601500	0.38418500	-0.49332100
H	-2.26402500	0.07169100	-1.41904300
H	-2.79238600	1.49163300	-0.50687100
N	-4.09907400	-0.16960300	-0.51815100
C	-4.72047800	0.06645500	-1.80377200
H	-5.70917600	-0.39721000	-1.82805000
H	-4.11537900	-0.37478700	-2.59875600
H	-4.84512500	1.14193200	-2.02583100
C	-4.93497000	0.34515500	0.54500500
H	-5.04522800	1.44406200	0.49960800

H	-4.52913600	0.08568400	1.52371900
H	-5.93079100	-0.09674000	0.47164700
H	-2.45083300	0.19022100	1.61001800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -943.385766

203) Conformer **32C6**

C	0.50123100	-0.63167400	0.77105400
C	-0.21397100	-0.71801700	-0.58586200
H	0.29451900	-1.36213100	-1.30057500
C	-1.64425700	-1.19462700	-0.37304900
C	-2.42881300	-0.22672100	0.48630900
H	-2.59646100	-0.75508600	1.43426800
C	-1.48391400	0.94807000	0.80723300
H	-2.00622600	1.73325200	1.35285100
C	-0.28409500	0.41635600	1.62287200
C	0.72965300	1.49978100	2.01468000
H	0.27051600	2.48824200	2.09206300
H	1.14197100	1.26139200	2.99881700
C	1.83710900	1.42708100	0.96922000
H	2.77786700	1.84568400	1.32953000
H	1.57097900	1.98001300	0.06352900
C	1.95007700	-0.06453100	0.67311000
O	-2.06205800	-2.22937900	-0.82853400
O	-0.30077900	0.58086800	-1.20717500
C	-0.94158700	1.51082600	-0.47187100
O	-1.00839200	2.64552900	-0.86406300
H	-0.70442200	-0.05788300	2.51329800
C	0.52070800	-2.01835200	1.40929000
H	-0.47745100	-2.45049500	1.51167100
H	0.95673800	-1.95645400	2.40817500
H	1.12524100	-2.71296000	0.81960100
C	-3.82169300	0.15833000	-0.05760500
H	-4.13094300	1.02661600	0.53621800
C	-4.83330300	-0.95377500	0.19209900
H	-4.57514400	-1.85158900	-0.37266900
H	-5.83052600	-0.63168900	-0.11734500
H	-4.87807600	-1.21989300	1.25142300
C	-3.82861500	0.56881000	-1.52570400
H	-3.17243700	1.41648600	-1.72935800
H	-4.83853300	0.86391200	-1.81931600
H	-3.52962000	-0.26183300	-2.17061700
C	2.70062000	-0.41339100	-0.60142200

H	2.20807400	0.07367800	-1.44799700
H	2.64420800	-1.50526900	-0.78196300
N	4.08387000	0.03120400	-0.60088100
C	4.64404800	-0.05596500	-1.93253500
H	5.66715000	0.32660100	-1.92976300
H	4.05456800	0.54665400	-2.62694500
H	4.67078900	-1.09195600	-2.31665400
C	4.90576300	-0.70187100	0.33778600
H	4.92252800	-1.78658600	0.12568200
H	4.55295700	-0.56231000	1.36051800
H	5.93230700	-0.33299700	0.28820900
H	2.47841000	-0.51994200	1.51804700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -943.384252

204) Conformer **33aC1**

H	3.15177100	1.03466800	-1.65937200
H	1.75797000	0.18135300	-2.33755400
H	1.76285100	3.12443700	-0.09075500
H	1.46931300	2.29679700	1.43354900
H	3.02890300	2.12239400	0.61334800
H	-1.09078700	-0.89075500	2.08552000
H	-0.80261200	0.84686000	2.11460900
H	1.48389300	0.38930500	2.40065400
H	1.17888300	-1.32498100	2.22923400
H	-0.40870200	1.17150100	-1.56546100
H	-0.48850400	2.09452100	-0.06731500
C	3.15050300	-0.70222700	0.50556700
C	1.95093700	2.19875100	0.45882400
C	2.06258600	1.03728000	-1.72926100
O	1.42069300	-2.38331700	-0.93257300
C	-0.50610100	-0.08778700	1.63673800
C	1.00196000	-0.35306900	1.76390100
C	1.68175100	-0.34598600	0.37802600
C	0.95173100	-1.41169900	-0.41112300
O	-0.38820200	-1.20441000	-0.47804600
C	-0.81728700	-0.00296600	0.15780800
Br	-2.74785900	0.08626600	-0.13326700
C	-0.13053500	1.16389800	-0.51019300
C	1.40988300	1.01994900	-0.34768100
H	1.76761100	1.94419900	-2.26274700
H	3.25897000	-1.65609700	1.02446800
H	3.68220600	0.05603400	1.08229600
H	3.63081500	-0.80460000	-0.46682400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -3113.812846

205) Conformer **33bC1**

C	-1.92533000	0.58900700	-2.17140400
C	-3.49439300	-0.68953400	0.31109000
C	-0.06704600	-1.93600900	-0.95433100
O	-1.70962200	-0.78044200	2.47061700
H	0.46890000	0.64948300	-1.71031900
Br	0.95431900	2.01609000	0.25929400
H	-1.86620700	-2.82232100	-0.13018300
H	-2.13261400	-1.99975400	-1.65223600
H	0.19239800	-1.78949400	-2.00408400
H	0.39183700	-2.87059400	-0.63400200
H	-3.14672700	1.86707800	-0.20837400
H	-1.65237800	2.74780300	-0.51355200
H	-1.87085300	1.89694400	1.01662900
H	-1.61292700	1.52339400	-2.64332900
H	-3.01138600	0.52393100	-2.25590700
H	-1.48893900	-0.23033500	-2.74451400
H	-4.04833700	-0.56501400	-0.62066100
H	-3.79420000	0.09193400	1.00720200
H	-3.78606800	-1.64574700	0.74878500
C	-2.06682800	1.84987000	-0.05590900
C	-1.57803900	-1.94645000	-0.71500600
C	-1.99889300	-0.68096300	0.05434600
C	-1.24806800	-0.77057300	1.36713800
C	-1.48392800	0.59767300	-0.70469900
C	0.08625700	0.54672800	-0.69758800
C	0.52963200	-0.79938300	-0.13631400
Br	2.46667800	-1.00160000	-0.11286400
O	0.09742200	-0.90038600	1.20882700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -5687.074861

206) Conformer **33cC1**

C	-1.10440600	-0.31171500	-0.32222400
C	-0.24943800	-1.40592000	-1.01331800
H	-0.64070900	-2.40340900	-0.79777500
H	-0.27099100	-1.28054400	-2.09877900
C	1.18710700	-1.32671900	-0.54470200
O	1.69536000	-0.01941600	-0.89209700
C	1.00417600	0.99700800	-0.35311400
C	-0.12789300	0.55238700	0.55426300

C	0.55076700	-0.33418700	1.62163300
H	-0.20433800	-0.68137900	2.32845700
H	1.24244100	0.28903900	2.19344000
C	1.29455500	-1.49950700	0.95869900
H	0.86571000	-2.46658400	1.23187900
H	2.34567300	-1.51750100	1.25231000
H	1.82515100	-2.02732800	-1.08276900
O	1.32681500	2.13208500	-0.59163400
C	-1.77937600	0.55180900	-1.38755500
H	-2.46392200	1.27889600	-0.94640900
H	-1.05022900	1.09569800	-1.99436000
H	-2.36073400	-0.08407300	-2.06019900
C	-2.19370300	-0.96167000	0.52914900
H	-2.86291100	-1.53213500	-0.12025800
H	-1.78785300	-1.65647800	1.26712400
H	-2.79971700	-0.21955100	1.05288900
C	-0.78113400	1.75621200	1.20682300
H	-0.04700600	2.30314100	1.80098300
H	-1.18548800	2.45100400	0.47148800
H	-1.58640700	1.44365900	1.87390600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -540.538163

207) Conformer **34aC1**

C	-5.10909500	1.95339700	-0.23351900
H	-5.51616700	2.76132500	-0.85238500
H	-5.33342900	2.22262500	0.80308800
C	-5.82364400	0.66143300	-0.57920400
H	-5.64389800	0.44970200	-1.64575800
C	-5.29611200	-0.55449000	0.20038100
C	-3.75690100	-0.59662400	-0.01268700
C	-2.95507500	0.69256900	0.31036100
C	-3.60920800	1.85075000	-0.46801600
H	-3.14254400	2.80278700	-0.20001300
H	-3.42899100	1.70320500	-1.54055300
C	-3.06384800	-1.81472200	0.58626600
H	-2.95794700	-1.71220800	1.67081900
H	-3.66201100	-2.71398000	0.42446000
C	-1.70410200	-2.02099800	-0.06683100
H	-1.87751900	-2.20926900	-1.13106700
H	-1.23175500	-2.91950400	0.33950400
C	-0.76121900	-0.82159800	0.10283500
C	-1.52029500	0.47513000	-0.28349400
C	0.51215800	-0.99570600	-0.84762000

C	1.42935200	0.23252700	-0.66763100
C	0.65163600	1.49548700	-0.97660400
H	0.31249400	1.35382900	-2.01143400
C	-0.59165800	1.66906000	-0.11596400
H	-0.28978100	1.81022400	0.92509000
H	-1.08767700	2.59004400	-0.43487800
C	1.24804900	-2.27972400	-0.44387100
H	1.32548500	-2.35533300	0.64081800
H	0.67187800	-3.14304700	-0.78350800
C	2.64433400	-2.33170400	-1.01179000
H	2.62372500	-2.25693900	-2.10257000
H	3.12575200	-3.28155600	-0.76695600
C	3.48309100	-1.19736700	-0.46781300
C	2.73634800	0.13096800	-0.35433500
C	4.69615900	-0.95260600	-1.40120400
H	5.16459900	-1.91545100	-1.62008500
H	4.30249300	-0.56001900	-2.34105800
C	5.68137700	0.01465400	-0.75693500
H	5.95376400	0.82743000	-1.42857600
H	6.60065500	-0.49352900	-0.45562700
C	5.04419000	0.59799400	0.49531500
C	3.67353700	1.24923500	0.15346500
C	5.99181400	1.52245500	1.22294400
H	5.63042100	1.76015000	2.22318900
H	6.10596000	2.44845400	0.65889700
H	6.97008200	1.04670800	1.31577300
C	-5.73180300	-0.51599900	1.66664600
H	-6.81225300	-0.65691000	1.73478000
H	-5.25491700	-1.32445700	2.22640200
H	-5.49092900	0.42231100	2.16441200
H	-3.65238500	-0.70658300	-1.10457400
H	-1.72196300	0.39264400	-1.35816300
C	0.12937100	-1.14598000	-2.33582500
H	1.02261700	-1.07404900	-2.95977600
H	-0.56932500	-0.39178800	-2.69585700
H	-0.32031400	-2.12253000	-2.52376500
O	-7.22756500	0.77515200	-0.35979800
H	-7.54735300	1.50767500	-0.89416500
C	-5.92147300	-1.80443500	-0.43392600
H	-5.71798800	-2.70311500	0.15166400
H	-5.54265200	-1.96529600	-1.44828400
H	-7.00518600	-1.68617400	-0.48909300
C	-2.94708100	1.07560900	1.79855500
H	-2.07974400	1.69386000	2.03787300

H	-3.82631500	1.66566500	2.05701000
H	-2.93925600	0.21567400	2.46834600
C	-0.28722100	-0.77070900	1.56659600
H	-1.04865400	-0.35654000	2.22108000
H	0.61231100	-0.16402600	1.68620300
H	-0.06135800	-1.77036600	1.94152900
O	3.98722000	2.21958100	-0.83225500
H	3.12497000	2.59806700	-1.08335100
O	4.79452000	-0.51237300	1.40441400
C	4.03542400	-1.49972000	0.90946100
O	3.85138900	-2.49819000	1.56214200
O	1.43381900	2.68705500	-0.95478000
H	0.90607700	3.39702200	-1.33256600
C	3.08447000	1.89317400	1.40961900
H	3.70523900	2.73337900	1.72528400
H	3.03031400	1.17104600	2.22725100
H	2.08295100	2.26667700	1.21175700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1545.095197

208) Conformer **34aC2**

C	-5.10983700	1.95328300	-0.26133700
H	-5.52130500	2.74881900	-0.88967900
H	-5.32755800	2.24185300	0.77375300
C	-5.83336500	0.66092000	-0.58624700
H	-5.68234400	0.44232300	-1.65042400
C	-5.29402700	-0.55440200	0.19918500
C	-3.75621000	-0.59759300	-0.01794900
C	-2.95478000	0.69287400	0.29763800
C	-3.60903800	1.84518500	-0.48905300
H	-3.14240700	2.79917900	-0.22780400
H	-3.42788700	1.68983100	-1.56024500
C	-3.06189100	-1.81455900	0.58205600
H	-2.95525000	-1.71027100	1.66647400
H	-3.66052800	-2.71384300	0.42180500
C	-1.70244200	-2.02160700	-0.07108100
H	-1.87598900	-2.21106800	-1.13508500
H	-1.22997700	-2.91957600	0.33624400
C	-0.76019300	-0.82169900	0.09731700
C	-1.51910200	0.47367300	-0.29366500
C	0.51471500	-0.99790000	-0.85066000
C	1.43133100	0.23081100	-0.67146900
C	0.65421200	1.49291800	-0.98545000
H	0.31754900	1.34884000	-2.02071200

C	-0.59104400	1.66836100	-0.12794700
H	-0.29116000	1.81232500	0.91330300
H	-1.08656700	2.58843900	-0.45016300
C	1.24978300	-2.28117200	-0.44296500
H	1.32403100	-2.35539200	0.64204500
H	0.67488400	-3.14511700	-0.78317300
C	2.64774000	-2.33359000	-1.00674500
H	2.63027300	-2.26037800	-2.09769000
H	3.12867800	-3.28297900	-0.75917900
C	3.48461400	-1.19822900	-0.46211000
C	2.73736300	0.13022900	-0.35391800
C	4.70088100	-0.95527900	-1.39180200
H	5.17003500	-1.91855000	-1.60724200
H	4.31047600	-0.56444800	-2.33374600
C	5.68388000	0.01317600	-0.74594700
H	5.95889600	0.82448300	-1.41827400
H	6.60194900	-0.49452200	-0.44016700
C	5.04216700	0.59927400	0.50269200
C	3.67272700	1.24975500	0.15443100
C	5.98716200	1.52528700	1.23175500
H	5.62224600	1.76498100	2.23024500
H	6.10324100	2.45014600	0.66623700
H	6.96512600	1.04979500	1.32899300
C	-5.72627900	-0.50538500	1.66679600
H	-6.80229900	-0.68450800	1.74730900
H	-5.23020600	-1.29228100	2.23956700
H	-5.50764100	0.44444500	2.15517300
H	-3.65615900	-0.71113100	-1.11003500
H	-1.71924400	0.38782500	-1.36834500
C	0.13442300	-1.15149100	-2.33911400
H	1.02914600	-1.08358200	-2.96139700
H	-0.56163300	-0.39666500	-2.70288900
H	-0.31724600	-2.12747600	-2.52515400
O	-7.24319300	0.82010700	-0.45510200
H	-7.42475300	1.12126500	0.44080400
C	-5.92333900	-1.80723600	-0.42280700
H	-5.73465900	-2.70019300	0.17649200
H	-5.53761000	-1.98548400	-1.43155300
H	-7.00564100	-1.67842100	-0.48981200
C	-2.94921400	1.08393200	1.78364600
H	-2.08358200	1.70522500	2.02100000
H	-3.82967900	1.67398700	2.03838700
H	-2.94026800	0.22752200	2.45798400
C	-0.28882700	-0.76688000	1.56177400

H	-1.05104300	-0.35003700	2.21369800
H	0.61095200	-0.16056300	1.68119900
H	-0.06448300	-1.76558200	1.94016400
O	3.98971300	2.21772600	-0.83254600
H	3.12825700	2.59535200	-1.08761300
O	4.78921200	-0.50911300	1.41330800
C	4.03215200	-1.49767500	0.91769900
O	3.84596500	-2.49482500	1.57179900
O	1.43623600	2.68460600	-0.96453900
H	0.91038400	3.39301300	-1.34785900
C	3.07935800	1.89673200	1.40699200
H	3.69922000	2.73752700	1.72286400
H	3.02214700	1.17654500	2.22612700
H	2.07866000	2.27007500	1.20473500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1545.095693

209) Conformer **34aC3**

C	-5.10629200	1.96100800	-0.23920000
H	-5.51603100	2.76323200	-0.85995600
H	-5.33100300	2.23255200	0.79694100
C	-5.82284900	0.67519500	-0.58322800
H	-5.64214000	0.46232700	-1.64918600
C	-5.29701700	-0.54616100	0.20383800
C	-3.75781200	-0.59556400	-0.01163100
C	-2.95437300	0.69339200	0.30944300
C	-3.60690400	1.85228600	-0.46883000
H	-3.13924600	2.80302000	-0.19809000
H	-3.42405500	1.70623800	-1.54109600
C	-3.06356700	-1.81244700	0.58977100
H	-2.95710800	-1.70625200	1.67388600
H	-3.65928800	-2.71385000	0.43200500
C	-1.70421400	-2.02049500	-0.06362200
H	-1.87821500	-2.21054100	-1.12744600
H	-1.23255200	-2.91869700	0.34416100
C	-0.76077400	-0.82148300	0.10374000
C	-1.51995600	0.47430100	-0.28490600
C	0.51229300	-0.99780700	-0.84668800
C	1.42961300	0.23060500	-0.66900200
C	0.65210200	1.49302200	-0.98068400
H	0.31309300	1.34933500	-2.01526200
C	-0.59128500	1.66867900	-0.12054400
H	-0.28935300	1.81258600	0.92011600
H	-1.08718500	2.58882200	-0.44189200

C	1.24793600	-2.28133500	-0.44086700
H	1.32507300	-2.35550400	0.64392400
H	0.67181500	-3.14510700	-0.77948700
C	2.64443700	-2.33421300	-1.00820000
H	2.62426100	-2.26101700	-2.09909600
H	3.12570600	-3.28373800	-0.76180200
C	3.48306200	-1.19911700	-0.46562500
C	2.73645900	0.12951300	-0.35498100
C	4.69678000	-0.95627300	-1.39866200
H	5.16515100	-1.91961100	-1.61551400
H	4.30382800	-0.56526700	-2.33947400
C	5.68177600	0.01190900	-0.75545300
H	5.95488800	0.82335400	-1.42839800
H	6.60068800	-0.49596000	-0.45250400
C	5.04380300	0.59777100	0.49521400
C	3.67351700	1.24864900	0.15112000
C	5.99110000	1.52340400	1.22176600
H	5.62904900	1.76307500	2.22130100
H	6.10583400	2.44830800	0.65604200
H	6.96920700	1.04763800	1.31618700
C	-5.73299900	-0.50260100	1.66883700
H	-6.81561000	-0.62964100	1.73944300
H	-5.26764700	-1.31646800	2.23043400
H	-5.48162300	0.43332100	2.16538700
H	-3.65442400	-0.70728600	-1.10360700
H	-1.72232700	0.38948500	-1.35927200
C	0.12910600	-1.15076300	-2.33449800
H	1.02241400	-1.08126900	-2.95863400
H	-0.56866300	-0.39649200	-2.69614500
H	-0.32173400	-2.12718200	-2.52034300
O	-7.21341600	0.91473500	-0.38883400
H	-7.70177900	0.15425600	-0.71598900
C	-5.92049200	-1.79970200	-0.42523700
H	-5.67483900	-2.70204500	0.13716300
H	-5.58463700	-1.93771100	-1.45750700
H	-7.01324200	-1.73729500	-0.42887000
C	-2.94514300	1.07822000	1.79729800
H	-2.07532400	1.69325300	2.03568100
H	-3.82175500	1.67284400	2.05432300
H	-2.94088600	0.21956700	2.46878600
C	-0.28668800	-0.76810700	1.56731500
H	-1.04885100	-0.35476000	2.22145600
H	0.61167500	-0.15957200	1.68615800
H	-0.05887500	-1.76689900	1.94333700

O	3.98797300	2.21687600	-0.83642100
H	3.12594300	2.59502000	-1.08878100
O	4.79323500	-0.51083600	1.40623100
C	4.03443500	-1.49903400	0.91256300
O	3.84984300	-2.49630400	1.56693400
O	1.43449500	2.68445900	-0.96117000
H	0.90715200	3.39368600	-1.34091200
C	3.08383900	1.89533200	1.40557600
H	3.70462200	2.73606100	1.71981300
H	3.02904500	1.17495100	2.22470500
H	2.08254000	2.26869700	1.20635600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1545.095305

210) Conformer **34aC4**

C	-5.12625400	1.95321900	-0.28130000
H	-5.53383600	2.74751600	-0.91380600
H	-5.35428000	2.24175900	0.75164000
C	-5.84405300	0.65915700	-0.61208500
H	-5.68271600	0.44018500	-1.67467800
C	-5.30969800	-0.55456100	0.17919500
C	-3.76972400	-0.59443600	-0.02275600
C	-2.97374100	0.69780400	0.29851600
C	-3.62320200	1.84796000	-0.49504100
H	-3.15939000	2.80242400	-0.23107000
H	-3.43177900	1.69161000	-1.56430800
C	-3.07866900	-1.80864000	0.58619700
H	-2.98358900	-1.70193100	1.67150300
H	-3.67331400	-2.70990800	0.42174500
C	-1.71165200	-2.01405100	-0.05156700
H	-1.87262300	-2.20879900	-1.11676000
H	-1.24226600	-2.90929900	0.36521400
C	-0.77480600	-0.81026400	0.12089800
C	-1.53230700	0.48223600	-0.27989400
C	0.50737900	-0.98510800	-0.81511400
C	1.42417000	0.24308500	-0.63009400
C	0.65523300	1.52176700	-0.93994600
H	0.32974200	1.36493100	-1.98093900
C	-0.60926000	1.67681800	-0.10874400
H	-0.32614400	1.82585600	0.93709700
H	-1.09025900	2.59829300	-0.44315400
C	1.23596000	-2.27079200	-0.40406400
H	1.32125100	-2.33605900	0.68089000
H	0.65072000	-3.13289400	-0.73076800

C	2.62586700	-2.34081900	-0.98414700
H	2.59559800	-2.28075800	-2.07541200
H	3.10318300	-3.29053100	-0.73123000
C	3.47909900	-1.20706200	-0.46238100
C	2.73725000	0.12532800	-0.34318100
C	4.67914100	-0.97938600	-1.41475600
H	5.13858500	-1.94639300	-1.63330600
H	4.27516000	-0.59065500	-2.35181200
C	5.68046700	-0.01519700	-0.79125900
H	5.95579000	0.78647600	-1.47568900
H	6.59894200	-0.52802100	-0.49656400
C	5.06461900	0.58044100	0.46586200
C	3.68419100	1.23334800	0.14366500
C	6.03281700	1.49747500	1.17862000
H	5.66907400	1.78171200	2.16530200
H	6.21712000	2.40217600	0.59535300
H	6.98903300	0.98568300	1.29971100
C	-5.75635200	-0.50522900	1.64247200
H	-6.83296100	-0.68531500	1.71269600
H	-5.26507200	-1.29129700	2.22052300
H	-5.54318100	0.44515900	2.13216200
H	-3.65859000	-0.70949200	-1.11362500
H	-1.72433200	0.39267900	-1.35557200
C	0.13994300	-1.13461600	-2.30782500
H	1.03572600	-1.04322200	-2.92544500
H	-0.56835300	-0.38996800	-2.66772800
H	-0.29061000	-2.11862000	-2.50294800
O	-7.25558700	0.81533700	-0.49415300
H	-7.44567700	1.11709300	0.39977200
C	-5.93039600	-1.80915600	-0.44781700
H	-5.74467700	-2.70145100	0.15344000
H	-5.53518400	-1.98678000	-1.45301100
H	-7.01241700	-1.68322400	-0.52457200
C	-2.98296500	1.09046200	1.78419600
H	-2.12011300	1.71295900	2.02811600
H	-3.86665000	1.67951500	2.03045700
H	-2.97895800	0.23474300	2.45960400
C	-0.31329100	-0.75046800	1.58832800
H	-1.08409500	-0.34160300	2.23527400
H	0.57891600	-0.13395700	1.71363400
H	-0.08005500	-1.74655700	1.96836100
O	3.89965400	2.17402800	-0.92452900
H	4.38278100	2.93144600	-0.57267600
O	4.81880500	-0.51579200	1.38884000

C	4.04698700	-1.50485900	0.90985200
O	3.86652100	-2.49507700	1.57357400
O	1.33068500	2.75584300	-0.88171100
H	2.26036400	2.63238500	-1.14516700
C	3.13126200	1.92384200	1.38573200
H	3.75518900	2.77630200	1.66723100
H	3.11190000	1.22672100	2.22524300
H	2.12333700	2.28462200	1.19973500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1545.092814

211) Conformer **34bC1**

C	-5.13421200	2.13022500	-0.01154900
H	-5.43514300	3.08356500	-0.46166400
H	-5.50027400	2.15192200	1.01961100
C	-5.81309900	0.99819500	-0.75616000
H	-5.48491700	1.03766900	-1.80760800
C	-5.42316300	-0.39257600	-0.23014600
C	-3.86950300	-0.46157900	-0.23949900
C	-3.09859700	0.66900700	0.49557700
C	-3.61834100	2.01050700	-0.05748800
H	-3.18179700	2.84585100	0.49624800
H	-3.28587900	2.11604800	-1.09830000
C	-3.29603300	-1.82564300	0.12524500
H	-3.37342500	-2.00769200	1.20153100
H	-3.87101100	-2.62067800	-0.35493900
C	-1.85039900	-1.93533400	-0.34158600
H	-1.85760100	-1.85296100	-1.43214600
H	-1.46142400	-2.93049900	-0.10453800
C	-0.92398200	-0.86341100	0.25529600
C	-1.59496700	0.53192000	0.07175200
C	0.47882900	-0.86382700	-0.50149000
C	1.36747700	0.28428200	0.05646400
C	0.66819700	1.63262900	-0.07051200
H	1.28476100	2.42177100	0.36808000
H	0.54875900	1.88845500	-1.13059100
C	-0.69201100	1.63691700	0.61255800
H	-1.15535000	2.61484300	0.46365500
H	-0.54747000	1.52820400	1.69249500
C	1.22619300	-2.18715700	-0.26134600
H	1.32641700	-2.37001600	0.80843900
H	0.64982500	-3.01979100	-0.67502800
C	2.62424100	-2.21190100	-0.86302100
H	2.57647600	-2.16587800	-1.95541400

H	3.11239500	-3.15896300	-0.61466800
C	3.49817300	-1.06424500	-0.38533600
C	2.78724800	0.30227600	-0.53853700
C	4.81643600	-0.99830600	-1.17767000
H	5.27714200	-1.98852100	-1.22187400
H	4.57947700	-0.69642000	-2.20166000
C	5.77247500	0.02823600	-0.55880700
H	6.58651300	-0.48930500	-0.03650600
C	5.01386900	0.81031000	0.52492100
C	3.68128300	1.41595900	0.05916800
H	3.21395800	1.76830100	0.98689100
C	5.90449900	1.79130600	1.24707800
H	5.34759800	2.31207200	2.02877200
H	6.30206700	2.52500900	0.54729300
H	6.74437000	1.26513200	1.70548600
C	-5.97686400	-1.42339900	-1.22318100
H	-5.87972200	-2.44379200	-0.84733200
H	-7.03827200	-1.23554500	-1.39554100
H	-5.45820800	-1.36367200	-2.18540500
H	-3.61161500	-0.30923400	-1.30054000
H	-1.64271800	0.69130200	-1.01213100
C	0.28946200	-0.71222700	-2.02144800
H	1.23346800	-0.49737500	-2.52253800
H	-0.39755100	0.08684900	-2.29810800
H	-0.08760500	-1.63858200	-2.45937300
O	-7.23240100	1.12887100	-0.70943000
H	-7.45655400	1.99025500	-1.07297500
C	-6.06018100	-0.67531000	1.13191100
H	-5.69012100	-1.62056800	1.53670300
H	-7.14310100	-0.76157200	1.02275800
H	-5.86379300	0.10311000	1.86801400
C	-3.29533200	0.68196100	2.02118400
H	-4.15862900	1.28598200	2.30369900
H	-2.43040800	1.12072800	2.52174200
H	-3.45533500	-0.30910800	2.44555900
C	-0.72687300	-1.20872000	1.73956300
H	-0.34198100	-2.22322800	1.85325000
H	-1.67065900	-1.17378600	2.27700600
H	-0.04297100	-0.53520400	2.25680500
H	2.71698100	0.48151800	-1.61682700
C	3.83529100	2.61020600	-0.87545200
H	2.85282300	3.00787300	-1.13552900
H	4.34279300	2.32622000	-1.79755400
H	4.40509700	3.41650600	-0.40870500

O	6.32073800	0.93158000	-1.50097600
H	6.91640400	0.43687800	-2.07117500
H	1.49653500	0.09172400	1.13043300
O	4.66970700	-0.20792600	1.51312800
C	3.90049200	-1.21433200	1.06677300
O	3.62520900	-2.12267700	1.81210500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1471.123350

212) Conformer **34bC2**

C	-5.13617100	2.12975500	-0.01150300
H	-5.43839600	3.08234600	-0.46233100
H	-5.50087700	2.15239300	1.02012100
C	-5.81524100	0.99635800	-0.75387300
H	-5.48839800	1.03472900	-1.80577500
C	-5.42369000	-0.39347800	-0.22658900
C	-3.86998200	-0.46150300	-0.23780700
C	-3.09883400	0.67063800	0.49476200
C	-3.62028900	2.01105100	-0.05929400
H	-3.18361900	2.84737600	0.49286000
H	-3.28924800	2.11555600	-1.10066700
C	-3.29546300	-1.82476800	0.12819500
H	-3.37225600	-2.00559300	1.20472600
H	-3.87032000	-2.62067900	-0.35068100
C	-1.85004700	-1.93455800	-0.33926400
H	-1.85783600	-1.85480000	-1.43002000
H	-1.46035200	-2.92893200	-0.10006800
C	-0.92377800	-0.86077700	0.25447800
C	-1.59577600	0.53388300	0.06888200
C	0.47806300	-0.86161200	-0.50400100
C	1.36646700	0.28706900	0.05319500
C	0.66731500	1.63509900	-0.07792000
H	1.28403400	2.42593400	0.35761500
H	0.54760700	1.88728900	-1.13881500
C	-0.69280600	1.64112600	0.60550900
H	-1.15670200	2.61827500	0.45330500
H	-0.54785800	1.53633700	1.68578300
C	1.22584200	-2.18519100	-0.26573800
H	1.32641300	-2.36972100	0.80370000
H	0.64930600	-3.01718300	-0.68039300
C	2.62389000	-2.20949200	-0.86779300
H	2.57640600	-2.16161500	-1.96012000
H	3.11187100	-3.15702200	-0.62095300
C	3.49750900	-1.06255700	-0.38799700

C	2.78576400	0.30343000	-0.54154900
C	4.81321300	-0.99197600	-1.18286900
H	5.27013600	-1.98184300	-1.25090300
H	4.57888800	-0.66630200	-2.19985000
C	5.77276800	0.01215600	-0.55222200
H	6.57184700	-0.51798600	-0.01910000
C	5.00824600	0.80788000	0.52717100
C	3.68191300	1.41780300	0.05170700
H	3.21087700	1.78173100	0.97308200
C	5.89841300	1.78791000	1.25251400
H	5.34797300	2.28458200	2.05402000
H	6.26620100	2.55604200	0.57103900
H	6.75599100	1.26954200	1.68714900
C	-5.97799100	-1.42593700	-1.21758300
H	-5.87971100	-2.44578300	-0.84055100
H	-7.03974200	-1.23899500	-1.38881800
H	-5.46060800	-1.36712500	-2.18054800
H	-3.61349900	-0.31050200	-1.29937500
H	-1.64552100	0.69069200	-1.01524500
C	0.28698700	-0.71010600	-2.02384400
H	1.23047400	-0.49574400	-2.52613200
H	-0.40005800	0.08899400	-2.30018600
H	-0.09074800	-1.63650600	-2.46107200
O	-7.23455300	1.12613100	-0.70548900
H	-7.45985500	1.98640700	-1.07093300
C	-6.05879300	-0.67484700	1.13664300
H	-5.68801500	-1.61959200	1.54197400
H	-7.14184100	-0.76145500	1.02903100
H	-5.86154500	0.10441600	1.87162700
C	-3.29331400	0.68535200	2.02064500
H	-4.15626600	1.28961500	2.30372800
H	-2.42768300	1.12471300	2.51945600
H	-3.45254800	-0.30524200	2.44638300
C	-0.72499100	-1.20294900	1.73920300
H	-0.33295300	-2.21450700	1.85451200
H	-1.66947100	-1.17427500	2.27583300
H	-0.04648900	-0.52385200	2.25623100
H	2.71427300	0.48001200	-1.62015200
C	3.84661500	2.60182600	-0.89438800
H	4.36230800	2.30750700	-1.80896600
H	4.41106400	3.41431400	-0.43162400
H	2.86685300	2.99712400	-1.16845000
O	6.33519000	0.81349600	-1.57262300
H	7.09308100	1.28322800	-1.21204200

H	1.49445700	0.09668800	1.12766100
O	4.65809700	-0.20495400	1.51850500
C	3.89600100	-1.21453200	1.06574800
O	3.62017900	-2.12503600	1.80803700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1471.124073

213) Conformer **34bC3**

C	-5.13200700	2.13705900	-0.04026800
H	-5.43572700	3.08076000	-0.50341400
H	-5.49070000	2.17837000	0.99514300
C	-5.82351800	0.99994300	-0.76552600
H	-5.52567700	1.03359800	-1.82061500
C	-5.42248500	-0.39236200	-0.23234600
C	-3.86959000	-0.46142800	-0.24492700
C	-3.09825900	0.67244700	0.48321600
C	-3.61642300	2.00989800	-0.08056600
H	-3.17895600	2.84914000	0.46661200
H	-3.28300500	2.10649900	-1.12184500
C	-3.29517300	-1.82457700	0.12230500
H	-3.37268500	-2.00457500	1.19899600
H	-3.87034900	-2.62021700	-0.35672800
C	-1.84938100	-1.93520100	-0.34351900
H	-1.85592700	-1.85435900	-1.43417700
H	-1.46073300	-2.93005500	-0.10470100
C	-0.92366200	-0.86224200	0.25233700
C	-1.59392800	0.53259500	0.06252700
C	0.48073600	-0.86584800	-0.50145600
C	1.36849100	0.28450000	0.05347800
C	0.66955000	1.63233100	-0.08052200
H	1.28547700	2.42335200	0.35553900
H	0.55144800	1.88346700	-1.14184100
C	-0.69150800	1.63933800	0.60073700
H	-1.15434100	2.61689800	0.44806500
H	-0.54824500	1.53399200	1.68116100
C	1.22761000	-2.18813200	-0.25396500
H	1.32609900	-2.36601300	0.81680400
H	0.65192700	-3.02264400	-0.66480400
C	2.62669800	-2.21563300	-0.85317400
H	2.58072800	-2.17419200	-1.94580800
H	3.11421300	-3.16172600	-0.59991400
C	3.49996900	-1.06614400	-0.37871900
C	2.78944300	0.29985500	-0.53870400
C	4.81955800	-1.00331700	-1.16904700

H	5.28029200	-1.99369800	-1.20890400
H	4.58441200	-0.70495500	-2.19446000
C	5.77467700	0.02536300	-0.55225700
H	6.58735400	-0.49046700	-0.02617500
C	5.01413600	0.81188900	0.52693400
C	3.68256400	1.41590400	0.05610400
H	3.21352500	1.77228600	0.98137800
C	5.90357800	1.79567200	1.24676500
H	5.34552200	2.31857900	2.02620000
H	6.30141600	2.52732800	0.54501900
H	6.74326900	1.27146800	1.70775200
C	-5.98127700	-1.42881100	-1.21500700
H	-5.89747200	-2.44627900	-0.82793100
H	-7.04022200	-1.23050800	-1.39366700
H	-5.45876900	-1.38534300	-2.17592200
H	-3.61554600	-0.31279000	-1.30755200
H	-1.63966900	0.68765300	-1.02205500
C	0.29427200	-0.72083400	-2.02245800
H	1.23883400	-0.50635900	-2.52258600
H	-0.39365600	0.07582900	-2.30378900
H	-0.08033100	-1.64970600	-2.45717300
O	-7.23520500	1.19555000	-0.79060400
H	-7.53693100	1.28175000	0.11926900
C	-6.05722100	-0.66560300	1.13340200
H	-5.67047200	-1.59481100	1.55802000
H	-7.13865400	-0.79166600	1.02703000
H	-5.88113700	0.12701500	1.86083800
C	-3.29797500	0.69488900	2.00819700
H	-4.16253300	1.29953300	2.28570100
H	-2.43487900	1.13832700	2.50770400
H	-3.45685700	-0.29376200	2.43863400
C	-0.72984000	-1.20264500	1.73812900
H	-0.34832100	-2.21793700	1.85608800
H	-1.67412100	-1.16263400	2.27433500
H	-0.04440900	-0.52932400	2.25358900
H	2.72131100	0.47476700	-1.61778900
C	3.83856000	2.60606900	-0.88339400
H	2.85663700	3.00259900	-1.14723800
H	4.34797800	2.31805600	-1.80317500
H	4.40739600	3.41441300	-0.41899900
O	6.32520100	0.92472400	-1.49679400
H	6.92463200	0.42840600	-2.06159600
H	1.49529400	0.09648900	1.12849000
O	4.66788700	-0.20221400	1.51854700

C	3.89948000	-1.21035500	1.07472300
O	3.62338000	-2.11609500	1.82291100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1471.123652

214) Conformer **34bC4**

C	-5.13164700	2.13848900	-0.01759100
H	-5.43507000	3.08627000	-0.47236800
H	-5.49788800	2.16400800	1.01361900
C	-5.81314300	1.01089100	-0.75739800
H	-5.48579100	1.04788200	-1.80894600
C	-5.42468700	-0.38612700	-0.22459100
C	-3.87075700	-0.46073500	-0.23864500
C	-3.09835600	0.67074800	0.49382900
C	-3.61704000	2.01196300	-0.06035100
H	-3.18021500	2.84621200	0.49474600
H	-3.28202800	2.11750400	-1.10030500
C	-3.29596200	-1.82398700	0.12925800
H	-3.37299100	-2.00240100	1.20612000
H	-3.86855600	-2.62248300	-0.34766400
C	-1.85047400	-1.93495300	-0.33771300
H	-1.85792400	-1.85480500	-1.42841900
H	-1.46224200	-2.92992100	-0.09865100
C	-0.92370100	-0.86236000	0.25675600
C	-1.59489400	0.53226600	0.06947600
C	0.47899700	-0.86517100	-0.50012900
C	1.36774100	0.28432100	0.05481100
C	0.66851600	1.63228800	-0.07655600
H	1.28508600	2.42283100	0.35947900
H	0.54903200	1.88458900	-1.13744300
C	-0.69171700	1.63898800	0.60653500
H	-1.15475900	2.61648600	0.45429700
H	-0.54706200	1.53382200	1.68677700
C	1.22617200	-2.18800500	-0.25652500
H	1.32664500	-2.36806500	0.81367100
H	0.64962800	-3.02162900	-0.66798100
C	2.62423700	-2.21451900	-0.85814000
H	2.57650200	-2.17108500	-1.95061900
H	3.11211400	-3.16109000	-0.60737800
C	3.49830800	-1.06592600	-0.38302600
C	2.78767600	0.30038400	-0.53978000
C	4.81677600	-1.00201500	-1.17512100
H	5.27723900	-1.99242700	-1.21729300
H	4.58025500	-0.70184700	-2.19969000

C	5.77297500	0.02540000	-0.55792300
H	6.58609700	-0.49149200	-0.03358300
C	5.01398200	0.81050500	0.52338900
C	3.68192200	1.41544800	0.05516900
H	3.21424500	1.77081200	0.98151200
C	5.90453800	1.79306700	1.24349900
H	5.34759600	2.31490500	2.02444200
H	6.30157000	2.52569600	0.54231000
H	6.74474900	1.26803800	1.70259800
C	-5.97676100	-1.42339700	-1.21194400
H	-5.83822300	-2.44344900	-0.84993900
H	-7.05516000	-1.29974600	-1.35358900
H	-5.49438400	-1.33889100	-2.19056200
H	-3.61447400	-0.31034300	-1.30048200
H	-1.64319100	0.68846600	-1.01483500
C	0.28948800	-0.71769300	-2.02052500
H	1.23319500	-0.50293300	-2.52216000
H	-0.39856000	0.07977600	-2.29922400
H	-0.08640900	-1.64570500	-2.45597100
O	-7.21348700	1.26801300	-0.70018200
H	-7.66345600	0.62621400	-1.25649600
C	-6.06079300	-0.66280200	1.13810700
H	-5.69775600	-1.60995200	1.54475600
H	-7.14533000	-0.74234400	1.03461500
H	-5.85813700	0.11624300	1.87149500
C	-3.29406000	0.68672700	2.01959600
H	-4.15502100	1.29440800	2.30133800
H	-2.42734700	1.12387100	2.51839100
H	-3.45667300	-0.30288300	2.44633700
C	-0.72667200	-1.20403000	1.74182800
H	-0.34046000	-2.21772600	1.85796500
H	-1.67061600	-1.16916300	2.27895400
H	-0.04384500	-0.52831700	2.25760300
H	2.71770600	0.47686900	-1.61849500
C	3.83691500	2.60671200	-0.88309300
H	2.85470900	3.00386400	-1.14495100
H	4.34485700	2.31967500	-1.80399800
H	4.40671000	3.41430200	-0.41856400
O	6.32269700	0.92596100	-1.50178200
H	6.92166000	0.43034300	-2.06769900
H	1.49628500	0.09491800	1.12935800
O	4.66886100	-0.20500600	1.51396100
C	3.89989500	-1.21248700	1.06960500
O	3.62478300	-2.11937400	1.81676300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1471.123256

215) Conformer **34bC5**

C	-5.13407700	2.13649800	-0.04026800
H	-5.43929700	3.07932000	-0.50421400
H	-5.49104500	2.17896100	0.99569800
C	-5.82592100	0.99784800	-0.76276500
H	-5.52984600	1.03020200	-1.81839200
C	-5.42301400	-0.39336200	-0.22820900
C	-3.87008200	-0.46140900	-0.24323400
C	-3.09834000	0.67419800	0.48189800
C	-3.61846900	2.01042100	-0.08293000
H	-3.18074000	2.85074400	0.46237100
H	-3.28683700	2.10582600	-1.12489400
C	-3.29448800	-1.82365500	0.12541600
H	-3.37127100	-2.00221800	1.20239600
H	-3.86959700	-2.62027700	-0.35206600
C	-1.84897000	-1.93448900	-0.34120100
H	-1.85626300	-1.85672400	-1.43208600
H	-1.45953800	-2.92843600	-0.09987900
C	-0.92334700	-0.85941000	0.25093600
C	-1.59471500	0.53463500	0.05866300
C	0.48002300	-0.86366000	-0.50470300
C	1.36750400	0.28739200	0.04916200
C	0.66876400	1.63486200	-0.08960900
H	1.28484800	2.42773100	0.34308500
H	0.55051500	1.88195500	-1.15182600
C	-0.69223500	1.64394600	0.59194600
H	-1.15565000	2.62060200	0.43535700
H	-0.54857700	1.54321900	1.67276400
C	1.22718700	-2.18626700	-0.25898300
H	1.32545800	-2.36608200	0.81145200
H	0.65148700	-3.02001400	-0.67126500
C	2.62662800	-2.21345300	-0.85779800
H	2.58162000	-2.17049200	-1.95041700
H	3.11380200	-3.15996200	-0.60549600
C	3.49931100	-1.06453900	-0.38108500
C	2.78803500	0.30080300	-0.54255900
C	4.81691000	-0.99733900	-1.17307800
H	5.27367200	-1.98755700	-1.23681900
H	4.58509800	-0.67474800	-2.19160400
C	5.77532600	0.00842900	-0.54341300
H	6.57154900	-0.52034300	-0.00466300

C	5.00777000	0.80984300	0.52970000
C	3.68312200	1.41788000	0.04730600
H	3.20969200	1.78708100	0.96530500
C	5.89611300	1.79322200	1.25270800
H	5.34364200	2.29344700	2.05059400
H	6.26540100	2.55820600	0.56851300
H	6.75268600	1.27698100	1.69184100
C	-5.98274300	-1.43165100	-1.20838400
H	-5.89765500	-2.44848000	-0.81991600
H	-7.04210400	-1.23428700	-1.38560900
H	-5.46183200	-1.38929700	-2.17021500
H	-3.61780600	-0.31435200	-1.30650000
H	-1.64286200	0.68660600	-1.02621200
C	0.29190200	-0.71896600	-2.02559700
H	1.23630800	-0.50660900	-2.52694900
H	-0.39480600	0.07870500	-2.30686700
H	-0.08474100	-1.64744000	-2.45934200
O	-7.23780400	1.19236400	-0.78578300
H	-7.53795500	1.28040700	0.12443400
C	-6.05524700	-0.66496900	1.13902100
H	-5.66761600	-1.59358700	1.56412100
H	-7.13685000	-0.79131300	1.03473900
H	-5.87795000	0.12860200	1.86512800
C	-3.29531600	0.69867800	2.00721300
H	-4.15945700	1.30361000	2.28544000
H	-2.43136800	1.14278700	2.50464000
H	-3.45329100	-0.28941000	2.43924000
C	-0.72770400	-1.19610700	1.73728800
H	-0.33802000	-2.20802600	1.85724600
H	-1.67285200	-1.16322500	2.27249000
H	-0.04849900	-0.51634000	2.25249000
H	2.71885300	0.47229400	-1.62209000
C	3.85115700	2.59659600	-0.90483000
H	4.37000800	2.29712000	-1.81593300
H	4.41407000	3.41164800	-0.44470300
H	2.87234400	2.99037900	-1.18443300
O	6.34282500	0.80433600	-1.56514100
H	7.10079500	1.27357800	-1.20407600
H	1.49310600	0.10200700	1.12475200
O	4.65431400	-0.19805000	1.52486300
C	3.89380100	-1.20987700	1.07441000
O	3.61642200	-2.11732200	1.81984100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1471.124363

216) Conformer **34bC6**

C	-5.13350200	2.13808900	-0.01723400
H	-5.43827200	3.08522600	-0.47243700
H	-5.49824700	2.16434100	1.01450200
C	-5.81513400	1.00924400	-0.75499800
H	-5.48906600	1.04526500	-1.80699300
C	-5.42513900	-0.38686400	-0.22109400
C	-3.87117900	-0.46062800	-0.23714000
C	-3.09847600	0.67230500	0.49288200
C	-3.61885300	2.01254200	-0.06203300
H	-3.18171600	2.84766300	0.49151000
H	-3.28539900	2.11718600	-1.10259300
C	-3.29538500	-1.82308500	0.13203400
H	-3.37177600	-2.00016500	1.20917900
H	-3.86795500	-2.62248300	-0.34341000
C	-1.85016000	-1.93418800	-0.33567400
H	-1.85825200	-1.85663700	-1.42658600
H	-1.46124500	-2.92839000	-0.09456100
C	-0.92348700	-0.85980100	0.25567000
C	-1.59559700	0.53414600	0.06639600
C	0.47829600	-0.86305500	-0.50283200
C	1.36680200	0.28698100	0.05130200
C	0.66778300	1.63466600	-0.08397700
H	1.28450700	2.42677400	0.34921700
H	0.54821300	1.88364600	-1.14562600
C	-0.69240200	1.64304400	0.59936400
H	-1.15597800	2.61977300	0.44388400
H	-0.54744400	1.54176300	1.67996300
C	1.22574500	-2.18623900	-0.26115900
H	1.32603200	-2.36824600	0.80871300
H	0.64916700	-3.01911200	-0.67400000
C	2.62405800	-2.21237300	-0.86256800
H	2.57712700	-2.16743100	-1.95503700
H	3.11170600	-3.15933600	-0.61289300
C	3.49763500	-1.06431700	-0.38539400
C	2.78619800	0.30135900	-0.54315000
C	4.81380600	-0.99608000	-1.17966500
H	5.27040700	-1.98625500	-1.24529200
H	4.58018500	-0.67246600	-2.19746200
C	5.77335600	0.00902000	-0.55062200
H	6.57121600	-0.52028800	-0.01484100
C	5.00807900	0.80837000	0.52558500
C	3.68242500	1.41730600	0.04704600

H	3.21082800	1.78467400	0.96675300
C	5.89792800	1.79033800	1.24867100
H	5.34700800	2.28945600	2.04832200
H	6.26630900	2.55635400	0.56513600
H	6.75510400	1.27310500	1.68544800
C	-5.97789800	-1.42567500	-1.20637100
H	-5.83786400	-2.44522600	-0.84352800
H	-7.05664900	-1.30311600	-1.34624800
H	-5.49722800	-1.34181500	-2.18589100
H	-3.61631600	-0.31156400	-1.29952100
H	-1.64595800	0.68782700	-1.01816600
C	0.28718800	-0.71551900	-2.02306400
H	1.23077900	-0.50297100	-2.52590200
H	-0.39945100	0.08319500	-2.30152300
H	-0.09096100	-1.64292500	-2.45780000
O	-7.21561700	1.26541300	-0.69634400
H	-7.66569600	0.62295500	-1.25179800
C	-6.05909400	-0.66232300	1.14286400
H	-5.69553500	-1.60918300	1.54973800
H	-7.14381400	-0.74185700	1.04122200
H	-5.85513100	0.11727500	1.87531500
C	-3.29188000	0.68981300	2.01896200
H	-4.15255600	1.29763000	2.30141600
H	-2.42452200	1.12751300	2.51613700
H	-3.45366400	-0.29939000	2.44697400
C	-0.72497600	-1.19843200	1.74122600
H	-0.33204800	-2.20933000	1.85905000
H	-1.66963600	-1.16944400	2.27750200
H	-0.04734500	-0.51744900	2.25688800
H	2.71498100	0.47477000	-1.62227500
C	3.84847300	2.59792300	-0.90306800
H	4.36503600	2.30018900	-1.81604800
H	4.41269100	3.41188100	-0.44261700
H	2.86909900	2.99252700	-1.17952000
O	6.33788900	0.80694600	-1.57249000
H	7.09616000	1.27642000	-1.21237800
H	1.49448600	0.09971700	1.12633700
O	4.65668100	-0.20137000	1.51965500
C	3.89502800	-1.21225800	1.06906500
O	3.61865300	-2.12072700	1.81363000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1471.123977

217) Conformer **35aC1**

C	0.28205900	-1.32465200	1.57988000
H	-0.51899900	-1.92976000	1.14033900
H	0.53783500	-1.81533200	2.52254800
C	-0.24373500	0.06701600	1.88150500
H	-1.13909500	-0.00750100	2.50179900
H	0.49262200	0.64167900	2.45127900
C	-0.63359500	0.87678100	0.63099600
C	-1.57513400	0.06358800	-0.25051700
C	-1.07781600	-0.37485800	-1.59340900
H	-1.88766100	-0.88366300	-2.11664400
H	-0.83393000	0.53186300	-2.16010600
C	0.15731900	-1.27725600	-1.54120500
H	0.47972600	-1.43236500	-2.57216100
H	-0.12333300	-2.26024400	-1.15466800
C	1.34612800	-0.75975100	-0.72178200
C	1.50112600	-1.34570000	0.67493800
H	1.82030200	-2.38300200	0.53501200
H	2.33875200	-0.83086700	1.15769700
O	1.42234800	0.68548300	-0.73034900
C	0.55661600	1.47218900	-0.08936600
O	0.75258200	2.66275400	-0.10092400
O	-2.68609500	-0.19029800	0.15209700
H	2.25692500	-1.01947800	-1.26147100
H	-1.21163100	1.74101200	0.96354600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -575.272552

218) Conformer **35aC2**

C	1.38050400	0.69510300	1.53649200
H	1.65248300	1.31689900	2.39227200
H	2.23780700	0.04173900	1.34936700
C	1.12531000	1.59307700	0.33157700
H	0.52331400	2.45852700	0.61943100
H	2.06878400	1.97202200	-0.06604100
C	0.35997000	0.87483300	-0.79255200
C	-1.15361000	0.87737800	-0.56923600
C	-1.87234100	-0.43123300	-0.70561300
H	-2.94421300	-0.24749100	-0.77366500
H	-1.54780200	-0.88707400	-1.64781100
C	-1.56188100	-1.39485200	0.44904500
H	-1.79557800	-2.41061400	0.12423300
H	-2.21157600	-1.17251100	1.29935000
C	-0.12613200	-1.33140700	0.94756800
C	0.16314100	-0.14317000	1.89323300

H	0.28704700	-0.55467400	2.89676900
H	-0.71538100	0.50754800	1.94717600
O	0.79164100	-1.45438100	-0.16553400
C	0.97994100	-0.47662600	-1.05571700
O	1.69096300	-0.69068300	-2.00592700
O	-1.71977000	1.92060000	-0.34435400
H	0.08047400	-2.25064600	1.49403600
H	0.49256900	1.44337700	-1.71738800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -575.268334

219) Conformer **35bC1**

C	1.72625900	1.86567200	-1.09256800
H	2.03816400	2.84449500	-1.46523500
H	1.35778200	1.32150000	-1.96974600
C	2.93704800	1.14931200	-0.52323800
H	3.40847400	1.75061700	0.25960800
H	3.68115900	1.00796300	-1.30932700
C	2.62475100	-0.24517700	0.05143100
C	1.85758000	-1.07134800	-0.97263800
C	0.43435100	-1.43818900	-0.67921400
H	0.06887800	-2.07127000	-1.48748700
H	0.42455300	-2.03869200	0.23757100
C	-0.50594900	-0.25006000	-0.48906800
H	-0.65393800	0.25795500	-1.44572900
C	-0.03229000	0.82590500	0.51974500
C	0.60005300	2.06707200	-0.09520500
H	-0.21473700	2.61120400	-0.58186900
H	0.93814800	2.69843200	0.73320100
O	0.74915700	0.25307700	1.58433900
C	1.99885400	-0.19796000	1.42658300
O	2.59648900	-0.56329800	2.40645800
O	2.42052000	-1.43047600	-1.97918600
H	-0.90927600	1.17920300	1.06192000
H	3.57413100	-0.76275200	0.19994000
C	-1.86904600	-0.76951400	-0.06678500
O	-2.07957700	-1.85948400	0.40108400
O	-2.80457200	0.15197500	-0.26389700
C	-4.14302000	-0.18615400	0.14871500
H	-4.45418800	-1.08216100	-0.39203700
H	-4.12702600	-0.42155100	1.21488700
C	-5.02889200	0.99015700	-0.15470900
H	-4.70336500	1.87817200	0.39015800
H	-6.05189700	0.75930100	0.14826800

H	-5.03118300	1.21493000	-1.22280000
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No imaginary frequency.
Gibbs Free Energies (a.u.) = -842.215353

220) Conformer **35bC2**

C	-1.92031200	-0.84579400	-1.88783900
H	-1.62295000	0.12329400	-2.30468700
H	-2.33091100	-1.41204300	-2.72750500
C	-3.01259900	-0.63939700	-0.85482400
H	-3.42607600	-1.59972700	-0.53317100
H	-3.83227000	-0.07088400	-1.29813400
C	-2.55346200	0.13887100	0.39264100
C	-1.86220100	1.43053100	-0.02414200
C	-0.39465800	1.57947700	0.24185800
H	-0.08924000	2.57820300	-0.06926600
H	-0.24116200	1.51272300	1.32501600
C	0.48787100	0.53473700	-0.43750100
H	0.49155700	0.70272600	-1.51761200
C	0.07162300	-0.94090000	-0.21638100
C	-0.70113100	-1.58080900	-1.36179900
H	-0.97876100	-2.58931500	-1.03769900
H	0.01782500	-1.70828900	-2.17645300
O	-0.54520300	-1.13581900	1.06943700
C	-1.77629100	-0.70896700	1.37349000
O	-2.23366600	-1.01726600	2.44424000
O	-2.51627000	2.30931500	-0.53309200
H	0.98293500	-1.52933500	-0.10970500
H	-3.44674800	0.44326800	0.94091600
C	1.92059200	0.72708400	0.02844600
O	2.24761700	1.32267200	1.02292300
O	2.76528000	0.13256900	-0.80804500
C	4.16676300	0.16059900	-0.47027100
H	4.67620600	0.08151100	-1.43002400
H	4.39777800	1.12681000	-0.02124500
C	4.53243800	-0.98043000	0.44467100
H	4.28044400	-1.94058800	-0.00950200
H	4.01910900	-0.89675600	1.40387100
H	5.60840900	-0.96338800	0.63138500

No imaginary frequency.
Gibbs Free Energies (a.u.) = -842.214317

221) Conformer **35bC3**

C	-2.12763400	0.31069900	-1.97456900
H	-1.39845600	1.12033600	-2.09319200

H	-2.69734900	0.29200700	-2.90705900
C	-3.07121400	0.64527200	-0.83366100
H	-3.90174000	-0.06589300	-0.79868300
H	-3.50450700	1.63387400	-0.99664000
C	-2.39842900	0.67397400	0.55207700
C	-1.16316800	1.56295300	0.52392800
C	0.18483300	0.92591700	0.71239200
H	0.93681300	1.71246600	0.73637500
H	0.18517600	0.42208600	1.68620100
C	0.53137400	-0.09384100	-0.38680800
H	0.65127200	0.45596300	-1.32519600
C	-0.51029800	-1.19994900	-0.60554200
C	-1.40805400	-1.01822700	-1.82135300
H	-2.13118000	-1.84046900	-1.81495100
H	-0.77174500	-1.17976400	-2.69674300
O	-1.24554200	-1.50884400	0.59769000
C	-2.17060900	-0.70514400	1.12804000
O	-2.80377100	-1.10882400	2.07082200
O	-1.29184900	2.75295800	0.36671700
H	0.04146500	-2.12675500	-0.75551300
H	-3.09224900	1.15205600	1.24612700
C	1.89755900	-0.68324200	-0.06694100
O	2.10351800	-1.83167600	0.23420800
O	2.84255700	0.24306000	-0.15675400
C	4.18717100	-0.17203100	0.15234100
H	4.20130800	-0.56722400	1.17010400
H	4.46421200	-0.97912800	-0.52886800
C	5.08444100	1.02480600	0.00056600
H	5.05613600	1.41007500	-1.02026500
H	6.11226000	0.73640000	0.22876200
H	4.79345400	1.82347100	0.68525500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -842.215407

222) Conformer **35bC4**

C	-1.88665500	-1.27519300	-1.66530700
H	-1.39892000	-0.52755900	-2.30131800
H	-2.29508600	-2.02136800	-2.35135200
C	-3.03103400	-0.62705800	-0.90808600
H	-3.62274300	-1.38191600	-0.38204500
H	-3.70067600	-0.13035000	-1.61269700
C	-2.58271400	0.43959600	0.10880700
C	-1.65611400	1.44448500	-0.56293200
C	-0.21888500	1.49133900	-0.14014900

H	0.27148000	2.30131400	-0.67955300
H	-0.19001400	1.74301900	0.92611900
C	0.55044300	0.18931200	-0.35183000
H	0.68527000	0.01279100	-1.42229800
C	-0.11409700	-1.08336600	0.23029400
C	-0.85845700	-1.95031800	-0.77604800
H	-0.08982600	-2.40930700	-1.40483700
H	-1.32266200	-2.76779900	-0.21436000
O	-0.88138000	-0.79286400	1.41313400
C	-2.05350900	-0.14787200	1.39699000
O	-2.66019400	-0.05030500	2.43299900
O	-2.10612700	2.19229400	-1.39804300
H	0.67718200	-1.71358100	0.63566100
H	-3.46727300	1.00465700	0.40799600
C	1.94463700	0.34421100	0.23062600
O	2.26897600	1.18772600	1.02690000
O	2.75377000	-0.59719700	-0.24404000
C	4.10915200	-0.62051500	0.24727300
H	4.10505500	-0.33030600	1.29813500
H	4.40819100	-1.66506400	0.16566900
C	5.00207800	0.27478700	-0.57364700
H	4.69905400	1.31926600	-0.48705900
H	4.98143400	-0.01396100	-1.62614100
H	6.03009900	0.18648400	-0.21547900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -842.214062

223) Conformer **35bC5**

C	-2.30650300	-0.21934500	-1.85757000
H	-2.96444100	-0.47963900	-2.69051200
H	-1.65339900	0.57483200	-2.23711300
C	-3.15220000	0.32428600	-0.72027400
H	-3.92080400	-0.39850600	-0.43124400
H	-3.67091600	1.22628900	-1.05042200
C	-2.34743300	0.70538100	0.53715500
C	-1.19144300	1.62431300	0.16856400
C	0.21248400	1.11429600	0.33406600
H	0.90249100	1.92105400	0.09341200
H	0.35060400	0.84834700	1.38870600
C	0.51900200	-0.11285100	-0.54262400
H	0.49798200	0.21031100	-1.58762100
C	-0.45200400	-1.29080600	-0.38162800
C	-1.48005500	-1.44084400	-1.49407900
H	-2.13629800	-2.27297600	-1.21855100

H	-0.92598500	-1.76995600	-2.37833900
O	-1.03595700	-1.34832900	0.93730900
C	-1.96027800	-0.49079600	1.37683800
O	-2.46358800	-0.69678600	2.45242200
O	-1.42389300	2.73921000	-0.23189800
H	0.14984200	-2.19834400	-0.38150400
H	-3.00165900	1.29535900	1.18181900
C	1.95194100	-0.53944200	-0.25902300
O	2.27053600	-1.56022600	0.29592400
O	2.80659600	0.37366600	-0.70436400
C	4.21000200	0.14317300	-0.46734900
H	4.41110700	-0.92325600	-0.57131900
H	4.71021300	0.68147100	-1.27165300
C	4.62791000	0.65935800	0.88605200
H	4.12294600	0.11768900	1.68736200
H	4.40557800	1.72366600	0.98289400
H	5.70464700	0.52305200	1.00816500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -842.213856

224) Conformer **35bC6**

C	-1.99437300	0.17322800	-2.05383400
H	-2.48281000	0.09017000	-3.02797000
H	-1.35986600	1.06461800	-2.11925400
C	-3.05798700	0.38823300	-0.99231100
H	-3.79709400	-0.41793600	-1.01815600
H	-3.59293500	1.31799600	-1.19503700
C	-2.50494500	0.49337600	0.44199000
C	-1.38832100	1.52585200	0.50545300
C	0.00912500	1.05668100	0.79804000
H	0.65615200	1.92872700	0.87329400
H	-0.00202500	0.55352000	1.77203400
C	0.55910900	0.08975700	-0.26521100
H	0.68029300	0.65239800	-1.19566000
C	-0.31973700	-1.13516800	-0.55387100
C	-1.13535100	-1.06055900	-1.83687000
H	-0.41770000	-1.14199600	-2.65880100
H	-1.75305500	-1.96359300	-1.88109900
O	-1.10355200	-1.53399500	0.59094500
C	-2.15758700	-0.84984100	1.04257500
O	-2.80883700	-1.32990800	1.93591300
O	-1.64860000	2.69227200	0.33477100
H	0.35039600	-1.98772000	-0.65337800
H	-3.30406600	0.88143800	1.07636900

C	1.95955900	-0.32678900	0.16053000
O	2.27548400	-1.43901700	0.49909100
O	2.78639500	0.71095000	0.12035000
C	4.15383900	0.48977400	0.52042500
H	4.48542000	1.45790600	0.89447100
H	4.16661700	-0.23298800	1.33642600
C	4.99524200	0.03032800	-0.64314300
H	6.03435100	-0.06746300	-0.32128200
H	4.95775500	0.75311800	-1.46027700
H	4.66000400	-0.93983800	-1.01287700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -842.214011

225) Conformer **35cC1**

C	1.49413100	0.94998100	1.26166600
H	1.73700400	1.79054900	1.91199600
H	2.43674000	0.46548300	0.97957100
C	0.87842400	1.47863000	0.00312200
C	0.52772800	0.48048500	-1.09493500
C	-0.99876800	0.40269100	-1.27706600
H	-1.31211300	1.35168400	-1.71833600
H	-1.22554800	-0.37864300	-2.01043500
C	-1.78699200	0.16482800	0.00251500
H	-1.60490700	1.01523700	0.67270900
C	-1.36795800	-1.10838000	0.72305400
H	-1.58914800	-1.97907300	0.09434500
H	-1.98689700	-1.21726000	1.61984000
C	0.07447900	-1.23186500	1.19286100
C	0.62214100	-0.05783300	2.01377400
H	-0.22205600	0.46030800	2.47553300
H	1.22734100	-0.45138000	2.83219700
O	0.97714500	-1.61741100	0.13027700
C	1.18502200	-0.87489700	-0.95774000
O	1.90393900	-1.31591200	-1.82070400
H	0.10760400	-2.11840100	1.82638300
H	0.94662600	0.89435300	-2.01413200
C	-3.27859700	0.13420500	-0.29765900
H	-3.60043400	1.05692100	-0.78621900
H	-3.86122700	0.01607500	0.61899200
H	-3.52365200	-0.70082000	-0.96100600
O	0.66554200	2.65431100	-0.17944700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -614.526070

226) Conformer **36aC1**

H	-1.43801600	1.55776800	-2.13501300
H	-1.27336500	-0.16541100	-2.41408200
H	0.43754400	-1.88950000	1.21349000
H	-0.94339500	-0.25699600	2.54034800
H	0.72699700	0.18731500	2.23816700
H	-3.26399900	0.57591500	-1.02718100
H	-2.40355600	2.34054800	0.26620000
H	-2.81396800	1.08030300	1.41639400
H	-0.61442600	2.17809500	1.90467600
H	0.89202400	0.99055600	-1.88022200
O	-3.41198300	-1.70597900	-0.30057500
O	-1.35223300	-1.69448000	0.40663100
C	-0.10492300	-1.06793200	0.74751800
C	-2.40362100	-1.06905500	-0.14655700
C	-0.24640000	0.05653000	1.75868300
C	0.64944000	-0.65508100	-0.51370400
O	0.82308500	2.78186200	-0.09085500
C	-1.22030400	0.60664700	-1.64135400
C	-2.29270400	0.37923900	-0.57187000
C	-2.12341400	1.34053000	0.60927200
C	-0.68992600	1.39017400	1.15323200
C	0.21487200	1.74414900	-0.00054200
C	0.21119000	0.68689700	-1.08428500
H	0.57139400	-1.44182700	-1.26355800
Br	2.56247300	-0.59087400	-0.08123400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -3186.623780

227) Conformer **36bC1**

C	-0.41399600	-1.01617300	0.75768000
O	-1.60976100	-1.74025000	0.41420400
O	0.21285100	2.89000300	-0.09271000
C	0.31078500	-0.55218000	-0.50234300
C	-0.65353800	0.09802500	1.76215200
I	2.41998800	-0.35129200	-0.05135600
O	-3.65570500	-1.91850200	-0.31023800
H	0.42611600	1.10780300	-1.87695500
H	-1.18741200	2.18460800	1.89520900
H	-3.29044200	0.91454400	1.40091900
H	-2.97476000	2.19810800	0.24650300
H	-3.68517500	0.36570900	-1.04283400
H	-1.63458300	-0.21987700	-2.41609000
H	-1.93609900	1.48618700	-2.14332600

H	0.29651500	-1.34613500	-1.24820500
H	0.30172400	0.30823300	2.25028800
H	-1.33056700	-0.26631400	2.53928400
H	0.18125200	-1.79299000	1.23563800
C	-2.70210000	-1.20291100	-0.15081600
C	-1.64718200	0.55612300	-1.64558200
C	-2.70402800	0.24813900	-0.58134600
C	-2.61829800	1.22489800	0.59588400
C	-0.22821800	0.75017200	-1.08140400
C	-0.31462400	1.80872600	-0.00278600
C	-1.19630100	1.38995000	1.14713000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -910.485731

228) Conformer **36cC1**

C	-1.01036400	-0.04115500	-1.12948700
H	-1.72848200	0.03809700	-1.94815700
C	-1.62746400	-0.83804800	-0.00129800
C	-0.70527300	-0.96358500	1.18575000
H	-1.21875700	-1.53149200	1.96369100
C	0.54016600	-1.73235900	0.72896500
H	1.23861700	-1.83189800	1.56474700
H	0.24248700	-2.74638000	0.44684200
C	1.23810900	-1.10035700	-0.48007600
H	1.95891500	-1.82246100	-0.86541300
C	0.24441100	-0.78737700	-1.60406900
H	0.73244500	-0.22409400	-2.40451600
H	-0.07296800	-1.73737100	-2.04170600
O	-2.71746100	-1.35053000	-0.07031900
C	-0.66992800	1.35555100	-0.63980100
H	-0.16234600	1.92801200	-1.42225700
C	-0.37478500	0.43856500	1.70422500
H	0.34195600	0.38300900	2.52807700
H	-1.28400900	0.89256200	2.10740500
C	2.10900200	0.08249500	-0.11142600
C	0.16099800	1.37848700	0.63915500
H	0.11680200	2.39966400	1.01990300
O	1.55534900	1.21154200	0.35959000
F	-1.85942600	2.01511400	-0.34669800
O	3.30472900	0.05936600	-0.23676600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -712.550373

229) Conformer **36dC1**

C	0.74828800	0.43994700	-1.10023800
H	1.47174600	0.58418700	-1.90374700
C	1.02282400	1.44452900	-0.00155300
C	0.07618200	1.29680000	1.16351000
H	0.34805000	2.03104600	1.92394500
C	-1.33673100	1.59597800	0.64745100
H	-1.37904000	2.63991200	0.32403100
H	-2.05580100	1.49103000	1.46474700
C	-1.74725600	0.72289600	-0.54294300
H	-2.65177900	1.15149700	-0.97616400
C	-0.66863100	0.70888800	-1.63036300
H	-0.91597800	-0.01563200	-2.41135000
H	-0.66449800	1.69220800	-2.10856100
O	1.86639700	2.30270400	-0.08460200
C	0.87360700	-0.97727200	-0.55367000
H	0.59343000	-1.70822700	-1.31301800
C	0.20127500	-0.11459500	1.74220600
H	-0.53647200	-0.26785600	2.53435000
H	1.18624100	-0.22638500	2.20231300
C	-2.19060700	-0.66568200	-0.13589100
C	0.05506400	-1.22193100	0.71329100
H	0.40044800	-2.15620200	1.15467900
O	-1.30806500	-1.53134000	0.38810600
Cl	2.59505300	-1.31824300	-0.17009300
O	-3.32287500	-1.04421400	-0.27981000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1072.826965

230) Conformer **37C1**

H	6.89804400	-0.65453900	2.23070700
H	6.19278400	0.94760700	1.94414400
H	5.17194200	-1.20621100	-3.38507100
H	1.96509000	-0.34103800	-2.30322300
H	7.40247400	-1.47355200	-1.14172300
H	2.12096700	2.39616500	1.39560300
H	4.90435800	-1.71233000	1.20860600
H	0.91768400	2.19129100	2.67837300
H	1.17488300	3.77541000	1.95737000
H	-0.16686400	0.51894600	-2.87042100
H	-1.01267300	-1.23445800	-1.51462700
H	-6.17586700	-2.01099000	-1.55591000
H	-7.15414900	-2.92709200	-0.39257000
H	-5.59788700	-3.58401900	-0.95007900
H	-4.27499600	-4.12021200	1.39409600

H	-2.67839100	-3.90252400	2.14518600
H	-0.71319800	2.56374800	-2.57929300
H	-1.63486900	1.07833400	2.18387600
H	-2.82443600	-3.92791700	0.36999600
O	2.82196000	-0.78302500	-2.40258900
H	-3.80414100	-2.08660100	-0.66136000
H	-5.64817900	-0.29893000	1.47568100
H	-1.79377200	2.92892500	-1.24978100
H	1.25035100	2.78602500	-1.06974900
H	0.22347000	4.15831300	-0.63704600
H	-0.87014900	2.88478300	1.09560600
H	-3.33187300	1.24054800	-2.61628500
H	-3.50378100	-0.51940600	-2.56250600
H	-1.39348300	-0.56492700	1.57696900
H	2.79280600	-1.40868800	0.17422800
H	3.89702100	0.80846000	-1.61833800
H	4.75977500	-2.09619000	-1.32056900
H	6.18833900	0.46063100	-0.51068100
O	-3.08743100	2.97250900	0.94181900
O	5.28300700	-0.24719500	3.37931700
C	-1.53532200	0.47102500	1.28352700
C	-2.73559900	0.58603400	0.37139700
H	4.42310300	0.17553700	3.28232900
O	-5.54082800	-2.03484200	0.43413600
C	-6.13611200	-2.66942300	-0.68223500
O	-1.80041000	-1.15671500	-0.95561600
C	5.95938600	-0.10577100	2.15074000
O	5.69860400	-0.84158500	-2.66668400
O	7.03996300	-1.40800600	-0.25099200
O	-3.45062800	-2.21184300	1.35081100
C	-4.17282600	-1.69718800	0.29130000
C	-3.37132700	1.98388100	0.32602900
C	1.13303900	2.70598000	1.73742000
C	-3.30781000	-3.61696300	1.30356700
O	-4.84989600	0.24818900	1.47377200
O	-4.41948700	1.94338000	-0.51103700
O	1.94020800	0.44725600	-0.03361300
C	-0.84489300	2.45281900	-1.50008300
C	0.27294000	3.06781600	-0.66864500
H	-5.53318300	0.40438700	-1.30255700
C	-0.83694100	0.97997600	-1.09955200
O	0.05151800	0.26690300	-1.96552400
C	-0.33282700	0.95348500	0.41931700
C	-3.38199400	0.37556400	-1.95336800

C	-4.09524700	-0.16806100	0.36674400
C	0.04986100	2.44635700	0.70515600
O	0.85146300	-0.95802100	1.32542900
C	0.84912100	0.02469400	0.63476600
C	-4.51944000	0.57018600	-0.94646100
C	-2.17062100	0.20918500	-1.01566600
C	5.15703100	-0.66260000	0.99765300
O	3.96289300	0.10848900	0.92932900
C	3.08217500	-0.37371400	-0.04265100
C	3.68773300	-0.25403800	-1.43017200
C	4.98794000	-1.02921000	-1.46112100
C	5.89861600	-0.58560700	-0.33090400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1948.147810

231) Conformer **37C2**

H	5.28047200	2.38026200	2.25463100
H	3.79599500	2.91787300	1.44638500
H	5.76336600	-0.31013700	-2.98596200
H	2.86161900	-1.57790800	-2.74876200
H	7.03378900	1.53401100	-0.66239700
H	0.94432500	-3.25187400	-1.80194000
H	4.82473500	0.05264200	1.53120700
H	0.32994100	-4.81059000	-1.26336600
H	1.37132500	-3.87226400	-0.19675600
H	-0.02844600	-1.68248700	2.54577500
H	-1.03841900	0.42219300	2.21212000
H	-3.72100900	4.63727400	0.79353000
H	-5.05096800	3.45162800	0.81214800
H	-5.07286300	4.79057600	-0.35255000
H	-1.50425600	4.68780500	-0.79635500
H	0.03050200	3.82858500	-1.05358700
H	-3.18479100	-2.89748500	0.71590900
H	-1.03129700	-1.05293100	-1.95514200
H	-0.75980700	3.76817900	0.54177400
O	3.69554800	-1.49858100	-2.27686000
H	-2.70369200	2.51238600	0.73956900
H	-4.12963300	1.90845600	-2.22273200
H	-2.65591800	-3.11479300	2.38122500
H	-0.50902100	-4.07480100	1.59241800
H	-1.70626300	-4.84413700	0.54997000
H	-1.43897100	-3.13061500	-1.14261600
H	-4.33589600	-0.80695400	1.90978300
H	-3.78724100	0.84626500	2.21562300

H	-0.43300600	0.26939000	-0.94976700
H	3.38127800	-1.43262600	0.37137100
H	3.15829200	0.48711700	-2.00133100
H	5.61121600	-0.80251000	-0.74187300
H	4.74183700	2.10778400	-0.72664800
O	-3.43709400	-2.19685700	-1.69044200
O	3.57992100	1.73854600	3.14295200
C	-1.05180300	-0.62290200	-0.95340800
C	-2.44856200	-0.26144700	-0.50408200
H	2.71356700	1.40959400	2.88113000
O	-3.75634300	3.33131300	-0.82264100
C	-4.42953500	4.08347100	0.16974900
O	-1.48957600	0.77324400	1.42491900
C	4.27481600	2.07558800	1.96395100
O	5.77749700	0.44025000	-2.38227700
O	6.51092800	1.47804900	0.14520300
O	-1.58601500	2.61735900	-0.97164400
C	-2.79910200	2.40439600	-0.34405700
C	-3.53500200	-1.23344100	-0.98335000
C	0.56701600	-3.79657000	-0.93362100
C	-0.92976800	3.79248400	-0.54096300
O	-3.67257200	1.06420700	-2.10094200
O	-4.72036000	-0.79510000	-0.53288500
O	1.59433900	-0.79312100	-0.42324200
C	-2.31136800	-2.89991200	1.36931900
C	-1.27901400	-3.88098300	0.83727400
H	-5.36717900	1.01418500	0.20601500
C	-1.57093000	-1.56433400	1.35743900
O	-0.95342700	-1.37881500	2.61675500
C	-0.55821500	-1.65032300	0.11146200
C	-3.79511800	0.03920500	1.48400000
C	-3.30085600	1.01398600	-0.74883300
C	-0.67985100	-3.14972300	-0.35857300
O	1.36671900	-1.81946700	1.54745800
C	0.87451100	-1.42198900	0.51265500
C	-4.44272500	0.44406800	0.15677300
C	-2.35541800	-0.27877000	1.03872600
C	4.36969000	0.90770300	1.01016900
O	3.03542700	0.58267400	0.63731400
C	2.96254700	-0.56555500	-0.15354500
C	3.66473800	-0.33588200	-1.48267600
C	5.10385000	0.05786100	-1.20451300
C	5.17951300	1.22411800	-0.23858700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1948.150102

232) Conformer **37C3**

H	5.28047200	2.38025500	2.25463700
H	3.79599300	2.91786700	1.44639400
H	5.76335800	-0.31012500	-2.98596700
H	2.86161300	-1.57790300	-2.74876100
H	7.03378800	1.53401400	-0.66239200
H	1.37132200	-3.87226600	-0.19676400
H	4.82473500	0.05263600	1.53120600
H	0.94431900	-3.25187700	-1.80194700
H	0.32993500	-4.81059100	-1.26337100
H	-0.02844400	-1.68249000	2.54577200
H	-1.03841400	0.42219200	2.21211700
H	-5.05097700	3.45162400	0.81214400
H	-5.07285500	4.79058300	-0.35254200
H	-3.72101100	4.63726200	0.79354700
H	-0.75980200	3.76817900	0.54176900
H	-1.50425200	4.68780600	-0.79635900
H	-2.65591700	-3.11479300	2.38122400
H	-1.03130000	-1.05293000	-1.95514300
H	0.03050300	3.82858300	-1.05359500
O	3.69554700	-1.49857200	-2.27686700
H	-2.70368600	2.51238700	0.73957000
H	-4.12963300	1.90845900	-2.22272800
H	-3.18479200	-2.89748400	0.71590800
H	-0.50902200	-4.07480300	1.59241400
H	-1.70626500	-4.84413700	0.54996600
H	-1.43897500	-3.13061400	-1.14261900
H	-4.33589300	-0.80695200	1.90978700
H	-3.78723500	0.84626700	2.21562600
H	-0.43300600	0.26939000	-0.94976900
H	3.38127800	-1.43262800	0.37136600
H	3.15829100	0.48712500	-2.00133000
H	5.61121500	-0.80250800	-0.74187800
H	4.74183700	2.10778600	-0.72664200
O	-3.43709700	-2.19685500	-1.69044100
O	3.57992300	1.73853400	3.14295900
C	-1.05180400	-0.62290100	-0.95340900
C	-2.44856200	-0.26144600	-0.50408200
H	2.71356700	1.40958500	2.88113700
O	-3.75634000	3.33131700	-0.82263600
C	-4.42953500	4.08346900	0.16975600
O	-1.48957100	0.77324300	1.42491700

C	4.27481600	2.07558000	1.96395700
O	5.77749600	0.44025800	-2.38227700
O	6.51092800	1.47804700	0.14520800
O	-1.58601500	2.61736000	-0.97164800
C	-2.79909900	2.40439800	-0.34405600
C	-3.53500400	-1.23343900	-0.98334700
C	0.56701100	-3.79657100	-0.93362800
C	-0.92976500	3.79248400	-0.54096900
O	-3.67257400	1.06420800	-2.10094000
O	-4.72036100	-0.79509800	-0.53288000
O	1.59433800	-0.79312000	-0.42324500
C	-2.31136800	-2.89991200	1.36931700
C	-1.27901600	-3.88098400	0.83727100
H	-5.36717700	1.01418800	0.20602100
C	-1.57092900	-1.56433500	1.35743700
O	-0.95342400	-1.37881800	2.61675300
C	-0.55821500	-1.65032400	0.11145900
C	-3.79511500	0.03920700	1.48400300
C	-3.30085600	1.01398700	-0.74883100
C	-0.67985400	-3.14972300	-0.35857700
O	1.36671900	-1.81947100	1.54745300
C	0.87451100	-1.42199100	0.51265100
C	-4.44272400	0.44407000	0.15677700
C	-2.35541600	-0.27876900	1.03872600
C	4.36968900	0.90769900	1.01017100
O	3.03542600	0.58267100	0.63731600
C	2.96254700	-0.56555500	-0.15354700
C	3.66473700	-0.33587700	-1.48267800
C	5.10384900	0.05786500	-1.20451400
C	5.17951300	1.22411800	-0.23858300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1948.150102

233) Conformer **37C4**

H	5.31855200	2.16206100	2.46727300
H	3.82764100	2.78073900	1.73217400
H	5.73143000	-0.00070200	-3.01823500
H	2.82728300	-1.27503500	-2.87595900
H	7.03812200	1.59331800	-0.53885500
H	1.37630800	-3.81039600	-0.54465100
H	4.84540700	-0.08226300	1.52450100
H	0.31485800	-4.64116700	-1.67853600
H	0.91314400	-3.03285000	-2.06951800
H	0.02476300	-1.91079800	2.43395500

H	-0.99458400	0.21384000	2.32429200
H	-4.69591400	5.13318400	-0.03304400
H	-2.91588000	5.11165700	-0.03151200
H	-3.81586000	4.46839700	1.36659300
H	-0.51837600	3.63505000	-1.94342000
H	-2.27037500	3.73436300	-2.21984900
H	-2.59279600	-3.33191100	2.18381500
H	-1.06310000	-0.83787500	-1.96393800
H	-1.42901000	2.18063700	-2.41677300
O	3.66562500	-1.24651100	-2.40619200
H	-2.75040600	2.39606000	1.09373500
H	-4.26239000	2.04405700	-1.89848200
H	-3.16396900	-2.95596600	0.56180300
H	-0.46387900	-4.19854500	1.25494000
H	-1.68181100	-4.86599100	0.16749200
H	-1.45568800	-2.99249200	-1.35217400
H	-3.74453700	0.63199400	2.41966000
H	-4.28850700	-0.99494400	1.98878500
H	-0.45077200	0.37573500	-0.83565200
H	3.38743100	-1.44096200	0.23979100
H	3.13849700	0.70355800	-1.92874700
H	5.60159200	-0.71154700	-0.83396400
H	4.74928200	2.18634600	-0.51854600
O	-3.45567700	-2.03649200	-1.76130000
O	3.62507500	1.44163900	3.30737900
C	-1.07032300	-0.51246700	-0.92333500
C	-2.46224000	-0.20890800	-0.41593500
H	2.75264500	1.14741700	3.02516300
O	-3.89467900	3.30377700	-0.34604600
C	-3.81537800	4.57213300	0.27616400
O	-1.46451200	0.63852100	1.58582300
C	4.30855600	1.89040800	2.15937300
O	5.75383200	0.68737400	-2.34463200
O	6.52355600	1.46291500	0.26548200
O	-1.61312500	2.85231400	-0.44791000
C	-2.85928300	2.42664600	0.00957000
C	-3.54865800	-1.14909700	-0.96048800
C	0.55619400	-3.66452100	-1.25300500
C	-1.46427200	3.10455500	-1.83473200
O	-3.75970200	1.21936700	-1.85935300
O	-4.72630400	-0.77804100	-0.43721000
O	1.59025000	-0.72662300	-0.46157800
C	-2.27434900	-3.01646100	1.18986900
C	-1.25097700	-3.93411500	0.53995700

H	-5.37536100	0.95636900	0.47262200
C	-1.54011800	-1.68109700	1.29247800
O	-0.89799000	-1.61505400	2.55120000
C	-0.55283300	-1.63909800	0.02410200
C	-3.76552900	-0.11049800	1.62284900
C	-3.33960400	1.06842400	-0.52661800
C	-0.68009700	-3.08494100	-0.59004100
O	1.39825200	-1.94881300	1.39804700
C	0.88727300	-1.44846500	0.41854000
C	-4.44911600	0.40046600	0.35343300
C	-2.33498900	-0.37388600	1.11697500
C	4.38839000	0.82123300	1.09481200
O	3.04901500	0.53852900	0.70680400
C	2.96309200	-0.52635700	-0.19150000
C	3.64838700	-0.16794800	-1.50060200
C	5.09257900	0.19224500	-1.20241800
C	5.18618400	1.25598800	-0.12592100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1948.147665

234) Conformer **38C1**

C	0.16266700	-1.15093100	-0.80571000
C	-0.78164300	-0.08732300	-1.34070200
H	-1.19507000	-0.38238100	-2.30519900
C	-1.84241600	0.31250400	-0.29804800
C	-0.92079700	1.14397100	0.59594900
H	-1.45929900	1.83535300	1.24236900
C	0.04342600	0.27642700	1.42874200
C	0.71352400	-0.87718800	0.61557800
C	1.21895700	1.12110300	1.97999200
H	1.50328900	0.79408000	2.98215000
H	0.96558600	2.17956800	2.03802300
C	2.37659100	0.88030000	1.03496200
H	2.98908600	1.68526400	0.64497200
C	2.08520600	-0.33898200	0.27702000
C	2.41141200	-0.69764700	-1.12948300
O	1.30624200	-1.22217600	-1.68477900
O	3.45180000	-0.60494000	-1.71428300
C	-2.59960400	-0.84367100	0.36031200
H	-1.86195600	-1.51593800	0.80737100
C	-3.39474500	-1.65255400	-0.66060100
H	-2.77221300	-2.04136300	-1.46991500
H	-4.20111500	-1.06160900	-1.10501500
H	-3.86419900	-2.50661900	-0.16925200

C	-3.50978900	-0.34449700	1.47555100
H	-4.26016500	0.34511500	1.08411800
H	-2.95428700	0.17101700	2.26198300
H	-4.03086200	-1.18658500	1.93524300
H	-0.32456600	-2.12483500	-0.86174800
C	0.80204500	-2.16554100	1.42452000
H	-0.19209200	-2.56362900	1.63642900
H	1.30599400	-1.98354100	2.37452200
H	1.36479500	-2.93053300	0.88395300
O	-0.04422700	1.12856600	-1.55594500
O	0.33644400	2.99995300	-0.41065200
C	-0.15381600	1.90883600	-0.46058500
O	3.06969400	-0.34425600	1.27794100
H	-0.54037300	-0.14720500	2.24777100
O	-2.72947500	1.25565100	-0.87066400
H	-3.26248700	0.82261300	-1.54568000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1032.753176

235) Conformer **38C2**

C	0.15845700	-1.17194100	-0.76463200
C	-0.78247400	-0.12325000	-1.33212600
H	-1.20297300	-0.43909100	-2.28566200
C	-1.84096100	0.29981600	-0.30931200
C	-0.92119900	1.16181600	0.56853500
H	-1.45395000	1.87165400	1.20122900
C	0.04768400	0.32196300	1.42667000
C	0.71431800	-0.85548400	0.64592400
C	1.22536400	1.18290900	1.94775900
H	1.51354000	0.88667900	2.95839600
H	0.97233200	2.24271000	1.97472100
C	2.37945400	0.91329500	1.00613300
H	2.99077400	1.70587900	0.58982800
C	2.08483500	-0.32807500	0.28632600
C	2.40576400	-0.72996900	-1.10974500
O	1.29871600	-1.27250800	-1.64404500
O	3.44404800	-0.65659100	-1.70079500
C	-2.59764500	-0.83780200	0.38215300
H	-1.86511300	-1.46108900	0.90235000
C	-3.33580000	-1.71364800	-0.62372800
H	-4.06981500	-1.12795900	-1.18053000
H	-3.86537700	-2.51311700	-0.10187100
H	-2.66270200	-2.18276900	-1.34525600
C	-3.56310000	-0.30160400	1.43400000

H	-3.06562800	0.32448500	2.17822200
H	-4.03219100	-1.13315900	1.96292000
H	-4.36973600	0.28068700	0.97917400
H	-0.33208000	-2.14541300	-0.78837900
C	0.80534000	-2.11923600	1.49253700
H	-0.18830400	-2.50969500	1.72016900
H	1.31354400	-1.90970500	2.43454900
H	1.36496100	-2.90073000	0.97272700
O	-0.04086800	1.08581700	-1.57912300
O	0.32926000	2.99278400	-0.49107900
C	-0.15531800	1.89799800	-0.50902400
O	3.07303800	-0.30365900	1.28335400
H	-0.53318500	-0.07665400	2.26019000
O	-2.72422700	1.14353000	-1.02827200
H	-3.30214400	1.59158200	-0.40192200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1032.752926

236) Conformer **39C1**

C	-3.02569900	1.21715600	0.24706000
C	-3.40437900	-0.21610800	-0.15167800
H	-3.66082100	-0.19488900	-1.21660700
C	-2.37140200	-1.35672100	0.05740400
C	-0.96486200	-1.02250100	-0.39939500
C	-0.29121200	0.12792800	-0.27753700
C	-0.67458200	1.45669100	0.33138500
C	-1.89125000	1.36488900	1.24305000
H	-1.83871900	0.53114300	1.93929500
H	-1.99859900	2.29861900	1.80083500
O	-2.58586800	1.97301700	-0.91159200
C	-1.26464400	2.21471800	-0.85348400
O	-0.70585700	2.89916000	-1.66772500
C	1.06479300	0.05732800	-0.90391100
C	2.15193300	0.49697400	0.10051600
C	1.89288600	1.96714200	0.39119300
H	2.64924300	2.38151000	1.06116800
H	1.96975500	2.52295900	-0.54693400
C	0.51043200	2.16727900	1.01296200
H	0.28532200	3.23587000	1.06322200
H	0.53180600	1.81587000	2.04878700
C	1.24117200	-1.39852200	-1.34573200
C	2.46298200	-1.93170300	-0.60549700
O	3.58703100	-1.07446300	-0.96533500
C	3.46079700	0.21365600	-0.59110100

C	-0.10248300	-2.08638100	-1.04824700
H	0.00444300	-2.95679700	-0.39150700
H	-0.55676100	-2.46119800	-1.96896800
C	2.10099500	-0.42198800	1.35225500
H	1.09002200	-0.34095900	1.75750000
C	2.32635000	-1.87909700	0.90170900
H	1.51226400	-2.52906700	1.22754600
H	3.24468100	-2.27653600	1.34193200
C	-2.90710000	-2.57910100	-0.68980300
H	-2.29081600	-3.45301200	-0.47911300
H	-2.92290600	-2.41134900	-1.76913000
H	-3.92605000	-2.78678100	-0.36046100
O	-2.28327200	-1.67266500	1.45147900
H	-3.19224000	-1.81329600	1.74825900
O	-4.52783700	-0.61527400	0.62504500
H	-5.32768300	-0.24110400	0.24620400
H	-3.94073200	1.70612500	0.58209500
H	1.11568400	0.74690500	-1.75431400
H	1.46159100	-1.45168600	-2.41290600
H	2.75079300	-2.92271200	-0.95475600
C	3.08427900	-0.01160900	2.43858300
H	3.02455000	-0.71139700	3.27580300
H	2.87602100	0.98714900	2.82779900
H	4.11563700	-0.02450200	2.07238400
O	4.34448800	0.99884400	-0.83143700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1226.623323

237) Conformer **39C2**

C	-3.02670700	1.22575600	0.24287300
C	-3.42037300	-0.20480200	-0.15851200
H	-3.67277400	-0.17006700	-1.22219100
C	-2.38322600	-1.34438600	0.03717900
C	-0.97278000	-1.01167500	-0.41396400
C	-0.29407000	0.13521800	-0.28032800
C	-0.67437100	1.46146100	0.33532600
C	-1.89461600	1.37058100	1.24242600
H	-1.84242000	0.54087500	1.94362200
H	-2.00157000	2.30436700	1.80036400
O	-2.57943900	1.98420300	-0.91270000
C	-1.25962900	2.22536000	-0.84849400
O	-0.69577300	2.91274500	-1.65709800
C	1.06324000	0.06467500	-0.90342500
C	2.14984500	0.49443800	0.10566200

C	1.89475500	1.96354200	0.40494100
H	2.65038600	2.37113700	1.07986400
H	1.97647600	2.52485400	-0.52945800
C	0.51100400	2.16480900	1.02353900
H	0.28920300	3.23384500	1.07820500
H	0.52845600	1.80847000	2.05776700
C	1.23646100	-1.38794200	-1.35605500
C	2.45491200	-1.93032000	-0.61671800
O	3.58214000	-1.07433900	-0.96816100
C	3.45929100	0.21168600	-0.58522300
C	-0.11015500	-2.07411200	-1.06823100
H	-0.00352100	-2.95093200	-0.41942300
H	-0.56188900	-2.44120400	-1.99321400
C	2.09336800	-0.43282500	1.35098400
H	1.08185500	-0.35085000	1.75486600
C	2.31498400	-1.88754100	0.89060700
H	1.49842100	-2.53762300	1.21017000
H	3.23105700	-2.29099400	1.32997700
C	-2.91645100	-2.57080200	-0.69720600
H	-2.31113000	-3.45271000	-0.47550600
H	-2.90455300	-2.41535500	-1.77748800
H	-3.94290800	-2.76570200	-0.38683600
O	-2.39380000	-1.61517100	1.45516300
H	-2.15715800	-2.53773500	1.59324600
O	-4.59989700	-0.55495000	0.53892000
H	-4.30087800	-0.98609100	1.35298500
H	-3.94655800	1.70806400	0.57080300
H	1.11714000	0.76019200	-1.74876800
H	1.45933200	-1.43364700	-2.42300200
H	2.74019900	-2.91984100	-0.97213300
C	3.07597100	-0.03330700	2.44197000
H	3.01266500	-0.73876100	3.27415500
H	2.87015600	0.96337700	2.83768800
H	4.10784300	-0.04691200	2.07734400
O	4.34595000	0.99555700	-0.81826700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1226.624078

238) Conformer **39C3**

C	-3.02341800	1.21902900	0.24857000
C	-3.40345900	-0.20865900	-0.16200400
H	-3.64247800	-0.17420500	-1.22928600
C	-2.37310000	-1.35221400	0.06825000
C	-0.96413700	-1.02559900	-0.38861300

C	-0.28997600	0.12553100	-0.27327600
C	-0.67112700	1.45684500	0.33152400
C	-1.88771300	1.36897900	1.24303500
H	-1.83311600	0.53998000	1.94427200
H	-1.99677700	2.30600600	1.79490700
O	-2.58373800	1.97725800	-0.90824400
C	-1.26134900	2.21462700	-0.85331100
O	-0.70286500	2.89709800	-1.66934600
C	1.06450100	0.05297200	-0.90247100
C	2.15439500	0.49415100	0.09842100
C	1.89660500	1.96489700	0.38735800
H	2.65435600	2.37973700	1.05545400
H	1.97226800	2.51932700	-0.55168300
C	0.51531600	2.16688800	1.01106400
H	0.29125100	3.23572300	1.06079500
H	0.53769900	1.81618500	2.04712300
C	1.23920900	-1.40365500	-1.34202100
C	2.46337800	-1.93565500	-0.60472700
O	3.58620900	-1.07898500	-0.96944700
C	3.46134800	0.20959000	-0.59632600
C	-0.10344800	-2.09076200	-1.03846900
H	0.00667400	-2.95992600	-0.38058900
H	-0.56067300	-2.46761600	-1.95699900
C	2.10645200	-0.42289300	1.35168100
H	1.09621000	-0.34169700	1.75873200
C	2.33161600	-1.88055600	0.90284900
H	1.51940600	-2.53081800	1.23274100
H	3.25190900	-2.27629800	1.34051100
C	-2.90143500	-2.58893200	-0.66106600
H	-2.26612800	-3.45031100	-0.45654000
H	-2.94596500	-2.43208200	-1.74129100
H	-3.90503200	-2.83362900	-0.30672900
O	-2.30667300	-1.64413400	1.46742900
H	-3.22828200	-1.68232900	1.76148400
O	-4.57067700	-0.52589700	0.59590900
H	-5.17408000	-1.03721900	0.05089100
H	-3.94307600	1.69707700	0.58257600
H	1.11349400	0.74102400	-1.75422000
H	1.45596900	-1.45899900	-2.40982200
H	2.75011400	-2.92722400	-0.95325900
C	3.09165600	-0.01052900	2.43549000
H	3.03420900	-0.70944700	3.27359900
H	2.88338400	0.98847500	2.82405300
H	4.12226300	-0.02299200	2.06716600

O	4.34455600	0.99427400	-0.84000600
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No imaginary frequency.
Gibbs Free Energies (a.u.) = -1226.622998

239) Conformer **39C4**

C	-3.02670900	1.22575600	0.24287100
C	-3.42037400	-0.20480200	-0.15851600
H	-3.67277800	-0.17006800	-1.22219300
C	-2.38322600	-1.34438500	0.03717600
C	-0.97278100	-1.01167500	-0.41396600
C	-0.29407100	0.13521700	-0.28033100
C	-0.67437300	1.46145800	0.33532500
C	-1.89461900	1.37057600	1.24242500
H	-1.84242300	0.54086600	1.94361600
H	-2.00157200	2.30435800	1.80036700
O	-2.57944000	1.98420400	-0.91270200
C	-1.25962900	2.22536100	-0.84849400
O	-0.69577200	2.91274600	-1.65709500
C	1.06324000	0.06467400	-0.90342400
C	2.14984400	0.49443800	0.10566200
C	1.89475200	1.96354000	0.40494400
H	2.65038200	2.37113300	1.07987000
H	1.97647300	2.52485400	-0.52945300
C	0.51100100	2.16480300	1.02354200
H	0.28920000	3.23383900	1.07821200
H	0.52845200	1.80845800	2.05776800
C	1.23646200	-1.38794500	-1.35605200
C	2.45491900	-1.93031800	-0.61672300
O	3.58214200	-1.07433200	-0.96817000
C	3.45929000	0.21169200	-0.58522600
C	-0.11015100	-2.07411800	-1.06821800
H	-0.00351200	-2.95092500	-0.41939200
H	-0.56188200	-2.44123000	-1.99319400
C	2.09336900	-0.43282800	1.35098300
H	1.08185300	-0.35086300	1.75485900
C	2.31499900	-1.88754200	0.89060300
H	1.49844800	-2.53763400	1.21017400
H	3.23108300	-2.29098200	1.32996500
C	-2.91645600	-2.57080000	-0.69720900
H	-2.90455800	-2.41535200	-1.77749000
H	-3.94291500	-2.76569300	-0.38683700
H	-2.31114000	-3.45271000	-0.47550700
O	-2.39380000	-1.61516500	1.45516100
H	-2.15717000	-2.53773200	1.59324500

O	-4.59989500	-0.55495400	0.53892200
H	-4.30087000	-0.98609900	1.35298200
H	-3.94656100	1.70806500	0.57079900
H	1.11714200	0.76018900	-1.74876800
H	1.45932500	-1.43365100	-2.42300100
H	2.74020900	-2.91983700	-0.97214000
C	3.07596400	-0.03330500	2.44197400
H	4.10783700	-0.04689600	2.07735000
H	3.01266200	-0.73876400	3.27415400
H	2.87013500	0.96337400	2.83769500
O	4.34594900	0.99556400	-0.81826200

No imaginary frequency.

Gibbs Free Energies (a.u.) = 1226.624078

240) Conformer **40C1**

C	3.44756400	-0.89453900	0.28609500
C	3.60407600	0.60042600	0.22596500
H	4.63057800	0.96028000	0.24657100
C	2.63260900	1.52101500	0.24328200
C	1.15081000	1.20202500	0.19398100
C	0.78962300	-0.08716500	-0.57305800
C	1.15700600	-1.47613600	0.02516900
C	2.23836200	-1.33653800	1.09620200
H	1.97952100	-0.63476500	1.88924800
H	2.41592100	-2.31398100	1.55482300
O	3.25276100	-1.49115400	-1.02383400
C	2.01032000	-2.18986800	-1.02564000
H	1.59752800	-2.14837700	-2.03697700
H	2.16001900	-3.24239000	-0.74723200
C	-0.67121800	0.07570600	-1.01067100
C	-1.70651500	-0.62493600	-0.10315500
C	-1.36610700	-2.10472700	-0.10356700
H	-2.12989100	-2.68945300	0.41373700
H	-1.35541100	-2.45898500	-1.13934300
C	-0.01153100	-2.32347300	0.55806000
H	0.26750300	-3.37890700	0.47721100
H	-0.11670600	-2.13453400	1.63073700
C	-0.94326300	1.58873300	-1.07438000
C	-2.21581800	1.85777500	-0.28018400
O	-3.26597100	1.01807700	-0.84270500
C	-3.03390000	-0.30439200	-0.74627900
C	0.32997500	2.27231000	-0.55661100
H	0.90398100	2.61693100	-1.42002200
H	0.12343100	3.15350200	0.05507400

C	-1.74724200	0.00620900	1.31751900
H	-0.74446600	-0.08950500	1.73595100
C	-2.09305600	1.50118900	1.18481600
H	-1.34143400	2.13566500	1.65938400
H	-3.04552900	1.71870500	1.67530000
C	2.99539500	2.97386200	0.36187900
H	4.07288500	3.10071000	0.47563800
H	2.50574300	3.42138700	1.23377200
H	2.67408600	3.55341600	-0.50763800
H	4.37234600	-1.31406300	0.69339100
H	-0.79299800	-0.37485700	-2.00014700
H	-1.13784600	1.90152000	-2.10222200
H	-2.57328200	2.87706300	-0.42288800
C	-2.71053600	-0.70511200	2.25834100
H	-2.72975000	-0.19395800	3.22410100
H	-2.42190400	-1.74248100	2.43878300
H	-3.73162200	-0.70125600	1.86419200
O	-3.84777700	-1.08847900	-1.17022000
H	1.37542400	0.00238800	-1.49430200
H	0.79045600	1.15421000	1.23036300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1002.242517

241) Conformer **41C1**

C	3.12815500	-1.21546500	0.63007800
C	3.46225000	0.17754200	0.18740400
H	4.52540200	0.39481000	0.12910100
C	2.61065200	1.18260600	-0.04289500
C	1.10065600	1.05659600	-0.02784700
C	0.57675500	-0.28648700	-0.57663700
C	0.80984600	-1.58340500	0.27979300
C	1.82279300	-1.34258200	1.39395100
H	1.60676100	-0.47252300	2.01175200
H	1.85934000	-2.21995300	2.04514700
O	2.95329000	-2.14618600	-0.48720000
C	1.65081800	-2.45094200	-0.64338300
C	-0.87086900	-0.03449400	-1.01830100
C	-1.94327500	-0.50115900	-0.01384400
C	-1.77023800	-2.00057800	0.14328000
H	-2.58146900	-2.43772500	0.72914000
H	-1.81979600	-2.46161100	-0.84739000
C	-0.44000200	-2.30919000	0.81714700
H	-0.25418200	-3.38537000	0.77268800
H	-0.52690800	-2.06711600	1.87984700

C	-0.98798700	1.47792500	-1.27854900
C	-2.17844800	1.98606800	-0.47406500
O	-3.34188200	1.21619400	-0.89458800
C	-3.25299600	-0.10478600	-0.65349400
C	0.37660200	2.08022900	-0.92252300
H	0.93799200	2.20740500	-1.85082700
H	0.30948300	3.06323600	-0.45337000
C	-1.85650100	0.28906900	1.32224700
H	-0.85832200	0.11887600	1.72969000
C	-2.02501000	1.79054500	1.01848700
H	-1.18027900	2.37842900	1.38403800
H	-2.91798400	2.18165100	1.51276300
C	3.18588000	2.54491100	-0.31222000
H	2.85909100	2.91254800	-1.29142400
H	4.27907200	2.48184800	-0.32823100
H	3.97331600	-1.61182200	1.19247600
H	-1.05713600	-0.59493000	-1.93812900
H	-1.21251500	1.66944900	-2.32956700
H	-2.42385900	3.01698600	-0.72670300
C	-2.86490700	-0.18564300	2.35991700
H	-3.89129400	-0.09195800	1.99198600
H	-2.78244400	0.42500200	3.26227000
H	-2.70301500	-1.22621400	2.64825700
O	-4.16503400	-0.83410900	-0.95582800
H	1.13268900	-0.41425100	-1.51280000
H	0.76320600	1.20764900	1.00366700
O	1.28752600	-3.26896000	-1.44712500
O	2.74698700	3.42944600	0.71403000
H	2.91071400	4.32994100	0.42001400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1151.430540

242) Conformer **41C2**

C	-2.98844700	1.33815700	0.65134500
C	-3.38915800	-0.05924900	0.29169500
H	-4.45676100	-0.24656000	0.26202800
C	-2.58093800	-1.10807400	0.11494300
C	-1.06711800	-1.04721600	0.09441700
C	-0.50111000	0.23668000	-0.54424500
C	-0.66497200	1.59063100	0.23669900
C	-1.66352500	1.45893100	1.38141500
H	-1.46942800	0.62058700	2.04842800
H	-1.65069800	2.37540100	1.97751400
O	-2.79812700	2.20163100	-0.52075900

C	-1.48933700	2.43752400	-0.72089400
C	0.92594300	-0.09924500	-0.99717700
C	2.03796800	0.38399200	-0.04480800
C	1.92562500	1.89554800	0.02594700
H	2.76578300	2.33402100	0.56840700
H	1.97063900	2.29544500	-0.99118400
C	0.62362400	2.29468400	0.70679200
H	0.47881900	3.37318300	0.60416900
H	0.72411700	2.11011700	1.77985300
C	0.98009900	-1.62757100	-1.16681300
C	2.16949700	-2.13337100	-0.35912000
O	3.35011100	-1.43563800	-0.85051000
C	3.31681300	-0.10014500	-0.68651600
C	-0.39852000	-2.15428000	-0.74720400
H	-0.98125100	-2.32035400	-1.65561700
H	-0.34629600	-3.11076400	-0.22230600
C	1.95137700	-0.32182600	1.33764500
H	0.96849800	-0.09120700	1.75225800
C	2.05958000	-1.84378000	1.12182200
H	1.20417600	-2.37730100	1.54195600
H	2.95024900	-2.23714300	1.61843200
C	-3.16881400	-2.48257000	-0.04143300
H	-2.66812500	-3.14922400	0.67664600
H	-2.93784300	-2.86789400	-1.04226600
H	-3.80450900	1.80326400	1.20408400
H	1.11293500	0.39649900	-1.95319500
H	1.17102300	-1.89107900	-2.20872400
H	2.36986300	-3.18615200	-0.55476100
C	2.99713400	0.17563900	2.32645000
H	4.01169500	0.02313700	1.94568600
H	2.91186200	-0.37793900	3.26465000
H	2.87827900	1.23642900	2.55591400
O	4.24838700	0.57394100	-1.05069700
H	-1.07213900	0.33038500	-1.47525800
H	-0.71618100	-1.14937500	1.12872400
O	-1.10698900	3.18916700	-1.57966200
O	-4.56394800	-2.47469100	0.17318800
H	-4.90448900	-3.33550800	-0.08367700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1151.431190

243) Conformer 41C3

C	3.03166400	-1.32611800	0.81127100
C	3.40484400	0.11252900	0.62084400

H	4.47238900	0.31521100	0.65080200
C	2.58115600	1.15480700	0.46914500
C	1.07165100	1.04919500	0.38041300
C	0.58863300	-0.15205800	-0.45775200
C	0.76091000	-1.58788800	0.16334400
C	1.65491400	-1.56568100	1.40024400
H	1.37410300	-0.82168300	2.14367900
H	1.62886500	-2.54775700	1.88003500
O	2.97704600	-2.04902200	-0.46201800
C	1.69847400	-2.28162900	-0.81321200
C	-0.82183600	0.20112100	-0.94845900
C	-1.96891500	-0.45338800	-0.15339100
C	-1.79172800	-1.95434500	-0.28546700
H	-2.64698500	-2.49538900	0.12480800
H	-1.74626300	-2.20673200	-1.34882600
C	-0.52425500	-2.39922600	0.43025900
H	-0.32302100	-3.44608700	0.18918200
H	-0.70893300	-2.37352500	1.50753900
C	-0.93089300	1.73577600	-0.90037800
C	-2.19878200	2.07555700	-0.12565500
O	-3.30899500	1.41038200	-0.79476500
C	-3.22442600	0.06769000	-0.81198400
C	0.38191400	2.25113800	-0.29443000
H	1.01840900	2.62947300	-1.09416100
H	0.22434200	3.07771900	0.40253400
C	-2.00461100	0.05253000	1.31589500
H	-1.03851000	-0.19266700	1.76094200
C	-2.17643700	1.58371500	1.30521500
H	-1.38064600	2.08639600	1.85896100
H	-3.11856300	1.86512800	1.78267000
C	3.21085300	2.52096500	0.38190200
H	4.19418100	2.49666100	0.86347300
H	2.59212400	3.25152100	0.91601400
H	3.81620200	-1.82298600	1.38167600
H	-0.93029100	-0.15428200	-1.97645700
H	-1.05544400	2.14017300	-1.90665500
H	-2.43576700	3.13707700	-0.18790700
C	-3.08357900	-0.62224700	2.15205100
H	-4.07845600	-0.45901600	1.72637000
H	-3.08562800	-0.20370000	3.16141100
H	-2.92650000	-1.69909500	2.24029100
O	-4.09751300	-0.58375000	-1.33023200
H	1.21391400	-0.11190900	-1.35680000
H	0.68566900	0.97107000	1.40417100

O	1.42200400	-2.92360500	-1.79242600
O	3.34580000	2.89198100	-0.98853100
H	3.59078600	3.82184400	-1.01910200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1151.428992

244) Conformer **41C4**

C	-2.99693700	1.32922200	0.63668700
C	-3.38943800	-0.06792500	0.26536400
H	-4.45858300	-0.24595200	0.20503300
C	-2.57859100	-1.11621500	0.09627500
C	-1.06517700	-1.05074400	0.08684300
C	-0.50088500	0.23734400	-0.54475300
C	-0.67126500	1.58697000	0.24171400
C	-1.67830100	1.44852400	1.37822100
H	-1.48780500	0.60778700	2.04319100
H	-1.67209200	2.36248700	1.97820400
O	-2.79974300	2.19834300	-0.52876000
C	-1.48930600	2.43808700	-0.71747900
C	0.92775700	-0.09206400	-0.99605900
C	2.03614500	0.38782800	-0.03774700
C	1.91878900	1.89851500	0.04418400
H	2.75605000	2.33537600	0.59235700
H	1.96522900	2.30642000	-0.96968900
C	0.61366300	2.28861800	0.72439700
H	0.46715300	3.36779600	0.63186600
H	0.71022300	2.09355500	1.79597500
C	0.98541600	-1.61915100	-1.17528500
C	2.17626100	-2.12676900	-0.37067000
O	3.35488900	-1.42146600	-0.85571400
C	3.31761700	-0.08743200	-0.68087900
C	-0.39124000	-2.15326300	-0.75759600
H	-0.97328000	-2.32049900	-1.66621900
H	-0.33372600	-3.11059100	-0.23508500
C	1.94938500	-0.32855800	1.33922100
H	0.96480100	-0.10481100	1.75361300
C	2.06383500	-1.84844000	1.11227800
H	1.21016400	-2.38835700	1.52767600
H	2.95557400	-2.24194400	1.60681500
C	-3.16587600	-2.49832700	-0.07022400
H	-2.64456900	-3.17566500	0.62119500
H	-2.96468000	-2.87147500	-1.07743000
H	-3.81916700	1.78810900	1.18552900
H	1.11591200	0.41016500	-1.94844400

H	1.17636500	-1.87566100	-2.21889600
H	2.38033500	-3.17739500	-0.57384700
C	2.99126600	0.16550600	2.33381700
H	2.90664600	-0.39580300	3.26746700
H	2.86753400	1.22395100	2.57137200
H	4.00710000	0.02024500	1.95365100
O	4.24780700	0.59223400	-1.03806000
H	-1.07003400	0.33301700	-1.47671500
H	-0.71942700	-1.15685800	1.12240700
O	-1.10225900	3.19554100	-1.56861700
O	-4.56143600	-2.58759900	0.09784400
H	-4.77250500	-2.35066800	1.00657800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1151.431761

245) Conformer **41C5**

C	3.12814400	-1.21546700	0.63010800
C	3.46224600	0.17753700	0.18743200
H	4.52539800	0.39480000	0.12913000
C	2.61065200	1.18260100	-0.04288300
C	1.10065500	1.05659400	-0.02783700
C	0.57675200	-0.28648300	-0.57664400
C	0.80984100	-1.58340600	0.27977800
C	1.82276900	-1.34258900	1.39395500
H	1.60672700	-0.47253600	2.01176300
H	1.85930700	-2.21996500	2.04514500
O	2.95329900	-2.14618700	-0.48717800
C	1.65083300	-2.45093300	-0.64339000
C	-0.87087100	-0.03448100	-1.01830400
C	-1.94327800	-0.50115800	-0.01385500
C	-1.77024500	-2.00058000	0.14324600
H	-2.58147700	-2.43773400	0.72909900
H	-1.81980700	-2.46159600	-0.84743200
C	-0.44001000	-2.30920800	0.81710700
H	-0.25418900	-3.38538600	0.77261800
H	-0.52691900	-2.06716400	1.87981300
C	-0.98798800	1.47794300	-1.27853000
C	-2.17844700	1.98607600	-0.47403800
O	-3.34188300	1.21621100	-0.89457000
C	-3.25299800	-0.10477200	-0.65349800
C	0.37660200	2.08024000	-0.92249600
H	0.93799000	2.20743200	-1.85079900
H	0.30948400	3.06323900	-0.45332800
C	-1.85650100	0.28905000	1.32224900

H	-0.85832200	0.11884900	1.72968800
C	-2.02500800	1.79053100	1.01851200
H	-1.18027400	2.37840700	1.38407100
H	-2.91797900	2.18163100	1.51279400
C	3.18588800	2.54489700	-0.31223400
H	2.85910100	2.91251500	-1.29144700
H	4.27907900	2.48182600	-0.32824600
H	3.97329600	-1.61182500	1.19251700
H	-1.05713800	-0.59490200	-1.93814100
H	-1.21251800	1.66948200	-2.32954500
H	-2.42385500	3.01699800	-0.72666000
C	-2.86490800	-0.18567600	2.35991100
H	-2.78244200	0.42495400	3.26227300
H	-2.70302000	-1.22625300	2.64823300
H	-3.89129500	-0.09198100	1.99198200
O	-4.16504000	-0.83408900	-0.95584000
H	1.13268500	-0.41424200	-1.51280800
H	0.76320500	1.20763100	1.00367900
O	1.28755000	-3.26894000	-1.44714900
O	2.74700300	3.42945500	0.71399800
H	2.91076400	4.32994200	0.41997700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1151.430540

246) Conformer **41C6**

C	-2.98377500	1.33513700	0.66792100
C	-3.38373400	-0.06691500	0.32429700
H	-4.45317800	-0.25110700	0.32844300
C	-2.57725100	-1.11568000	0.14157600
C	-1.06364900	-1.04982900	0.10539000
C	-0.50224000	0.23256600	-0.54158000
C	-0.66411200	1.59025000	0.23357000
C	-1.65338100	1.46292800	1.38685100
H	-1.45264900	0.62899300	2.05740700
H	-1.63817400	2.38291100	1.97739700
O	-2.80496700	2.18904900	-0.51180400
C	-1.49829500	2.42882100	-0.72276700
C	0.92378900	-0.10418000	-0.99807300
C	2.03850900	0.38632300	-0.05272800
C	1.92545500	1.89818600	0.00744800
H	2.76711600	2.34123200	0.54381500
H	1.96680100	2.29066700	-1.01270800
C	0.62569900	2.30145800	0.69009100
H	0.47832900	3.37858100	0.57735100

H	0.73166000	2.12769200	1.76438900
C	0.97991700	-1.63337100	-1.15887500
C	2.17082200	-2.13311300	-0.34965900
O	3.34992800	-1.43819300	-0.84859900
C	3.31584800	-0.10156400	-0.69465500
C	-0.39813800	-2.15831700	-0.73640700
H	-0.98208200	-2.32246300	-1.64453000
H	-0.34757900	-3.11541100	-0.21224500
C	1.95659900	-0.30979300	1.33497100
H	0.97531800	-0.07592800	1.75153800
C	2.06396700	-1.83326300	1.12944400
H	1.20937400	-2.36389700	1.55487000
H	2.95553900	-2.22335500	1.62697500
C	-3.16788900	-2.50057300	0.00726000
H	-2.74834200	-3.12706100	0.80208600
H	-2.85056300	-2.95106800	-0.93957000
H	-3.79622500	1.80210200	1.22428700
H	1.10625800	0.38609800	-1.95774500
H	1.17056700	-1.90277600	-2.19932700
H	2.37124000	-3.18710800	-0.53844100
C	3.00593200	0.19450300	2.31653000
H	2.92362800	-0.35213200	3.25905400
H	2.88821900	1.25700300	2.53855500
H	4.01910300	0.03877600	1.93342800
O	4.24573800	0.57065200	-1.06646400
H	-1.07659400	0.32139000	-1.47099600
H	-0.70548800	-1.14687300	1.13766300
O	-1.12523400	3.17658000	-1.58876200
O	-4.56856700	-2.57968500	0.14194600
H	-4.97189500	-2.22492700	-0.65585800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1151.431094

247) Conformer **42C1**

C	-3.75501200	0.35266600	0.14401600
H	-3.87864300	0.73553200	-0.87747600
H	-4.70389700	0.58364800	0.63839400
C	-3.61771300	-1.14127700	0.13731800
H	-4.56270000	-1.68072900	0.18625100
C	-2.51145200	-1.88931100	0.14947500
C	-1.09382800	-1.36994900	0.05911600
C	-0.87443300	0.01195900	-0.59086100
C	-1.34796400	1.31545600	0.08989000
C	-2.64596800	1.10386800	0.87387500

H	-2.41458800	0.56266600	1.79782600
H	-3.01479300	2.08858400	1.17542300
C	0.61258500	0.02417700	-0.97432500
C	1.58901500	0.58689700	0.09707100
C	1.11334200	1.97934300	0.47180400
H	1.79071200	2.44861000	1.18802500
H	1.13205100	2.61421200	-0.41939900
C	-0.29686900	1.90574600	1.04707500
H	-0.62798800	2.90651100	1.33358100
H	-0.28689200	1.31677600	1.96967100
C	0.97891200	-1.42825700	-1.31191500
C	2.32021000	-1.72969700	-0.65251300
O	3.25415800	-0.67938700	-1.04340600
C	2.91489900	0.55604600	-0.62575400
C	-0.21053100	-2.27596900	-0.83344600
H	-0.79628800	-2.57600700	-1.70653200
H	0.09405800	-3.19574600	-0.33058600
C	1.76737000	-0.34275500	1.33494200
H	0.79146900	-0.44952000	1.80621600
C	2.25187200	-1.72322700	0.85779700
H	1.59860500	-2.52481900	1.20743900
H	3.25019100	-1.93524800	1.24971800
C	-2.63318900	-3.37983000	0.31830900
H	-3.67280700	-3.67284400	0.47335000
H	-2.05380300	-3.71911300	1.18466700
H	-2.25095100	-3.92922200	-0.54658300
H	0.74820500	0.66263900	-1.85220200
H	1.10967700	-1.54865200	-2.38914000
H	2.76472500	-2.64723800	-1.03654100
C	2.71184600	0.23687300	2.38163800
H	2.32374000	1.15318400	2.82975000
H	3.69781400	0.45508400	1.95917400
H	2.85373100	-0.48840100	3.18679600
O	3.63965600	1.49004500	-0.86905300
H	-1.42086200	-0.05438600	-1.54321500
H	-0.68366900	-1.38616200	1.07595000
C	-1.60064300	2.31458600	-1.04889000
H	-2.39718700	1.92568200	-1.69515100
H	-0.70000900	2.40994400	-1.66669100
O	-1.96921800	3.58021100	-0.52303000
H	-2.12136400	4.17398200	-1.26253700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1003.435264

248) Conformer 42C2

C	-3.75747800	0.36803000	0.13156600
H	-3.87409900	0.74150700	-0.89414300
H	-4.70896600	0.60615700	0.61731900
C	-3.62473000	-1.12649400	0.13840900
H	-4.57162000	-1.66204100	0.19252300
C	-2.52147500	-1.87879400	0.15394700
C	-1.10238900	-1.36568800	0.05919500
C	-0.87891200	0.01561600	-0.59011300
C	-1.34662600	1.32018000	0.08954300
C	-2.65233600	1.12431200	0.86262700
H	-2.43597300	0.59733000	1.79844300
H	-3.01978000	2.11649000	1.14302500
C	0.60819200	0.02253700	-0.97274600
C	1.58724800	0.57704800	0.10088700
C	1.11752000	1.96990800	0.48257200
H	1.79437500	2.43223500	1.20343900
H	1.14506100	2.60845600	-0.40630000
C	-0.29511600	1.89444600	1.05383100
H	-0.62189100	2.88876700	1.37547600
H	-0.28799200	1.29480100	1.96926100
C	0.96800500	-1.43038400	-1.31483200
C	2.31022200	-1.73804100	-0.65994200
O	3.24617800	-0.68829500	-1.04856800
C	2.91192100	0.54597700	-0.62441000
C	-0.22377900	-2.27463400	-0.83502800
H	-0.81198500	-2.57242500	-1.70724300
H	0.07847900	-3.19550500	-0.33286600
C	1.76603400	-0.35792300	1.33484100
H	0.79155900	-0.46495200	1.80900100
C	2.24569800	-1.73763000	0.85049300
H	1.59117900	-2.53882500	1.19856900
H	3.24437200	-1.95376400	1.23911800
C	-2.64803800	-3.36781500	0.33141000
H	-3.68834400	-3.65655200	0.48973600
H	-2.06808600	-3.70443700	1.19841200
H	-2.26915600	-3.92278400	-0.53144300
H	0.74764100	0.66300800	-1.84860900
H	1.09508100	-1.54833000	-2.39272300
H	2.75157800	-2.65497000	-1.04890900
C	2.71548400	0.21472600	2.38102000
H	2.85802000	-0.51477000	3.18217200
H	2.33139500	1.12976400	2.83517600
H	3.70059700	0.43228700	1.95631700

O	3.63819600	1.47950400	-0.86442000
H	-1.42484500	-0.04774200	-1.54333600
H	-0.69014500	-1.38323200	1.07514400
C	-1.58724600	2.32606100	-1.05684300
H	-2.39395800	1.95339300	-1.69215100
H	-0.69548500	2.39907100	-1.68912700
O	-1.99582700	3.61615900	-0.63588600
H	-1.22856800	4.08949500	-0.30385500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1003.435435

249) Conformer **42C3**

C	-3.74944000	0.34604400	0.16538700
H	-3.88851700	0.73489200	-0.85190500
H	-4.69075000	0.57238400	0.67583900
C	-3.61007600	-1.14748500	0.14663100
H	-4.55482300	-1.68717300	0.19435900
C	-2.50319500	-1.89473500	0.15037800
C	-1.08568600	-1.37447800	0.05978000
C	-0.86819200	0.00783500	-0.59085700
C	-1.34360700	1.31306700	0.08456400
C	-2.62866900	1.09023800	0.88491300
H	-2.38159000	0.54020900	1.79929800
H	-2.99826700	2.06476000	1.22656800
C	0.61825200	0.02299000	-0.97671700
C	1.59241100	0.59543500	0.09088400
C	1.11750800	1.99233500	0.44870700
H	1.79488000	2.47003300	1.15933600
H	1.13831100	2.61588800	-0.45036500
C	-0.29271600	1.92791200	1.02498800
H	-0.62639900	2.93631700	1.28341300
H	-0.28011700	1.36619900	1.96444400
C	0.98937200	-1.43058700	-1.30584100
C	2.32530900	-1.72794400	-0.63412100
O	3.26323700	-0.68270100	-1.02815500
C	2.92168400	0.55694200	-0.62551500
C	-0.20157200	-2.27868100	-0.83306700
H	-0.78533500	-2.57557000	-1.70857200
H	0.10152200	-3.20010900	-0.33224600
C	1.76320900	-0.32226800	1.33818200
H	0.78464500	-0.42144800	1.80594200
C	2.24606400	-1.70844000	0.87569300
H	1.58730400	-2.50494500	1.22680400
H	3.24058900	-1.92090900	1.27686100

C	-2.62477100	-3.38630700	0.30941900
H	-3.66394500	-3.68021200	0.46545800
H	-2.04292800	-3.73135200	1.17177000
H	-2.24505700	-3.92963400	-0.56034100
H	0.75086600	0.65658100	-1.85870800
H	1.12946800	-1.55545300	-2.38136100
H	2.77077200	-2.64964300	-1.00693700
C	2.70469800	0.26513300	2.38315300
H	2.84003100	-0.45178400	3.19685900
H	2.31776300	1.18774800	2.81924200
H	3.69346400	0.47521500	1.96315700
O	3.64760700	1.48846500	-0.87439900
H	-1.41519500	-0.06191100	-1.54296700
H	-0.67508100	-1.39088200	1.07644200
C	-1.61577900	2.30318100	-1.06868400
H	-2.38888300	1.88875300	-1.72696000
H	-0.71556700	2.42018600	-1.67496800
O	-1.96981800	3.61230800	-0.65919800
H	-2.85417800	3.58615900	-0.28370000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1003.435657

250) Conformer **43C1**

C	3.52913200	0.15243600	0.54300600
H	4.05436200	0.55230900	1.42037100
C	3.19836000	1.33283900	-0.37846300
H	4.08421100	1.96738800	-0.47275200
H	2.98203500	0.93893000	-1.37598700
C	2.04232100	2.14822200	0.12881000
C	0.65049900	1.54688800	0.03574700
C	0.57142500	0.16081200	-0.62504200
C	1.23128600	-1.05462500	0.07570000
C	2.31936600	-0.60406300	1.06423400
H	2.69034400	-1.48245300	1.60224800
H	1.84545600	0.02553700	1.82283200
C	-0.90150300	-0.00531000	-1.01165000
C	-1.78530600	-0.73322400	0.02984600
C	-1.14700800	-2.08839400	0.28166400
H	-1.76687600	-2.70535500	0.93574000
H	-1.08348900	-2.62669400	-0.66962900
C	0.23754600	-1.90976400	0.89527300
H	0.70153300	-2.88947500	1.04433900
H	0.13089500	-1.48120300	1.89703200
C	-1.43552900	1.41373000	-1.28118400

C	-2.76789600	1.53900000	-0.54992700
O	-3.60912900	0.42445900	-0.97242900
C	-3.13087500	-0.79397100	-0.65213000
C	-0.32143800	2.37536100	-0.82804300
H	0.21644300	2.73890800	-1.70754300
H	-0.69699000	3.25683000	-0.30393600
C	-2.00819700	0.09347700	1.32923000
H	-1.02967900	0.26191600	1.77812600
C	-2.63235900	1.45024200	0.95414800
H	-3.62642300	1.54963000	1.39791500
H	-2.03674800	2.28729200	1.32413200
C	2.23572700	3.34972300	0.67024000
H	3.22697600	3.78674600	0.73439800
H	1.41277900	3.93758500	1.06527100
H	-0.96232800	-0.61269600	-1.91976200
H	-1.63498700	1.55264300	-2.34552900
H	-3.31743500	2.42812300	-0.85722200
C	-2.85812200	-0.64084900	2.35885200
H	-3.02772100	0.00530300	3.22374500
H	-2.37664300	-1.55251900	2.71757300
H	-3.83827700	-0.91090200	1.95336300
O	-3.76468000	-1.78038900	-0.93793600
H	1.08439400	0.28404600	-1.58694300
H	0.25085200	1.49808700	1.05228500
C	1.82878100	-1.94425100	-1.03688500
H	2.37304200	-1.31628600	-1.75108300
H	1.01677800	-2.43118700	-1.58526900
O	2.67674400	-2.97013900	-0.56339900
H	3.50518300	-2.52439800	-0.33218300
O	4.38738100	-0.79060300	-0.10568900
H	5.16253200	-0.33439000	-0.44645900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1078.605464

251) Conformer 43C2

C	3.52913900	0.15245600	0.54293100
H	4.05443600	0.55229800	1.42026300
C	3.19839200	1.33290600	-0.37851200
H	4.08424300	1.96746900	-0.47267300
H	2.98213900	0.93903700	-1.37605800
C	2.04231500	2.14821900	0.12877600
C	0.65050900	1.54684600	0.03566600
C	0.57143500	0.16074400	-0.62507600
C	1.23126900	-1.05462800	0.07573300

C	2.31937600	-0.60402900	1.06422400
H	2.69038600	-1.48240300	1.60222800
H	1.84547900	0.02561600	1.82278600
C	-0.90149400	-0.00538000	-1.01166400
C	-1.78529700	-0.73321600	0.02988300
C	-1.14702700	-2.08837800	0.28176700
H	-1.76689200	-2.70528000	0.93589900
H	-1.08352500	-2.62673200	-0.66949200
C	0.23753400	-1.90972900	0.89537100
H	0.70151600	-2.88943700	1.04445000
H	0.13086800	-1.48111500	1.89710100
C	-1.43549700	1.41365300	-1.28126700
C	-2.76785000	1.53899000	-0.54997200
O	-3.60912600	0.42445400	-0.97239500
C	-3.13085200	-0.79398900	-0.65209600
C	-0.32136600	2.37527700	-0.82821900
H	0.21656300	2.73867000	-1.70775000
H	-0.69686500	3.25682500	-0.30420900
C	-2.00822600	0.09353600	1.32923900
H	-1.02975900	0.26184600	1.77829500
C	-2.63218400	1.45037500	0.95409400
H	-3.62613500	1.55002700	1.39803200
H	-2.03629300	2.28733300	1.32383400
C	2.23569000	3.34960700	0.67046000
H	3.22693200	3.78662100	0.73476900
H	1.41272900	3.93733900	1.06565700
H	-0.96234700	-0.61281600	-1.91974000
H	-1.63499500	1.55249800	-2.34561300
H	-3.31737000	2.42810000	-0.85732800
C	-2.85841700	-0.64068800	2.35873500
H	-3.02798900	0.00548200	3.22361700
H	-2.37712900	-1.55244300	2.71748600
H	-3.83856500	-0.91054200	1.95310900
O	-3.76464600	-1.78039500	-0.93794200
H	1.08440100	0.28389600	-1.58697700
H	0.25076900	1.49806300	1.05216500
C	1.82870300	-1.94437000	-1.03681200
H	2.37285100	-1.31646300	-1.75114100
H	1.01667400	-2.43147000	-1.58500000
O	2.67681200	-2.97009100	-0.56321000
H	3.50516100	-2.52414600	-0.33202800
O	4.38736600	-0.79060000	-0.10579200
H	5.16255600	-0.33442000	-0.44652200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1078.605463

252) Conformer 43C3

C	3.56004100	-0.00591700	0.63930600
H	4.10590300	0.39218200	1.50333300
C	3.26077200	1.16748300	-0.30357000
H	4.16029600	1.78341700	-0.39136200
H	3.04843900	0.76157900	-1.29669900
C	2.11316000	2.00396300	0.17864300
C	0.71624400	1.43612700	0.02431000
C	0.62309000	0.00108600	-0.52116000
C	1.18563400	-1.17706600	0.30029700
C	2.34194100	-0.72181100	1.20955200
H	2.71118000	-1.59014300	1.76749500
H	1.92107300	-0.04415600	1.95950100
C	-0.83792000	-0.14276000	-0.95300100
C	-1.81189600	-0.68488300	0.12701900
C	-1.25574300	-2.01425700	0.60725700
H	-1.92257800	-2.48444700	1.33281500
H	-1.20548900	-2.70182900	-0.24198400
C	0.12543200	-1.81382300	1.22869000
H	0.50863200	-2.78151000	1.57156200
H	0.02733300	-1.20513200	2.13303900
C	-1.27769100	1.25610900	-1.42149500
C	-2.64915400	1.52472300	-0.81092900
O	-3.51164500	0.39472600	-1.14182200
C	-3.11370700	-0.78725300	-0.63080500
C	-0.14777800	2.21177500	-0.99156900
H	0.46881300	2.45065800	-1.86237400
H	-0.50805500	3.16212000	-0.59188300
C	-2.08861400	0.31384100	1.28943200
H	-1.14209400	0.49841600	1.79551900
C	-2.61571700	1.63359800	0.69737500
H	-3.62957200	1.83414500	1.05340500
H	-2.00229800	2.48610500	0.99562500
C	2.31394200	3.19007100	0.75043500
H	3.31073300	3.60722000	0.85134500
H	1.48993100	3.78464600	1.13352200
H	-0.89506000	-0.85725100	-1.78009200
H	-1.39176200	1.27894200	-2.50698600
H	-3.13728300	2.38374700	-1.26996500
C	-3.05225700	-0.24368200	2.33099500
H	-3.25700400	0.52026900	3.08514100
H	-2.64619400	-1.11506200	2.84780900

H	-4.00997200	-0.52844000	1.88410100
O	-3.77431900	-1.77800000	-0.82713900
H	1.19093300	0.00853800	-1.45775400
H	0.23635000	1.49997000	1.00366500
C	1.63095600	-2.30310800	-0.65782900
H	0.75263400	-2.72161700	-1.15502000
H	2.07036800	-3.10536200	-0.04751300
O	2.51527200	-1.92339200	-1.68914800
H	3.34434700	-1.64552800	-1.25744400
O	4.40439100	-0.96967900	-0.00625100
H	5.20638300	-0.52603300	-0.30163000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1078.606421

253) Conformer **43C4**

C	3.56017600	-0.00182400	0.63670100
H	4.11404400	0.38971400	1.49826600
C	3.26486800	1.17197700	-0.29677100
H	4.16611600	1.78346200	-0.37807200
H	3.05815400	0.77116200	-1.29340600
C	2.11323100	2.00667200	0.18072500
C	0.71580300	1.43864300	0.02976600
C	0.62206800	0.00653500	-0.52250200
C	1.18694900	-1.17472800	0.29345200
C	2.33775300	-0.71828800	1.20814900
H	2.69851600	-1.58855000	1.77185700
H	1.91585400	-0.04191100	1.96003300
C	-0.83913000	-0.13678900	-0.95427100
C	-1.81064000	-0.68887600	0.12259100
C	-1.25280100	-2.02209000	0.58977800
H	-1.91904300	-2.50049800	1.31052200
H	-1.20133200	-2.70103200	-0.26637000
C	0.12770300	-1.82546600	1.21348600
H	0.51350300	-2.79630100	1.54463200
H	0.02785400	-1.22816200	2.12513600
C	-1.28234200	1.26482100	-1.41153800
C	-2.65211800	1.52754300	-0.79476900
O	-3.51490200	0.39984300	-1.13242500
C	-3.11440200	-0.78589300	-0.63252100
C	-0.15266200	2.21910600	-0.97866500
H	0.46114800	2.46441200	-1.84959500
H	-0.51342300	3.16638100	-0.57218700
C	-2.08390800	0.30016700	1.29393400
H	-1.13537300	0.48180100	1.79734200

C	-2.61439000	1.62406300	0.71430200
H	-3.62743600	1.82044100	1.07495000
H	-2.00106900	2.47481500	1.01774500
C	2.31245100	3.19966100	0.73825700
H	3.30911700	3.61757900	0.83714200
H	1.48763500	3.79922600	1.11168300
H	-0.89562600	-0.84503400	-1.78677300
H	-1.40004300	1.29512500	-2.49645800
H	-3.14200000	2.39005300	-1.24532500
C	-3.04269200	-0.26658900	2.33490400
H	-3.24522300	0.49103400	3.09600700
H	-2.63361200	-1.14169300	2.84300800
H	-4.00188300	-0.54882700	1.88957400
O	-3.77462100	-1.77565100	-0.83515700
H	1.18961500	0.01897800	-1.45914400
H	0.23980400	1.49705500	1.01147600
C	1.64236500	-2.29123600	-0.67176200
H	0.76635900	-2.71964600	-1.16454200
H	2.09513200	-3.09049300	-0.06686800
O	2.51467600	-1.89758400	-1.70818300
H	3.34340100	-1.60848900	-1.28276500
O	4.43666800	-0.87857300	-0.08867600
H	4.80555400	-1.51932100	0.52818400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1078.606468

254) Conformer **44C1**

C	3.34703900	-1.26028600	-0.36788900
H	4.25180200	-1.79806200	-0.07644300
C	3.00740100	-0.22772600	0.75324600
C	2.48388700	1.16232600	0.29072800
C	1.15271900	0.91759700	-0.37412100
C	0.59400700	-0.28551100	-0.32072100
C	1.12539800	-1.43306300	0.47535400
C	2.13425000	-2.21109100	-0.37176300
H	2.37480200	-3.16001400	0.11369400
H	1.79501800	-2.41004200	-1.38930300
C	-0.69520100	-0.36634400	-1.03647800
C	-1.78296500	-0.86533900	-0.05689100
C	-1.34059300	-2.25410000	0.39578700
H	-2.09494500	-2.72136100	1.03234800
H	-1.25183700	-2.89110800	-0.48983400
C	-0.00540500	-2.21023500	1.15754100
H	0.32675800	-3.23047200	1.36549800

H	-0.16349000	-1.73342700	2.12895800
C	-0.95657300	1.06560500	-1.53361300
C	-2.32994600	1.45124400	-0.98623700
O	-3.26704100	0.41577700	-1.40150100
C	-3.04161900	-0.81386800	-0.88198600
C	0.28349500	1.90569800	-1.11000000
H	0.01588600	2.74944300	-0.46996000
H	0.79056400	2.31730100	-1.98741900
C	-1.94724500	0.15111200	1.10411600
H	-0.94528700	0.34922700	1.49482700
C	-2.45687500	1.48574000	0.53053000
H	-3.53135300	1.57624100	0.73819700
H	-0.65181300	-1.08348600	-1.86511800
H	-1.04741700	1.07461200	-2.62102400
C	-2.83890100	-0.34927100	2.23076700
H	-2.97573800	0.43380700	2.98163800
H	-2.41257500	-1.21518700	2.74007400
H	-3.83050300	-0.62843700	1.86186200
O	-3.79438300	-1.71822800	-1.14055100
O	3.57085800	-0.62983600	-1.62580500
H	4.14630900	-1.18705800	-2.15622700
O	3.41849200	1.78681500	-0.58110900
H	3.62832700	1.12461700	-1.26031000
H	-2.71089900	2.37279500	-1.42477300
O	1.98749800	-0.88458700	1.49457600
O	-1.78411300	2.62360700	1.03311600
H	-2.01644000	2.72686500	1.96061600
H	3.86050200	-0.07526900	1.41717400
C	2.34297500	2.08723200	1.48922600
H	3.32331100	2.25898100	1.94076000
H	1.67723000	1.65302800	2.23552400
H	1.93620400	3.05029800	1.17384800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.527874

255) Conformer **44C2**

C	3.32108600	-1.28355700	-0.37372900
H	4.21962100	-1.83383400	-0.08685900
C	2.99092700	-0.25773000	0.75584200
C	2.48491100	1.14144800	0.29943200
C	1.15245900	0.91289500	-0.37121400
C	0.57674300	-0.28303300	-0.31828500
C	1.09613700	-1.44239500	0.46803700
C	2.09800700	-2.21977600	-0.38856700

H	2.32662500	-3.17649200	0.08691200
H	1.75744900	-2.40437500	-1.40833100
C	-0.70566000	-0.35348700	-1.04590100
C	-1.80069300	-0.85110600	-0.07173100
C	-1.37362900	-2.25072600	0.36192500
H	-2.13461900	-2.72009200	0.98869000
H	-1.28415800	-2.87661600	-0.53126700
C	-0.04157500	-2.22558400	1.13291100
H	0.28531100	-3.25084900	1.32269100
H	-0.20277000	-1.76879400	2.11335200
C	-0.95155800	1.08057200	-1.54324400
C	-2.29678500	1.49564000	-0.95291600
O	-3.27090500	0.49202100	-1.36712000
C	-3.06398700	-0.75625400	-0.88566800
C	0.32099000	1.89269600	-1.16385900
H	0.09718300	2.81059200	-0.61216500
H	0.85018900	2.21494800	-2.06553800
C	-1.94805000	0.13867300	1.11278300
H	-0.94484700	0.27145600	1.53059800
C	-2.39298100	1.50627800	0.57275300
H	-3.45390700	1.65306100	0.79702000
H	-0.65897000	-1.06949400	-1.87484500
H	-1.07730000	1.09017800	-2.62688000
C	-2.87103300	-0.35458100	2.21697100
H	-3.86371000	-0.59975200	1.82790800
H	-2.99261300	0.42650100	2.97135100
H	-2.47698500	-1.24008600	2.71868000
O	-3.83616600	-1.63914800	-1.15917000
O	3.55172700	-0.64322400	-1.62530400
H	4.12062500	-1.20123900	-2.16198900
O	3.42543000	1.76270800	-0.56565000
H	3.63214000	1.10315400	-1.24873600
H	-2.66243700	2.43466400	-1.36692500
O	1.96155100	-0.90894100	1.49118500
O	-1.73612200	2.59895300	1.18213400
H	-0.80615700	2.37978700	1.29303200
H	3.84358500	-0.11948200	1.42315500
C	2.35170100	2.06003400	1.50399100
H	1.70575900	1.61529400	2.26202100
H	1.93708300	3.02411900	1.20008000
H	3.33670800	2.23836300	1.94224600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.526750

256) Conformer 44C3

C	3.34703700	-1.26028700	-0.36788900
H	4.25179900	-1.79806600	-0.07644200
C	3.00739900	-0.22772800	0.75324700
C	2.48388500	1.16232500	0.29072900
C	1.15271900	0.91759600	-0.37412300
C	0.59400500	-0.28551200	-0.32072100
C	1.12539500	-1.43306400	0.47535400
C	2.13424600	-2.21109100	-0.37176600
H	2.37479700	-3.16001600	0.11368800
H	1.79501300	-2.41003900	-1.38930600
C	-0.69520200	-0.36634400	-1.03648100
C	-1.78296700	-0.86533800	-0.05689200
C	-1.34059600	-2.25410100	0.39578200
H	-2.09494800	-2.72136400	1.03234100
H	-1.25183900	-2.89110700	-0.48984000
C	-0.00540800	-2.21023800	1.15753900
H	0.32675400	-3.23047500	1.36549300
H	-0.16349500	-1.73343300	2.12895600
C	-0.95657400	1.06560500	-1.53361500
C	-2.32994400	1.45124800	-0.98623200
O	-3.26704300	0.41578600	-1.40149400
C	-3.04162100	-0.81386200	-0.88198500
C	0.28350000	1.90569400	-1.11001200
H	0.01589800	2.74945100	-0.46998600
H	0.79057200	2.31728000	-1.98743800
C	-1.94724200	0.15111000	1.10411700
H	-0.94528300	0.34922000	1.49482900
C	-2.45686500	1.48574300	0.53053600
H	-3.53134200	1.57625100	0.73820700
H	-0.65181300	-1.08348700	-1.86512000
H	-1.04742600	1.07461200	-2.62102600
C	-2.83890000	-0.34927400	2.23076700
H	-2.97573400	0.43380200	2.98164100
H	-2.41257700	-1.21519300	2.74007100
H	-3.83050300	-0.62843400	1.86186200
O	-3.79438800	-1.71821900	-1.14055200
O	3.57085900	-0.62983400	-1.62580200
H	4.14626800	-1.18708000	-2.15624500
O	3.41849400	1.78681400	-0.58110300
H	3.62833000	1.12462000	-1.26030600
H	-2.71089300	2.37280200	-1.42476600
O	1.98749600	-0.88459000	1.49457600
O	-1.78409400	2.62360500	1.03312000

H	-2.01643000	2.72687400	1.96061700
H	3.86049900	-0.07527200	1.41717500
C	2.34297000	2.08722900	1.48922800
H	3.32330400	2.25898000	1.94076400
H	1.67722400	1.65302300	2.23552400
H	1.93619700	3.05029400	1.17385200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.527874

257) Conformer **44C4**

C	3.30634200	-1.25488700	-0.44789700
H	4.26176300	-1.74994600	-0.27997600
C	3.01803100	-0.26180800	0.73314900
C	2.50535000	1.13735100	0.30498800
C	1.17860700	0.89933100	-0.37827500
C	0.61050500	-0.30404600	-0.32873400
C	1.13013000	-1.45732700	0.47427300
C	2.13494800	-2.24829300	-0.36655900
H	2.42144300	-3.15813600	0.16541900
H	1.77265700	-2.52666000	-1.35821500
C	-0.68569000	-0.36838100	-1.03635900
C	-1.77198400	-0.85448900	-0.04864200
C	-1.34507400	-2.24825200	0.40260400
H	-2.10284300	-2.70511700	1.04244200
H	-1.26807700	-2.88722900	-0.48260600
C	-0.00737300	-2.22078700	1.15960100
H	0.31407600	-3.24477700	1.36524900
H	-0.15542600	-1.74294700	2.13194800
C	-0.93443000	1.06746000	-1.53006000
C	-2.30225100	1.46616700	-0.97767600
O	-3.25051700	0.43976100	-1.38777200
C	-3.03531400	-0.79087000	-0.86692000
C	0.31191900	1.89666100	-1.10476900
H	0.05229800	2.73345400	-0.45272100
H	0.81803000	2.31674400	-1.97841300
C	-1.91908900	0.16504800	1.11217100
H	-0.91361000	0.35515900	1.49802300
C	-2.42072900	1.50355300	0.53990100
H	-3.49314400	1.60315000	0.75308600
H	-0.65814300	-1.08581200	-1.86505600
H	-1.02631600	1.07977000	-2.61720100
C	-2.80853200	-0.32560000	2.24482000
H	-3.80457300	-0.59643100	1.88187600
H	-2.93394400	0.46029000	2.99464900

H	-2.38716800	-1.19424100	2.75351600
O	-3.79902900	-1.68781300	-1.11752100
O	3.43062400	-0.64463500	-1.73178800
H	2.53857500	-0.46797700	-2.05515000
O	3.45645700	1.77468100	-0.54086100
H	3.68557600	1.12509800	-1.22521300
H	-2.67549300	2.39119400	-1.41526500
O	2.00158600	-0.91532000	1.48453300
O	-1.73540300	2.63571500	1.03781100
H	-1.97257000	2.75102800	1.96266700
H	3.89071400	-0.14177300	1.37769800
C	2.34637900	2.04179700	1.51583200
H	3.31862500	2.19482400	1.99053900
H	1.66091900	1.60099200	2.23973400
H	1.95641800	3.01446600	1.20906200

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.526970

258) Conformer **44C5**

C	3.34374400	-1.29311000	-0.39410300
H	4.22680200	-1.85540300	-0.07145600
C	3.00392600	-0.26843900	0.73990300
C	2.48026900	1.12541000	0.29101700
C	1.15692800	0.90244900	-0.38173300
C	0.58967300	-0.29622600	-0.33280300
C	1.11497800	-1.45525900	0.45071700
C	2.11816000	-2.22855600	-0.40687400
H	2.34320800	-3.18850200	0.06377000
H	1.77973900	-2.40481300	-1.42849000
C	-0.70367800	-0.35708000	-1.04260400
C	-1.79032700	-0.85682200	-0.06271200
C	-1.35906400	-2.25481700	0.37141900
H	-2.11481900	-2.72212400	1.00617800
H	-1.28051600	-2.88229000	-0.52186700
C	-0.02019100	-2.23190800	1.12721300
H	0.30528700	-3.25740400	1.31869600
H	-0.17031000	-1.76814000	2.10619300
C	-0.95521600	1.08156700	-1.52502500
C	-2.32027700	1.47548200	-0.96303100
O	-3.27077000	0.45446100	-1.38233600
C	-3.05399700	-0.78343500	-0.87899000
C	0.29517300	1.90702900	-1.10357100
H	0.03909100	2.74814000	-0.45557700
H	0.80081300	2.31918100	-1.98127100

C	-1.93862800	0.14781800	1.11082300
H	-0.93365400	0.32961500	1.50180200
C	-2.43427300	1.49551800	0.55505700
H	-3.50543100	1.59923300	0.77278500
H	-0.66747100	-1.06659200	-1.87775000
H	-1.05398300	1.10129600	-2.61145300
C	-2.83235600	-0.35602900	2.23430400
H	-2.95687300	0.41916100	2.99537400
H	-2.41466400	-1.23339100	2.73098400
H	-3.82855000	-0.61852400	1.86560700
O	-3.81765700	-1.67711100	-1.14159900
O	3.60291400	-0.75045900	-1.67322700
H	3.69714700	0.21124200	-1.56656300
O	3.37967500	1.70130300	-0.67595600
H	4.12022500	2.09817700	-0.20416200
H	-2.69438500	2.40567200	-1.38894000
O	1.97801400	-0.91907900	1.47661600
O	-1.74051400	2.61820700	1.06340600
H	-1.97088000	2.72136800	1.99138300
H	3.85401300	-0.12542700	1.41104800
C	2.36450300	2.05928100	1.48584100
H	3.34978700	2.23328500	1.93090200
H	1.71980800	1.62011300	2.24762200
H	1.94623600	3.02031000	1.18086000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.525797

259) Conformer **44C6**

C	3.34374300	-1.29311000	-0.39410500
H	4.22680400	-1.85540000	-0.07146200
C	3.00392700	-0.26843900	0.73990200
C	2.48027100	1.12541100	0.29101600
C	1.15692900	0.90245000	-0.38173300
C	0.58967400	-0.29622600	-0.33280200
C	1.11497900	-1.45525900	0.45071900
C	2.11816100	-2.22855700	-0.40687200
H	2.34321100	-3.18850200	0.06377300
H	1.77973900	-2.40481600	-1.42848800
C	-0.70367700	-0.35708000	-1.04260300
C	-1.79032600	-0.85682200	-0.06271000
C	-1.35906300	-2.25481600	0.37142300
H	-2.11481700	-2.72212200	1.00618300
H	-1.28051600	-2.88229100	-0.52186200
C	-0.02018900	-2.23190600	1.12721600

H	0.30528800	-3.25740200	1.31870100
H	-0.17030700	-1.76813600	2.10619400
C	-0.95521500	1.08156700	-1.52502400
C	-2.32027800	1.47547900	-0.96303400
O	-3.27076900	0.45445700	-1.38233900
C	-3.05399500	-0.78343800	-0.87899000
C	0.29517200	1.90703000	-1.10356800
H	0.03908800	2.74813700	-0.45556900
H	0.80081100	2.31918800	-1.98126500
C	-1.93862900	0.14781900	1.11082400
H	-0.93365400	0.32962000	1.50180100
C	-2.43427800	1.49551700	0.55505500
H	-3.50543600	1.59922700	0.77278000
H	-0.66747100	-1.06659300	-1.87774800
H	-1.05397900	1.10129400	-2.61145200
C	-2.83235500	-0.35602600	2.23430500
H	-2.95687300	0.41916400	2.99537400
H	-2.41466100	-1.23338700	2.73098700
H	-3.82854900	-0.61852400	1.86560900
O	-3.81765400	-1.67711500	-1.14159900
O	3.60290600	-0.75045800	-1.67323100
H	3.69715300	0.21124100	-1.56656500
O	3.37967700	1.70130400	-0.67595500
H	4.12022300	2.09818400	-0.20416100
H	-2.69438800	2.40566900	-1.38894400
O	1.97801600	-0.91907900	1.47661600
O	-1.74052500	2.61821000	1.06340300
H	-1.97087400	2.72135700	1.99138500
H	3.85401500	-0.12542700	1.41104600
C	2.36450400	2.05928100	1.48584100
H	3.34978800	2.23328500	1.93090200
H	1.71980800	1.62011200	2.24762100
H	1.94623800	3.02031100	1.18086000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.525797

260) Conformer **44C7**

C	3.32107200	-1.28356100	-0.37374100
H	4.21961000	-1.83383900	-0.08688600
C	2.99092200	-0.25774400	0.75584300
C	2.48491300	1.14143900	0.29944100
C	1.15246100	0.91289200	-0.37120800
C	0.57674000	-0.28303400	-0.31828100
C	1.09613000	-1.44240100	0.46803700

C	2.09799500	-2.21978200	-0.38857300
H	2.32661600	-3.17649800	0.08690400
H	1.75743500	-2.40438100	-1.40833600
C	-0.70566100	-0.35348400	-1.04590100
C	-1.80069700	-0.85110200	-0.07173300
C	-1.37363700	-2.25072500	0.36191900
H	-2.13462900	-2.72009200	0.98868000
H	-1.28416600	-2.87661200	-0.53127500
C	-0.04158400	-2.22559000	1.13290700
H	0.28530100	-3.25085700	1.32268300
H	-0.20277800	-1.76880500	2.11335000
C	-0.95155300	1.08057600	-1.54324400
C	-2.29677400	1.49565000	-0.95290800
O	-3.27090400	0.49203900	-1.36710900
C	-3.06398900	-0.75624100	-0.88567000
C	0.32100100	1.89269100	-1.16386500
H	0.09720600	2.81060500	-0.61219500
H	0.85020700	2.21492200	-2.06554800
C	-1.94805400	0.13867300	1.11278500
H	-0.94485500	0.27144600	1.53061400
C	-2.39295700	1.50629000	0.57276200
H	-3.45387600	1.65310400	0.79703900
H	-0.65896600	-1.06949000	-1.87484500
H	-1.07730400	1.09018400	-2.62688000
C	-2.87105800	-0.35457300	2.21695900
H	-2.99263600	0.42650600	2.97134200
H	-2.47703000	-1.24008600	2.71866800
H	-3.86373500	-0.59972700	1.82788400
O	-3.83617900	-1.63912700	-1.15916900
O	3.55169400	-0.64322300	-1.62532000
H	4.12073600	-1.20115100	-2.16194200
O	3.42543400	1.76269500	-0.56564000
H	3.63214700	1.10314000	-1.24872500
H	-2.66242000	2.43467900	-1.36691400
O	1.96154700	-0.90895500	1.49118500
O	-1.73606400	2.59894000	1.18214700
H	-0.80606900	2.37981300	1.29287900
H	3.84358400	-0.11950300	1.42315300
C	2.35170300	2.06001900	1.50400600
H	3.33670600	2.23832400	1.94227700
H	1.70573900	1.61529000	2.26202400
H	1.93711100	3.02411600	1.20009500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1188.526751

261) Conformer **45C1**

C	-2.19967500	1.91213500	-0.03415400
H	-2.73912100	2.81014300	0.28191900
H	-2.33801100	1.85441700	-1.11877200
C	-2.81640600	0.69923200	0.63895800
H	-3.90851300	0.78238900	0.62220100
H	-2.53305600	0.70300800	1.69870600
C	-2.45071500	-0.65763900	0.02446700
C	-0.94741700	-0.84891100	-0.21295200
C	-0.17986900	0.05538800	-1.20473500
C	0.22074900	0.97867000	-0.00403600
C	-0.73007500	2.12847800	0.29277300
H	-0.63040300	2.38407000	1.35400200
H	-0.37352900	3.00176600	-0.25898900
C	0.02989300	-0.32327100	0.85809800
C	1.31011200	-1.16356100	0.82556400
H	1.03088700	-2.21916000	0.75041200
C	2.02018800	-0.79940400	-0.48180800
C	1.05837700	-0.70893900	-1.66306500
H	1.57859000	-0.19754300	-2.47884700
H	0.78980500	-1.71092100	-2.00539500
C	-3.18678700	-0.85664500	-1.30041700
H	-2.91598800	-1.81502200	-1.75309600
H	-2.95802700	-0.07181900	-2.02474900
H	-4.26835900	-0.85559100	-1.13917000
C	-2.90282400	-1.74829200	0.99764500
H	-3.96436000	-1.63433300	1.23481400
H	-2.34433300	-1.69836000	1.93680200
H	-2.75780400	-2.74387700	0.56906300
C	1.63852700	1.48250500	-0.05045800
O	2.55251900	0.54124400	-0.31200700
O	1.99763200	2.62238100	0.12233700
H	-0.33391400	-0.17708600	1.87719200
C	2.19199500	-0.97944100	2.05024700
H	3.13126000	-1.52530300	1.94693300
H	1.67286500	-1.35870600	2.93293500
H	2.42926000	0.07114300	2.23026200
H	-0.80677100	-1.91283200	-0.43721500
H	-0.71049800	0.52312800	-2.03404800
O	3.09648600	-1.63147600	-0.68834900
H	3.44046700	-1.48853800	-1.57755900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -809.597387

262) Conformer **45C2**

C	-2.20141000	1.91077100	-0.03039900
H	-2.74022700	2.80867300	0.28700400
H	-2.34447300	1.85165900	-1.11430300
C	-2.81404000	0.69810400	0.64692600
H	-3.90627200	0.78034000	0.63506900
H	-2.52588800	0.70334000	1.70538800
C	-2.45010200	-0.65920200	0.03231200
C	-0.94785700	-0.84941500	-0.21232200
C	-0.18509900	0.05448300	-1.20822300
C	0.21971100	0.97931500	-0.00976500
C	-0.73060900	2.12874400	0.28994800
H	-0.62652600	2.38589300	1.35034600
H	-0.37709200	3.00159100	-0.26453500
C	0.03341500	-0.32183800	0.85392900
C	1.31476600	-1.16033200	0.81103400
H	1.03539200	-2.21629000	0.73798700
C	2.01748900	-0.79530700	-0.50646000
C	1.04933500	-0.70826300	-1.67734600
H	1.56793500	-0.19905100	-2.49327700
H	0.78102300	-1.71046900	-2.01784600
C	-3.19211100	-0.86030700	-1.28896000
H	-2.92246600	-1.81886200	-1.74192700
H	-2.96753100	-0.07602000	-2.01516200
H	-4.27290600	-0.86016500	-1.12262300
C	-2.89680000	-1.74916300	1.00875500
H	-3.95731500	-1.63583700	1.25072500
H	-2.33404400	-1.69777900	1.94529600
H	-2.75296200	-2.74508100	0.58054700
C	1.63743800	1.48268200	-0.05388000
O	2.55002400	0.54398300	-0.33119300
O	1.99826900	2.61937400	0.13454800
H	-0.32508500	-0.17623300	1.87507000
C	2.19550800	-0.97389000	2.03749700
H	2.45124600	0.07369500	2.20646400
H	3.12922000	-1.54040200	1.97423800
H	1.66554900	-1.33552100	2.92075500
H	-0.80726100	-1.91336700	-0.43629400
H	-0.72113100	0.52218400	-2.03397300
O	3.07860600	-1.60401700	-0.84313400
H	3.63782900	-1.73531000	-0.06899100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -809.597046

263) Conformer **45C3**

H	-0.35090300	0.06359100	1.87572200
H	-2.94319600	-2.53893600	-0.97239200
O	2.55738700	0.48532400	-0.37153400
H	3.45361800	-1.69235100	-1.33901500
O	3.09351100	-1.72032900	-0.44518900
H	-0.68965600	0.26361900	-2.09612200
H	-0.81284200	-1.95074800	-0.18044300
H	3.09608900	-1.27457100	2.14809000
H	2.39906000	0.34761700	2.21563900
H	1.62774400	-0.97716900	3.08767800
C	2.15855100	-0.71661100	2.16964600
O	2.00321300	2.60980700	-0.28046800
C	1.64446400	1.45696200	-0.26135100
H	-2.64721300	-2.16502400	1.48796300
H	-2.57672100	-0.52985100	2.14780100
C	-2.95938100	-1.13018500	1.31953500
H	-2.74201500	-1.20749900	-2.12194500
H	-4.20661900	-1.31186000	-1.13944100
C	-3.12483500	-1.47245100	-1.13217900
H	0.80267400	-1.95920500	-1.77552600
C	1.07430400	-0.92306900	-1.56165600
C	2.01941200	-0.86387500	-0.36538400
H	1.00499300	-2.10786900	1.02527700
C	1.28956600	-1.05249500	0.96820400
C	0.01387600	-0.20687700	0.88402900
H	-0.80037800	2.64381300	-0.95700700
H	-0.23543400	2.87667800	0.67866100
C	-0.71772700	2.15122300	0.01866600
C	0.22691900	0.96826100	-0.13170900
H	-4.05160600	-1.09814700	1.36219400
H	1.60760200	-0.52279200	-2.42936900
C	-0.16289600	-0.10309200	-1.21377300
C	-0.95163700	-0.86442700	-0.12877400
C	-2.46502100	-0.63070400	-0.03796200
H	-3.95130600	0.90115100	-0.02052200
H	-2.79327700	1.07580500	-1.31876300
C	-2.88346900	0.82901500	-0.25380300
H	-2.66566900	2.80330200	0.54858300
H	-2.05731800	1.55578500	1.60181100
C	-2.11221200	1.85936600	0.55128800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -809.597531

264) Conformer **45C4**

H	-0.34174700	0.06272600	1.87367100
H	-2.94728300	-2.54003300	-0.96117400
O	2.55507100	0.48597000	-0.39013300
H	3.63048600	-1.73808600	0.18505000
O	3.07806600	-1.71266900	-0.60462100
H	-0.70008500	0.26467600	-2.09579600
H	-0.81345200	-1.95060400	-0.18100100
H	2.42864800	0.33960100	2.19087800
H	1.61636800	-0.95582200	3.07163000
H	3.08814900	-1.29922100	2.17997500
C	2.16159400	-0.71820400	2.15619400
O	2.00476300	2.60952700	-0.26460900
C	1.64367200	1.45741500	-0.26303200
H	-4.04499700	-1.09853100	1.37732100
H	-2.63927100	-2.16425200	1.49759000
C	-2.95295800	-1.12977600	1.32974700
H	-2.75150100	-1.20948000	-2.11264700
H	-4.21161200	-1.31322200	-1.12337700
C	-3.12979900	-1.47370400	-1.12096300
H	0.79411200	-1.95869400	-1.78954400
C	1.06545400	-0.92269500	-1.57666500
C	2.01715600	-0.86256500	-0.39124200
H	1.00855200	-2.10799000	1.00892700
C	1.29410900	-1.05263800	0.95211600
C	0.01751900	-0.20652300	0.87957000
H	-0.80536000	2.64290200	-0.95868300
H	-0.23374500	2.87741000	0.67445700
C	-0.71853800	2.15128700	0.01714300
C	0.22596600	0.96864500	-0.13663800
H	-2.56711500	-0.52845800	2.15584300
H	1.59696400	-0.52390700	-2.44408200
C	-0.16799100	-0.10315200	-1.21721500
C	-0.95221300	-0.86434400	-0.12875100
C	-2.46516900	-0.63099500	-0.03039700
H	-3.95198300	0.90021000	-0.00700100
H	-2.80005700	1.07460400	-1.31070100
C	-2.88522100	0.82839200	-0.24521200
H	-2.66431900	2.80329100	0.55472300
H	-2.05122600	1.55668300	1.60630100
C	-2.11070200	1.85945100	0.55577000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -809.597368

265) Conformer **46C1**

H	0.81516900	1.27862000	-1.84060900
C	-2.00674600	-0.64207600	-1.30793400
O	-1.77626400	1.32799600	-0.06423600
H	-3.23379000	-1.40368900	1.11754300
H	-4.12359500	1.17078400	0.40643700
C	-0.50974500	-0.65029700	0.63681800
O	2.37376100	-0.35127100	1.88821500
C	-1.86922500	-0.11664800	0.11321900
C	1.49178100	0.71789600	1.53475700
C	2.57996200	-0.14055700	-0.41874500
H	4.21053600	-0.01117100	0.97640300
C	0.05764400	0.26391600	1.75506200
H	1.70323300	1.56979200	2.18880000
C	-0.66147600	-0.90345300	-1.79686700
O	-0.55968900	3.09367100	-0.52562900
H	4.29003300	0.76116000	-1.36602900
C	0.28351400	-0.49475600	-0.69666200
H	3.53264100	-1.65233700	0.81919300
C	0.54658100	1.00230700	-0.81600400
H	3.93975300	-0.89248900	-1.89583100
H	2.34307800	2.01209600	-0.03638200
C	-0.54219200	-2.08314100	1.16304000
C	-3.06555300	-0.33076000	1.01344900
O	-1.55761200	-1.96978200	-1.51022500
C	3.28618000	-0.58878800	0.84042500
C	3.48923400	0.05941700	-1.60643400
H	-1.12266000	-2.12963000	2.08739300
O	-4.24610000	0.21832000	0.47618100
H	0.02526800	-0.26832700	2.70727100
C	-0.62069200	1.89518800	-0.45251900
H	-2.82821400	-0.29932200	-1.92590300
C	1.78837800	1.08122300	0.06422100
H	-2.85168800	0.07740600	2.00890500
H	2.93574300	0.44417600	-2.46498400
O	1.55041100	-1.10126100	-0.74663100
H	-0.95299600	-2.79548500	0.45372500
H	-0.36290800	-0.79318800	-2.83414200
H	-0.56154300	1.15187300	1.89600100
H	0.48002300	-2.37848700	1.40585400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1032.709392

266) Conformer **46C2**

H	0.83807400	1.34897800	-1.78817000
C	-2.01580500	-0.53991800	-1.32849300
O	-1.75025800	1.37345500	-0.00397900
H	-3.14769800	-1.41705700	1.13296400
H	-4.96799000	-0.00327200	0.95093200
C	-0.51760000	-0.65295600	0.61339800
O	2.37315000	-0.45159800	1.87159400
C	-1.87056400	-0.07366600	0.11349100
C	1.50853500	0.64498900	1.56101900
C	2.57944500	-0.15572100	-0.42609700
H	4.21427800	-0.10922100	0.96952800
C	0.06714100	0.20675900	1.76562400
H	1.73479700	1.46721900	2.24730800
C	-0.67568300	-0.80604400	-1.82818900
O	-0.50321900	3.13208200	-0.40048500
H	4.30329400	0.75251600	-1.34226900
C	0.27683200	-0.45803200	-0.71432600
H	3.50704200	-1.73074600	0.75070400
C	0.56584800	1.03675400	-0.77499700
H	3.92433200	-0.87365500	-1.93361500
H	2.38017400	1.98438600	0.03994400
C	-0.56362300	-2.10602100	1.07930700
C	-3.05799200	-0.33321400	1.00363500
O	-1.59084200	-1.86676600	-1.58340700
C	3.27947500	-0.66459900	0.81334900
C	3.49033100	0.07397900	-1.60723000
H	-1.12315700	-2.18402500	2.01415900
O	-4.21188400	0.20443100	0.39558900
H	0.02684200	-0.36182600	2.69627300
C	-0.58700800	1.93197300	-0.37332200
H	-2.83054800	-0.15823600	-1.93160400
C	1.80972300	1.05990200	0.10527300
H	-2.87779700	0.11585400	1.98823400
H	2.94204900	0.50025300	-2.44936500
O	1.53276200	-1.08499800	-0.78872100
H	-1.00152800	-2.78073300	0.34949900
H	-0.37593100	-0.65991500	-2.86073100
H	-0.53730000	1.09850600	1.94177300
H	0.45907100	-2.42699600	1.28504800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1032.707832

267) Conformer **46C3**

H	0.95975300	1.00346900	1.99957500
C	-1.91451900	1.70429800	0.23554200
O	-1.79879900	-0.35365800	1.35798900
H	-4.04508900	0.01977100	0.16231600
H	-3.28298900	-2.13231500	0.14262100
C	-0.63861900	-0.12803000	-0.78697000
O	2.11969700	-1.58860700	-1.30610700
C	-1.92919400	0.19687700	0.01581100
C	1.29513600	-1.72555700	-0.14489300
C	2.55816100	0.30374200	-0.03095700
H	3.36850800	-0.12742600	-2.00126200
C	-0.16280100	-1.58708500	-0.54938900
H	1.45643000	-2.72362400	0.27511200
C	-0.52910000	2.13798600	0.15406700
O	-0.50881500	-0.91445200	3.04103800
H	3.11678600	1.78788700	1.43178600
C	0.29453400	0.89792500	-0.07087300
H	4.04322400	-1.11141700	-0.67685100
C	0.58958100	0.26271700	1.28345700
H	4.36370800	0.56992200	1.11033500
H	2.31677100	-1.04461400	1.68994300
C	-0.75872300	0.09583100	-2.29101800
C	-3.24982600	-0.31166300	-0.51718100
O	-1.46454200	2.47960100	-0.86040400
C	3.13138200	-0.63763500	-1.06537400
C	3.57991800	1.17758500	0.65431900
H	0.22374800	-0.05901300	-2.74045200
O	-3.29660500	-1.70327500	-0.71850600
H	-0.31346200	-2.16596800	-1.46152300
C	-0.59687000	-0.39096600	1.96214000
H	-2.65778200	2.15457700	0.88490700
C	1.74143700	-0.64143100	0.85875800
H	-3.42731200	0.15920700	-1.48602000
H	4.04274300	1.85055300	-0.07080300
O	1.54999100	1.12636500	-0.65994300
H	-1.43799900	-0.64488400	-2.71890500
H	-0.11963200	2.96325000	0.72730600
H	-0.76812800	-2.08445700	0.20856700
H	-1.10969400	1.08971500	-2.55383100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1032.708561

268) Conformer **46C4**

H	-0.98504200	-1.58204600	1.57729400
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C	1.91923600	-1.69254300	-0.27184400
O	1.77688600	-0.09585100	1.43781300
H	4.02432600	-0.01343900	0.26817700
H	4.06216700	2.20570300	-0.31905500
C	0.64846700	0.36689300	-0.68734500
O	-2.10523000	1.92317600	-0.75686000
C	1.92925900	-0.19165600	-0.00689600
C	-1.29577100	1.68424800	0.39946900
C	-2.55513700	-0.27540200	-0.15188100
H	-4.03567200	1.27239000	-0.34127900
C	0.16696700	1.67851500	-0.01009800
H	-1.46543900	2.49889400	1.11098800
C	0.53703700	-2.07878400	-0.50536200
O	0.46280700	-0.09854900	3.19284200
H	-4.37934000	-0.88344300	0.81688700
C	-0.28963400	-0.83087800	-0.34304200
H	-3.33666100	0.75733400	-1.89799700
C	-0.60663700	-0.65385200	1.13732300
H	-4.03170700	-1.73089100	-0.69911800
H	-2.34310200	0.46138200	1.90962500
C	0.79066100	0.62446800	-2.18410100
C	3.24723700	0.44910200	-0.35312000
O	1.48893300	-2.08650300	-1.56155800
C	-3.11581200	0.94530700	-0.84516200
C	-3.58460400	-1.31862900	0.20809500
H	-0.18306400	0.92729200	-2.57291200
O	3.18888500	1.84168600	-0.14994100
H	0.32504600	2.51222900	-0.69533300
C	0.56885200	-0.25047100	2.00383900
H	2.65506700	-2.32344600	0.21540500
C	-1.75432500	0.33976800	1.00237900
H	3.46479600	0.20394200	-1.40015900
H	-3.13229800	-2.14194300	0.76420400
O	-1.53584200	-0.86153800	-0.99278100
H	1.48542900	1.45134600	-2.34661100
H	0.12382000	-3.04208200	-0.22487900
H	0.77043500	1.91265200	0.86695400
H	1.13494000	-0.24175300	-2.74182700

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1032.707844

269) Conformer **46C5**

H	-0.97808400	-1.54314400	1.61853800
C	1.92091700	-1.69676800	-0.23921600

O	1.78149000	-0.05626100	1.42951600
H	4.02936300	-0.01684400	0.24922900
H	2.90405200	2.30647400	-0.84363700
C	0.64572200	0.34830700	-0.70228900
O	-2.10930200	1.90268000	-0.79694400
C	1.93037500	-0.18948300	-0.01122400
C	-1.29525500	1.69298800	0.36080300
C	-2.55492400	-0.28077500	-0.13584400
H	-4.03758200	1.26029400	-0.35955300
C	0.16563300	1.67781800	-0.05869500
H	-1.45993700	2.52514600	1.05268600
C	0.53821200	-2.09121200	-0.45690200
O	0.47663100	-0.02166100	3.19132800
H	-4.03333200	-1.74951400	-0.64001400
C	-0.29016700	-0.84091400	-0.32196600
H	-3.34249700	0.70704900	-1.90497900
C	-0.60129600	-0.62617100	1.15445000
H	-3.12732900	-2.12389500	0.82913900
H	-2.33448100	0.50836400	1.90542400
C	0.77144800	0.55817100	-2.20857300
C	3.25572700	0.44984700	-0.36604100
O	1.48502000	-2.12362100	-1.51685800
C	-3.11917500	0.92137200	-0.85780800
C	-3.58232100	-1.31485700	0.25468500
H	-0.21258700	0.82364200	-2.59876100
O	3.32634100	1.83462600	-0.12078500
H	0.30586000	2.49470300	-0.76949500
C	0.57707400	-0.20134300	2.00603200
H	2.65976400	-2.31446100	0.26023400
C	-1.74959500	0.36364900	0.99914700
H	3.47809500	0.20900400	-1.41134900
H	-4.37425500	-0.86447700	0.85596700
O	-1.53834700	-0.88773700	-0.96572900
H	1.43843200	1.39714200	-2.42494200
H	0.12727400	-3.04758700	-0.15086900
H	0.77479400	1.93767900	0.80776800
H	1.13353800	-0.31756500	-2.73896300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1032.707038

270) Conformer **47C1**

C	3.64333400	-5.41396600	0.72905300
C	3.84796300	-6.80319800	0.74698800
C	4.91553400	-7.27340900	-0.01100400

C	5.67353200	-6.40062100	-0.76501600
C	5.57024000	-5.02902100	-0.66974700
C	4.51217700	-4.53173100	0.07953900
H	4.36423200	-3.46115600	0.19515300
C	6.85975800	-7.03798500	-1.37233700
C	8.08616000	-6.42997300	-0.63429100
C	8.08998600	-4.90310000	-0.83890500
H	8.40416400	-4.42432400	0.09013100
H	8.84227600	-4.64601300	-1.58706100
C	6.72663500	-4.28638900	-1.26991100
H	6.65187100	-4.33562200	-2.36183600
H	6.70928800	-3.22806300	-1.00385300
C	5.63677400	-8.60304100	0.03965900
H	4.99930300	-9.48722900	-0.00370500
C	6.69914800	-8.53117500	-1.07481700
O	6.40038900	-8.68533100	1.26396100
C	9.26158700	-7.16414500	-1.21328500
O	9.16279300	-8.49881800	-1.03995500
O	10.21651000	-6.71197800	-1.78899600
C	7.98197200	-8.98450000	-0.38907700
H	8.09798400	-10.06536600	-0.34344600
C	8.04571800	-6.84807500	0.87043000
H	7.21414300	-6.31390300	1.33657800
C	7.75257300	-8.35953400	0.98339400
H	8.35197100	-8.81154000	1.77504400
C	2.97585400	-7.68116200	1.58758900
H	3.27866800	-8.72513700	1.51304800
H	1.92896300	-7.60641200	1.28072900
H	3.01538400	-7.38820100	2.64040000
O	2.58314400	-4.95239700	1.44596900
H	2.55028500	-3.99193700	1.38963300
C	9.33049000	-6.49663000	1.60981900
H	9.21675700	-6.71614500	2.67352900
H	9.58434400	-5.43967100	1.51425200
H	10.18179100	-7.07863800	1.24460000
H	6.44006500	-9.11503400	-1.95600500
H	6.96324500	-6.83442900	-2.44224600

No imaginary frequency.

Gibbs Free Energies (a.u.) = -996.633220

271) Conformer **47C2**

C	3.64869100	-5.40717500	0.73590600
C	3.85018800	-6.79673100	0.75461300
C	4.91474500	-7.27275500	-0.00679800

C	5.67036800	-6.40304600	-0.76377100
C	5.56876000	-5.02936500	-0.66974100
C	4.51654000	-4.52771900	0.08102900
H	4.36008700	-3.46107500	0.20358300
C	6.85477800	-7.04255200	-1.37257400
C	8.08321600	-6.43348900	-0.63881200
C	8.08795700	-4.90716800	-0.84765400
H	8.40509500	-4.42609700	0.07918400
H	8.83848400	-4.65295000	-1.59854300
C	6.72408500	-4.29062000	-1.27665800
H	6.64551800	-4.34451700	-2.36810100
H	6.70848100	-3.23129600	-1.01475800
C	5.63428300	-8.60317500	0.04614200
H	4.99602900	-9.48706300	0.00598000
C	6.69409700	-8.53485000	-1.07085900
O	6.39986600	-8.68292500	1.26906700
C	9.25699000	-7.17006100	-1.21817600
O	9.15773100	-8.50422300	-1.04089900
O	10.21102300	-6.72011000	-1.79699000
C	7.97799700	-8.98722800	-0.38635200
H	8.09320900	-10.06805700	-0.33803100
C	8.04564000	-6.84745200	0.86720000
H	7.21559000	-6.31129200	1.33378500
C	7.75183900	-8.35838700	0.98491100
H	8.35242800	-8.80865100	1.77661500
C	2.98238200	-7.67857200	1.59946000
H	3.29251200	-8.72004200	1.52774300
H	1.93235100	-7.63373300	1.28870000
H	3.02488800	-7.39927600	2.65785500
O	2.62413500	-4.83671100	1.42530100
H	2.10233700	-5.51942500	1.85955600
C	9.33233300	-6.49497500	1.60278400
H	9.22071700	-6.71126900	2.66737000
H	9.58679300	-5.43851200	1.50357500
H	10.18235000	-7.07874400	1.23740000
H	6.43275900	-9.12100500	-1.94982700
H	6.95572700	-6.84170800	-2.44321300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -996.632870

272) Conformer **48C1**

C	4.22062300	-5.65175100	0.50630100
C	4.37086400	-7.04494600	0.41153100
C	5.54961900	-7.49901400	-0.16707200

C	6.48300500	-6.59705800	-0.65283400
C	6.39825200	-5.23454300	-0.45458400
C	5.22172600	-4.76188900	0.12133700
H	5.08687300	-3.69998300	0.31187000
C	7.69902800	-7.26105100	-1.17048200
C	8.91972000	-6.59625200	-0.49802000
C	8.92985100	-5.15777600	-1.00709300
H	9.77770400	-4.60185400	-0.60327400
H	9.08293700	-5.19667500	-2.08861100
C	7.62216700	-4.38073200	-0.69644400
H	7.44017300	-3.67184100	-1.51014800
H	7.76870900	-3.76356200	0.19562100
C	6.08951900	-8.90753900	-0.27784200
H	6.05588900	-9.42579000	0.68587700
H	5.50012300	-9.51758000	-0.96860700
C	7.53754600	-8.74284200	-0.81048300
C	10.08336200	-7.45318100	-0.90887000
O	9.91890600	-8.74229700	-0.55097700
O	11.07727000	-7.11929100	-1.50385500
C	8.68052300	-9.05032500	0.15237200
H	8.75108800	-10.11461200	0.37694900
C	8.82218800	-6.72175700	1.04735300
H	7.92381200	-6.18029300	1.34871400
C	8.65360900	-8.20982000	1.41131300
H	9.46661100	-8.53704800	2.06422600
H	7.72251200	-8.38800500	1.95320000
C	3.31042700	-7.95574200	0.94542900
H	3.60309600	-9.00073000	0.84506800
H	2.36469800	-7.81704400	0.41338700
H	3.10675600	-7.75572500	2.00102700
O	3.05604900	-5.20770600	1.05538600
H	3.06784000	-4.24602400	1.09579900
C	10.00960700	-6.09989500	1.76900200
H	9.89008000	-6.22174800	2.84823200
H	10.10077800	-5.03111900	1.56609300
H	10.95166700	-6.58040300	1.48772900
H	7.68470300	-9.37317200	-1.68885600
H	7.80808700	-7.12539100	-2.25176300

No imaginary frequency.

Gibbs Free Energies (a.u.) = -922.653677

273) Conformer **48C2**

C	4.22579600	-5.63896400	0.50741400
C	4.37302900	-7.03355700	0.42697300

C	5.54888600	-7.49850000	-0.15241000
C	6.47973900	-6.60403000	-0.65187900
C	6.39716600	-5.23766400	-0.46777300
C	5.22649300	-4.75546600	0.10723200
H	5.08163700	-3.69574100	0.29147600
C	7.69240000	-7.27499500	-1.16825100
C	8.91715400	-6.60434500	-0.50911800
C	8.92690800	-5.17172700	-1.03448600
H	9.77711100	-4.61249500	-0.64032200
H	9.07587100	-5.22316700	-2.11606500
C	7.62139400	-4.38938600	-0.72772500
H	7.43544200	-3.69192900	-1.55031500
H	7.77282900	-3.75979100	0.15466500
C	6.08533500	-8.90925500	-0.24929100
H	6.05646000	-9.41610900	0.72070400
H	5.49155000	-9.52642500	-0.92995300
C	7.53084600	-8.75249100	-0.79110000
C	10.07773800	-7.46742300	-0.91580700
O	9.91323700	-8.75230900	-0.54279000
O	11.06927900	-7.14163400	-1.51908300
C	8.67796500	-9.05073400	0.16978200
H	8.74809600	-10.11254700	0.40593000
C	8.82670700	-6.71240100	1.03799100
H	7.93046400	-6.16643900	1.33759200
C	8.65803000	-8.19611800	1.41935900
H	9.47375700	-8.51707600	2.07197300
H	7.72938300	-8.36701600	1.96776600
C	3.31698400	-7.94363500	0.97677500
H	3.61004300	-8.98800900	0.87695400
H	2.36295500	-7.82764900	0.44972800
H	3.12898600	-7.75949100	2.04047500
O	3.10522000	-5.08173400	1.04445800
H	2.48837700	-5.77452600	1.30157100
C	10.01822300	-6.08401300	1.74712300
H	9.90348700	-6.19356300	2.82818500
H	10.10975100	-5.01770800	1.53178800
H	10.95837500	-6.56888900	1.46695500
H	7.67262600	-9.39288100	-1.66302700
H	7.79627200	-7.15116600	-2.25147500

No imaginary frequency.

Gibbs Free Energies (a.u.) = -922.653677

274) Conformer **49C1**

H	9.29566500	0.20641600	-0.98537300
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C	7.20674800	0.20117600	-0.53395600
H	7.97753800	2.07325100	0.25337600
H	4.81096800	-0.44977900	4.09877500
H	4.98818300	-2.17438200	-1.50006900
O	3.99185700	2.19748300	-1.16617400
H	9.42532000	-0.94603400	-4.26485100
C	8.32517100	-1.52422600	-1.80501000
H	2.07746100	0.41342000	2.89993200
H	11.50815800	-2.88359600	-1.81533300
H	3.80710200	0.90384500	4.63913400
C	2.87071600	0.05433700	2.23565400
C	5.25891000	0.35773800	1.55202700
O	7.05346400	-3.33481400	-2.63962200
C	6.58473100	1.13524200	1.65922200
H	11.03622200	-1.61127800	-3.95493600
C	3.49629600	-0.43255300	-0.13801000
H	6.45838800	2.07094800	2.20590600
C	10.62775900	-2.42556000	-1.35649200
C	2.41526900	0.10646300	0.78630700
H	6.15082900	-3.66806100	-2.66370200
C	4.88079700	1.65194800	-0.56015700
H	1.50799100	-0.49153000	0.66071700
H	5.49183600	1.18225600	4.19177300
H	5.43904100	-0.68168300	1.84706900
C	5.98959600	-0.46069800	-0.65930200
H	3.06098000	-0.99094100	2.51204200
C	4.14452600	0.86903900	2.49997300
C	9.58287700	-2.09543100	-2.42196200
H	9.30668600	-3.02845000	-2.91696100
C	7.09049400	-2.16990100	-1.93514100
H	3.18556700	-0.36091000	-1.18361500
H	3.63632800	-1.49597100	0.08448600
C	7.07840700	1.46069100	0.25588600
C	4.84127000	0.25232400	0.03943600
H	2.15349000	1.12891800	0.50184400
H	10.23044600	-3.12154400	-0.61368200
H	10.47089100	-0.20655500	-3.04598100
H	7.34907600	0.55621900	2.17978600
C	4.59467000	0.61076300	3.93888000
O	6.05206600	2.28249600	-0.37861500
H	10.95757000	-1.52465900	-0.83112100
H	3.50156700	2.63687800	1.35467800
C	3.83585400	2.36186500	2.35557000
C	8.35452800	-0.32432100	-1.09493400

H	4.69660400	2.98650000	2.60353500
C	10.15919800	-1.15917200	-3.48388700
H	3.03461700	2.62919000	3.05039200
C	5.92627100	-1.64435500	-1.37051400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1002.297182

275) Conformer **49C2**

H	9.35941100	0.26156100	-0.94168800
C	7.26705100	0.28291300	-0.48706500
H	8.05689200	2.14384700	0.30843500
H	5.55944700	1.25887500	4.24146100
H	5.02993600	-2.06659700	-1.46710100
O	4.07299000	2.31449700	-1.11191900
H	9.31509100	-4.12254000	-2.03943700
C	8.37436100	-1.44971000	-1.76769700
H	2.13910500	0.52716100	2.94429400
H	10.58197000	-2.34945000	-4.29014800
H	4.86352700	-0.36631000	4.14035000
C	2.92935000	0.16451200	2.27837600
C	5.32053300	0.44947900	1.59777200
O	7.07304500	-3.24284300	-2.60867400
C	6.65328400	1.21434100	1.70946200
H	10.11930700	-3.30237300	-0.69278600
C	3.55141500	-0.31578400	-0.09751100
H	6.53460900	2.14949600	2.25885000
C	9.60894200	-2.04080900	-3.89798100
C	2.47514200	0.22864800	0.82913300
H	6.16494700	-3.56173800	-2.63229800
C	4.95657700	1.75739100	-0.50845600
H	1.56216100	-0.35981100	0.69989800
H	3.87192300	0.99398500	4.68656800
H	5.49110700	-0.59297900	1.88777200
C	6.04500000	-0.36530200	-0.61637300
H	3.11002400	-0.88392900	2.54926900
C	4.21033100	0.96626500	2.54751000
C	9.65026700	-1.99741800	-2.37001000
H	10.43538800	-1.28624100	-2.09065700
C	7.12957800	-2.08202500	-1.90081800
H	3.24201300	-0.23555600	-1.14289700
H	3.68108800	-1.38171700	0.11927300
C	7.15179500	1.54015800	0.30793400
C	4.90275700	0.35520400	0.08433600
H	2.22344200	1.25512900	0.55004900

H	9.37484700	-1.05721100	-4.31294600
H	11.01788800	-3.66149000	-2.17293100
H	7.41150300	0.62681800	2.22945600
C	4.65716500	0.69694400	3.98536300
O	6.13375800	2.37528100	-0.32365200
H	8.85889200	-2.74919600	-4.25305400
H	3.11516900	2.73352000	3.10484900
C	3.91539700	2.46254900	2.41025900
C	8.40948900	-0.25406600	-1.05114600
H	3.58572400	2.74595400	1.41016700
C	10.04437300	-3.35285800	-1.78200300
H	4.78123300	3.07806100	2.66333100
C	5.97275800	-1.54563500	-1.33391800

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1002.294952

276) Conformer **49C3**

H	9.35920600	0.14140100	-0.79694400
C	7.25693000	0.18195700	-0.42954700
H	8.05342800	2.00288500	0.44766300
H	5.40552900	1.05488400	4.26496500
H	5.01926100	-2.11278800	-1.54795900
O	4.12480600	2.29520200	-1.10071300
H	9.82295600	-0.65099400	-3.92658800
C	8.37421000	-1.53553700	-1.71030100
H	2.01871700	0.42744600	2.83238000
H	11.74142800	-2.30989300	-2.06807700
H	4.68346300	-0.55277400	4.09245600
C	2.82443800	0.06917300	2.18282800
C	5.24220900	0.32695600	1.59208800
O	6.96633800	-3.28008600	-2.62836300
C	6.58481600	1.06118900	1.77160600
H	8.79829100	-2.01389600	-4.38281000
C	3.51831300	-0.35295600	-0.18430300
H	6.46546600	1.98195500	2.34471900
C	10.90685600	-1.75772500	-1.63048700
C	2.42136700	0.18484500	0.72171700
H	7.82491700	-3.62325200	-2.89680700
C	4.97625400	1.70242500	-0.48520900
H	1.50257600	-0.38159700	0.54422700
H	3.69906700	0.81023900	4.64497500
H	5.38270700	-0.72674500	1.85650500
C	6.02652500	-0.43918500	-0.61852600
H	2.97644400	-0.99007900	2.42797200

C	4.10997700	0.83773600	2.51863500
C	9.61461600	-2.12231300	-2.35123000
H	9.54034000	-3.21826700	-2.29319000
C	7.12353300	-2.14111600	-1.89977100
H	3.24671600	-0.23599300	-1.23667800
H	3.62075400	-1.42716900	0.00356100
C	7.13749000	1.41777600	0.39812300
C	4.87517800	0.28513200	0.06320500
H	2.19829000	1.22390600	0.46581300
H	10.85822200	-2.00092800	-0.56674000
H	10.55388600	-2.21808200	-4.30815000
H	7.31332100	0.44333600	2.29888500
C	4.50224600	0.51834300	3.96214500
O	6.15831300	2.29072900	-0.24287300
H	11.13497000	-0.69325400	-1.72948600
H	3.02998600	2.60944100	3.09121500
C	3.84783300	2.34287700	2.41569500
C	8.41133300	-0.35874900	-0.96240800
H	3.55720800	2.66121900	1.41400200
C	9.69859600	-1.73297600	-3.83094200
H	4.71605600	2.93374100	2.71516700
C	5.95562000	-1.60043900	-1.36344900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1002.295314

277) Conformer **49C4**

H	9.24452300	0.35066500	-1.12877200
C	7.17353200	0.27390200	-0.61695700
H	7.89412200	2.19819700	0.08796800
H	5.55204000	1.34727100	4.12005700
H	5.02930200	-2.21874600	-1.46108400
O	3.86942000	2.13015400	-1.22069500
H	11.05795500	-0.52654700	-1.94233600
C	8.32480700	-1.44758300	-1.86153100
H	2.13645800	0.40339700	2.95366100
H	9.45522000	-3.87386100	-1.25936400
H	4.93445500	-0.31218400	4.09943000
C	2.92446200	0.05417900	2.27794600
C	5.27837700	0.42663700	1.51614800
O	6.98993500	-3.34307700	-2.56369400
C	6.57619100	1.25582300	1.56164600
H	10.22473000	-0.22771100	-3.47686900
C	3.50192100	-0.48322000	-0.09755500
H	6.42916500	2.20362400	2.08168900

C	10.17939700	-3.09814600	-1.51972400
C	2.42690500	0.04206300	0.84156600
H	7.81541300	-3.56856000	-3.00516300
C	4.79435700	1.63710700	-0.62353900
H	1.54116900	-0.59476900	0.76116400
H	3.89284800	1.01851300	4.62507400
H	5.50598300	-0.59541700	1.83786900
C	5.97913200	-0.43591600	-0.68726300
H	3.16388200	-0.97344700	2.58102200
C	4.17164800	0.92590100	2.47919100
C	9.58333000	-2.04294000	-2.45744300
H	9.31133600	-2.54196700	-3.39930700
C	7.10817600	-2.14135300	-1.93553600
H	3.15964300	-0.45568800	-1.13533000
H	3.69002700	-1.53327700	0.15097300
C	7.01929700	1.55316200	0.13544300
C	4.82386400	0.25713100	0.02005500
H	2.11598600	1.04392600	0.53411300
H	10.51120900	-2.62768500	-0.59022000
H	11.45898300	-1.48954900	-3.35947700
H	7.37554100	0.72296800	2.07894600
C	4.67162100	0.73322000	3.91189500
O	5.94562500	2.31555800	-0.49533200
H	11.04256400	-3.58181200	-1.98404500
H	3.01022500	2.65974000	3.00619800
C	3.80028500	2.40005300	2.29582000
C	8.32649800	-0.22283400	-1.19410500
H	3.42557700	2.62787200	1.29738200
C	10.63568800	-1.00558800	-2.82953500
H	4.64276500	3.06541200	2.49626100
C	5.94041200	-1.64159900	-1.36064000

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1002.295436

278) Conformer **50C1**

C	8.55608900	-8.93814600	0.28551100
C	7.67773400	-8.46298400	1.46205900
H	7.26553600	-9.32620000	1.99264000
H	6.83397100	-7.91162500	1.03500500
C	8.45549100	-7.58910800	2.44671400
H	9.07098200	-8.24251700	3.07110600
H	7.75197900	-7.09999800	3.12306100
C	9.36194600	-6.54426500	1.78274000
C	10.08206000	-7.18201600	0.57797600

O	10.71776900	-8.43539600	1.01869900
C	9.85235100	-9.45204000	0.89513600
O	10.10658600	-10.56240000	1.28497300
C	10.28505600	-5.79868400	2.78580600
C	11.24087700	-4.89113100	1.99660100
H	10.65193900	-4.11307100	1.49302800
H	11.89837800	-4.37527400	2.70455200
C	12.05812800	-5.63767400	0.95577200
H	12.69363000	-6.38867600	1.43507300
H	12.73077000	-4.94789800	0.43809200
C	11.13590800	-6.29985900	-0.05243900
H	11.69135000	-6.89373100	-0.78424600
H	10.60229100	-5.52441000	-0.61479800
C	9.05348100	-7.68886300	-0.42888800
H	8.26171800	-6.96077400	-0.61044100
H	9.54522000	-7.93046000	-1.37194400
H	8.72401700	-5.76911000	1.33687300
C	7.82402200	-9.97456700	-0.54355300
H	6.90664200	-9.53183200	-0.94396000
H	7.49969300	-10.79547100	0.10665300
C	8.61261900	-10.58381900	-1.67439500
O	9.80357000	-10.30011800	-1.82266300
C	7.95452000	-11.52886700	-2.58351300
C	8.69740800	-12.10853700	-3.63550900
C	8.06975700	-13.00795700	-4.49657200
H	8.64726800	-13.44768600	-5.30106600
C	6.74036200	-13.33384100	-4.32731900
H	6.27078300	-14.03739200	-5.00805100
C	5.99573100	-12.76767100	-3.28895100
C	6.60340400	-11.87609000	-2.43039800
H	6.01183900	-11.44961500	-1.63029600
O	9.99174100	-11.82833800	-3.84304100
H	10.24738700	-11.18652000	-3.13543100
O	4.68134900	-13.06029900	-3.08413100
H	4.37846200	-13.68904100	-3.74680200
C	11.09815100	-6.74024900	3.68038300
H	11.79642000	-6.15305800	4.28437600
H	11.67284200	-7.47006100	3.10940700
H	10.45661600	-7.28987800	4.37274900
C	9.42813300	-4.90621900	3.68599900
H	8.75275800	-5.48917400	4.31686100
H	8.82661000	-4.20976000	3.09382900
H	10.06865300	-4.31663200	4.34873400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1190.728558

279) Conformer **50C2**

C	9.42795600	-9.33128500	0.01890200
C	8.60634300	-8.99694600	1.28000900
H	8.22153200	-9.91812600	1.72751800
H	7.74831500	-8.40345800	0.95878700
C	9.43489200	-8.23642300	2.31598700
H	10.08885500	-8.94767400	2.82815200
H	8.76754200	-7.83464300	3.08075300
C	10.29534900	-7.11209900	1.72527600
C	10.97065700	-7.60982000	0.43111400
O	11.62711500	-8.89847600	0.70956100
C	10.76148000	-9.89870000	0.50118900
O	11.05291800	-11.05009200	0.70088600
C	11.25127200	-6.45767500	2.76073200
C	12.16575400	-5.46181000	2.03230800
H	11.54947500	-4.64580000	1.63227400
H	12.84482900	-5.01034000	2.76343700
C	12.94945900	-6.08845000	0.89144500
H	13.61047800	-6.87537900	1.26766300
H	13.59475200	-5.34106300	0.42114500
C	11.99493700	-6.65708700	-0.14343900
H	12.52719600	-7.16747100	-0.95161800
H	11.43454000	-5.83519700	-0.60473400
C	9.90858300	-8.01867700	-0.58424700
H	9.11599600	-7.27945000	-0.68278300
H	10.37237900	-8.17512800	-1.56357800
H	9.62692900	-6.30775200	1.38954400
C	8.75247100	-10.32345000	-0.91132600
H	8.57120800	-11.25534000	-0.36682900
H	9.43662800	-10.58996100	-1.72616100
C	7.46326200	-9.87222500	-1.54687900
O	7.05237000	-8.71983600	-1.39267500
C	6.70920900	-10.82293800	-2.37479700
C	5.50630900	-10.40522800	-2.98609500
C	4.79279300	-11.30853300	-3.77317600
H	3.87089700	-10.97886200	-4.23747500
C	5.25093200	-12.59612400	-3.95859900
H	4.68114400	-13.28422300	-4.57582500
C	6.44034100	-13.02019800	-3.35989200
C	7.15549000	-12.13791500	-2.57796000
H	8.07501800	-12.48506900	-2.12432300
O	5.01741100	-9.16549600	-2.84033400

H	5.66117800	-8.68859400	-2.25937600
O	6.93062800	-14.28134500	-3.51522700
H	6.33844000	-14.79594700	-4.07248400
C	12.10859700	-7.47394900	3.52264500
H	12.82578700	-6.94188900	4.15487200
H	12.66660500	-8.13508800	2.85879400
H	11.50034700	-8.09889800	4.18021900
C	10.42302400	-5.67252200	3.77998600
H	9.77756700	-6.32475600	4.37300000
H	9.79329200	-4.92630100	3.28598100
H	11.08452100	-5.14629200	4.47465100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1190.727641

280) Conformer **50C3**

C	8.45887600	-8.79912100	0.06798200
C	7.46319900	-8.10550400	1.02168300
H	6.65245300	-8.79331700	1.27893300
H	7.01762400	-7.26962500	0.47295600
C	8.13685600	-7.61572300	2.30386700
H	8.28577400	-8.47592400	2.96228500
H	7.45561000	-6.94562800	2.83153000
C	9.48844800	-6.92516100	2.08051900
C	10.29950800	-7.71359900	1.03313400
O	10.32909800	-9.13170500	1.42964100
C	9.26564100	-9.76917900	0.91874500
O	9.01599300	-10.91637500	1.18534200
C	10.24453400	-6.60398000	3.39904700
C	11.63407600	-6.05091800	3.04876200
H	11.51023500	-5.09124600	2.52960000
H	12.17014600	-5.83518700	3.97917300
C	12.44832300	-6.98340300	2.16765300
H	12.63087500	-7.93246400	2.68116300
H	13.43079300	-6.54804800	1.96404300
C	11.72113800	-7.22912400	0.85732900
H	12.25409100	-7.94387600	0.22343000
H	11.66595400	-6.28914900	0.29541900
C	9.52660300	-7.77160500	-0.28155200
H	9.10826000	-6.80236700	-0.55647400
H	10.18022000	-8.12290500	-1.08095100
H	9.30301800	-5.95352600	1.60288900
C	7.72352600	-9.46295900	-1.07896700
H	7.16803600	-8.70233300	-1.63641700
H	6.96842700	-10.14842500	-0.67667100

C	8.57879900	-10.25061300	-2.03805000
O	9.78124400	-10.40606800	-1.81284100
C	7.96254500	-10.84235300	-3.23092000
C	8.76127400	-11.58849200	-4.12521900
C	8.17229900	-12.14903700	-5.25804000
H	8.79281100	-12.71924700	-5.93918500
C	6.82588200	-11.98296700	-5.50709300
H	6.38709800	-12.42792700	-6.39512700
C	6.02538800	-11.24839700	-4.62791100
C	6.59484700	-10.68762000	-3.50432500
H	5.95893400	-10.12381700	-2.83372700
O	10.07325700	-11.78186900	-3.92941900
H	10.29314300	-11.31744700	-3.08454000
O	4.69239600	-11.05836900	-4.83306300
H	4.42022200	-11.49618000	-5.64566300
C	10.39622300	-7.81571400	4.32466800
H	11.02419200	-7.54331500	5.17827500
H	10.85283600	-8.67101700	3.82583200
H	9.43237000	-8.13898800	4.72400800
C	9.48462900	-5.51497800	4.15923000
H	8.49888000	-5.85531300	4.48534100
H	9.35046300	-4.62205700	3.54098700
H	10.04292600	-5.22284300	5.05368400

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1190.728287

281) Conformer **50C4**

C	8.64859300	-8.98386900	0.37723800
C	7.82638700	-8.48291300	1.58360600
H	7.58523300	-9.32068900	2.24433600
H	6.88007200	-8.09567400	1.19249400
C	8.56534500	-7.40729900	2.38035100
H	9.31837700	-7.89917400	3.00209600
H	7.86685900	-6.93152000	3.07115700
C	9.25664600	-6.34586800	1.51486400
C	9.94389700	-7.03024900	0.31695400
O	10.78010600	-8.13351500	0.81957400
C	10.05280300	-9.25750300	0.89562700
O	10.49022100	-10.27430200	1.36921700
C	10.15495400	-5.37413300	2.32854200
C	10.90302100	-4.45681700	1.34955300
H	10.17024700	-3.82590500	0.82920300
H	11.54499800	-3.78032800	1.92381400
C	11.71719100	-5.21618800	0.31536600

H	12.49043500	-5.81769800	0.80327900
H	12.23958100	-4.51556100	-0.34225000
C	10.80697500	-6.10641300	-0.51250000
H	11.37012100	-6.71035900	-1.23000200
H	10.12413900	-5.47779300	-1.09641200
C	8.90549600	-7.77743700	-0.51541200
H	8.00942400	-7.17996600	-0.68853900
H	9.33746700	-8.06730900	-1.47400200
H	8.48106400	-5.71674400	1.05741000
C	7.98754500	-10.19413700	-0.25140400
H	6.98179800	-9.92059100	-0.58501200
H	7.84811700	-10.96749200	0.51312400
C	8.73282200	-10.82690200	-1.39862400
O	9.85758600	-10.42449100	-1.70481500
C	8.11223000	-11.93337600	-2.13583200
C	8.80610800	-12.52164900	-3.21611400
C	8.21067900	-13.56956400	-3.91737600
H	8.74902800	-14.01317600	-4.74654000
C	6.96179900	-14.03494300	-3.56206700
H	6.51575800	-14.85174700	-4.12147400
C	6.26883100	-13.46470700	-2.49062300
C	6.84372500	-12.42470200	-1.79137000
H	6.29281600	-11.99616300	-0.96390000
O	10.02303600	-12.11060600	-3.59984800
H	10.26963900	-11.37846700	-2.98272000
O	5.03606600	-13.89361100	-2.10164100
H	4.75268400	-14.62499900	-2.65910400
C	11.16567100	-6.09022400	3.23052400
H	11.82663600	-5.35070900	3.69251400
H	11.78358400	-6.80444900	2.68549000
H	10.66961600	-6.62945600	4.04059800
C	9.26794300	-4.49319900	3.21086700
H	8.73683200	-5.07482400	3.96818600
H	8.52710700	-3.95433600	2.61227900
H	9.87869200	-3.75225600	3.73531900

No imaginary frequency.

Gibbs Free Energies (a.u.) = -1190.728350

282) Conformer **51C1**

N	2.04889400	0.44607000	0.14712200
C	2.93624200	-0.34803100	-0.69490800
H	3.96018600	-0.00418000	-0.52190500
H	2.72064200	-0.16383700	-1.76365800
C	2.83557500	-1.83727800	-0.40901100

H	3.45563900	-2.37970900	-1.12770800
H	3.24616200	-2.03701500	0.58667700
C	1.39192700	-2.32450000	-0.45390100
H	1.32792800	-3.36166400	-0.11153700
H	1.01242100	-2.30491200	-1.48083600
C	0.56753000	-1.41853800	0.44276500
C	0.66879400	0.03365000	-0.01940300
C	-0.85989200	-1.83790400	0.74368400
C	-1.38668700	-1.11362800	1.97134300
H	-2.47219000	-1.23389200	2.00334600
H	-0.99591700	-1.61929500	2.85702100
C	-0.97929800	0.36582500	1.99817900
H	-0.20872100	0.52527600	2.75770900
H	-1.82548900	0.99185900	2.29605100
C	-0.42478700	0.88570500	0.67600800
C	0.01865300	2.29910300	0.84935100
H	-0.70659400	2.99177500	1.26895100
C	1.23422400	2.72863100	0.53300800
H	1.49597900	3.77208300	0.67996800
C	2.28784800	1.85990100	-0.05765300
H	2.38210600	2.11023300	-1.13331700
H	3.26079500	2.10899300	0.38055300
O	-1.78986600	-1.67833100	-0.35129100
C	-0.01399100	0.31866100	-1.38160700
H	0.42416700	1.18976800	-1.87235500
H	-0.09453900	-0.48975800	-2.10861600
C	-1.31029400	0.72760600	-0.63742400
C	-2.03005300	1.95945100	-1.14188100
H	-1.34027900	2.80186500	-1.19460000
H	-2.86163100	2.23303000	-0.48809100
H	-2.43647000	1.78078400	-2.13811900
C	-2.24247400	-0.46635500	-0.70848200
O	-3.33696500	-0.40659300	-1.21387300
H	-0.88489500	-2.91567700	0.91326500
H	1.05317400	-1.43261800	1.42824100

No imaginary frequency.

Gibbs Free Energies (a.u.) = -826.561323