

Supplementary materials

A Simple and Efficient Method for the Partial Synthesis of Pure (3*R*,3'*S*)-Astaxanthin from (3*R*,3'*R*,6'*R*)-Lutein and Lutein Esters via (3*R*,3'*S*)-Zeaxanthin and Theoretical Study of their Formation Mechanisms

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HPLC Analysis

Table S1. HPLC analytical conditions: Column: C₃₀, 5µm, 140Å, 250 x 4.6 mm; flow rate: 0.7 mL/min; detection at λ = 474 nm; injection volume: 10 µL, run time: 35 minutes; mobile phase: gradient of MeOH–methyl *ter*-butyl ether (MTBE)–H₂O as follow:

Time (minutes)	MeOH (%)	MTBE (%)	H ₂ O (%)
0	81	15	4
15	66	30	4
23	16	80	4
27	16	80	4
27.1	81	15	4
35	81	15	4

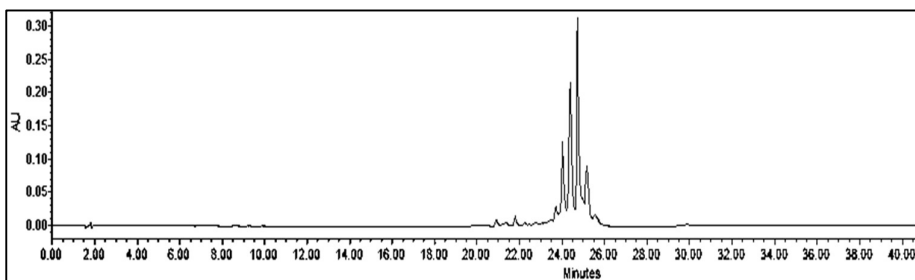


Figure S1. Chromatogram of the lutein esters extracted from the marigold oleoresin.

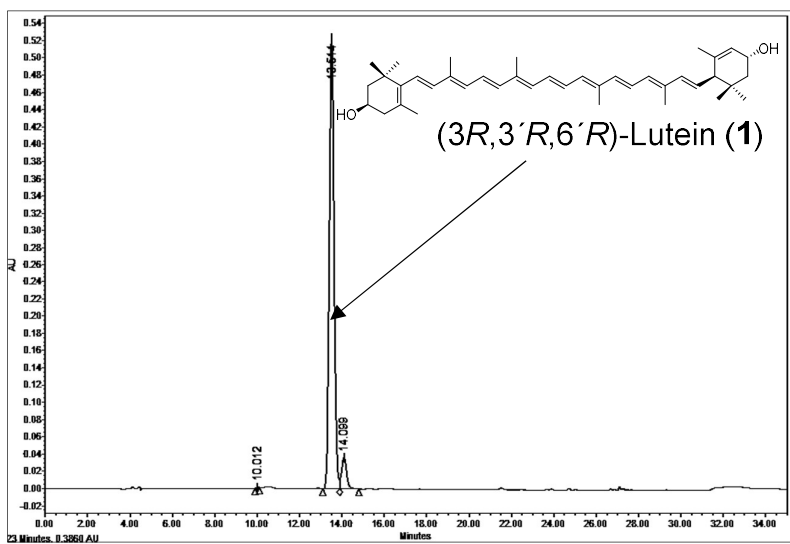


Figure S2. Chromatogram of lutein obtained from KOH-hydrolyzed lutein esters.

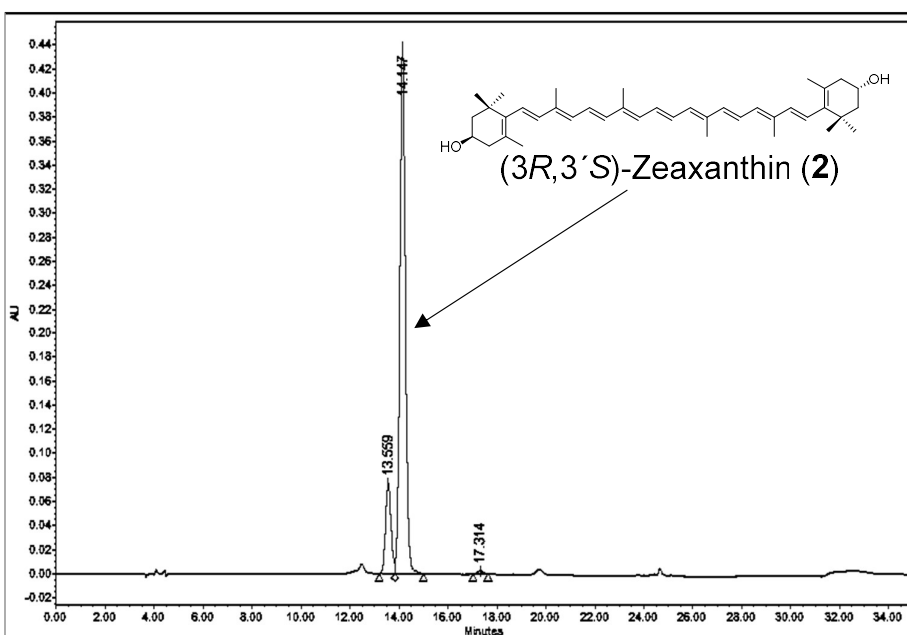


Figure S3. Chromatogram of zeaxanthin obtained from 1.

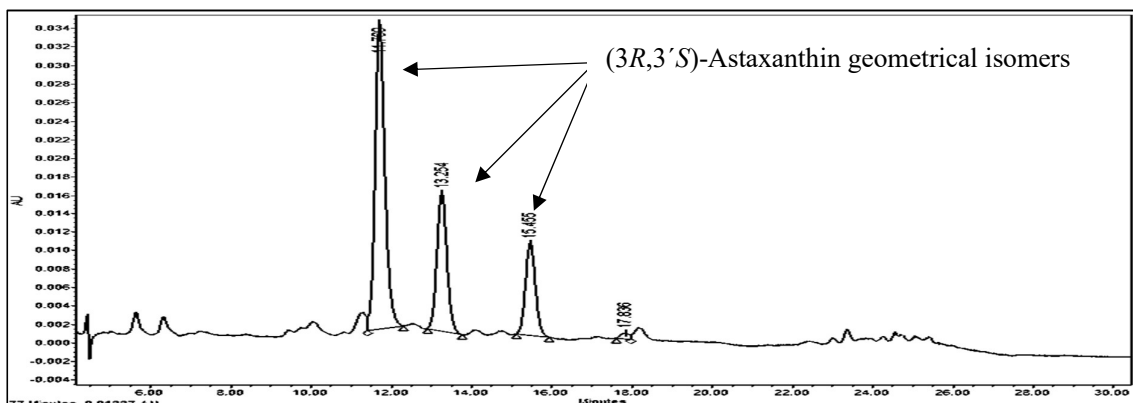


Figure S4. Chromatogram of the (3*R*,3'*S*)-astaxanthin obtained during the partial synthesis. The 3 peaks emerge as a consequence of the inherent *cis-trans* isomerization.

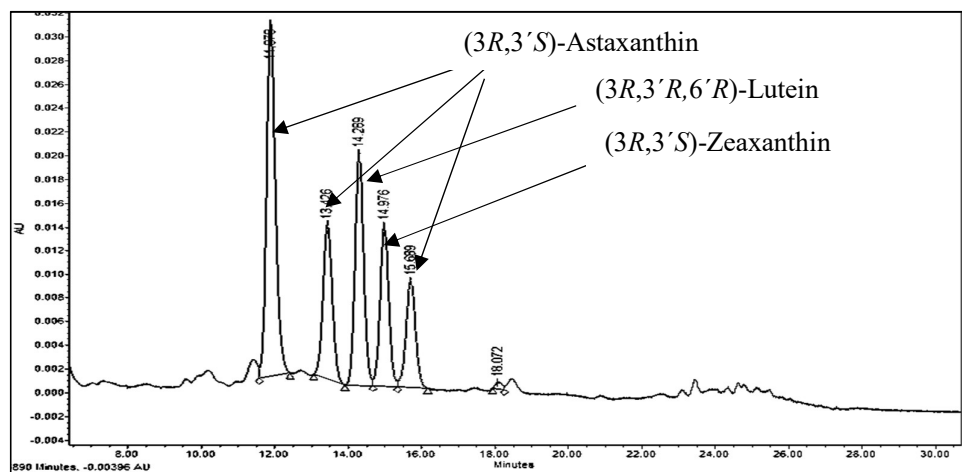


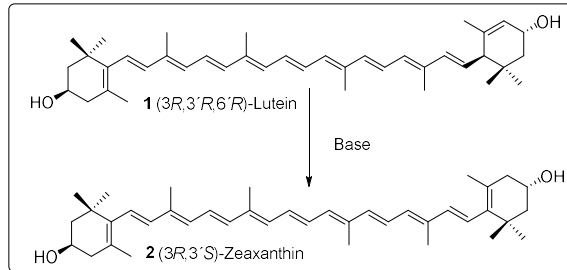
Figure S5. HPLC coelution of the obtained lutein, zeaxanthin and astaxanthin.

Table S2. Experimental UV λ_{\max} of the carotenoids.

Compound	λ_{\max} (nm)
Lutein	446 & 474
Lutein esters	446 & 474
Zeaxanthin	450 & 478
Astaxanthin	474

Implementation of the reaction conditions

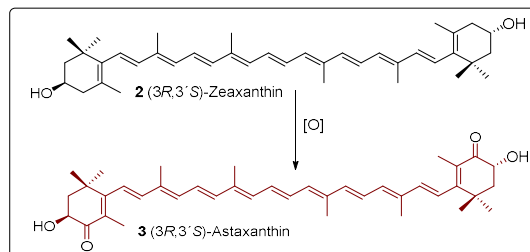
Table S3. Implementation of the reaction conditions for the conversion of 1 to 2.



Entry	Reaction time (Hours)	Solvent	Temperature (°C)	KOH (equivalents)	Yield (%)
1	8	No solvent	110	10	30
2	10	DMSO	110	10	75
3	12	Hexanes	Reflux	16	nr
4	14	Toluene	Reflux	12	nr
5	14	<i>n</i> -BuOH	115	10	92
6	16	<i>n</i> -BuOH	90	10	50
7	24	<i>n</i> -BuOH	rt	10	nr
8	12	<i>n</i> -BuOH	115	12	92

nr= no reaction

Table S4. Implementation of the reaction conditions for the conversion of 2 to 3.



Entry	I ₂ % mol	Solvent	Oxidant mixture Equivalents*	Reaction Time (Hours)	Yield (%)
1	20	CH ₂ Cl ₂	2:1	4	20
2	10	CH ₂ Cl ₂	1.5:1	4	10
3	10	CH ₂ Cl ₂	2:1	2	64
4	5	CH ₂ Cl ₂	1:1	2.5	5
5	2	CH ₂ Cl ₂	4:1	2.5	10
6	10	CH ₂ Cl ₂	2:1	4	42
7	10	acetone	2:1	6	nr
8	10	Water	2:1	6	nr

*Ratio between NaBrO₃ with Na₂S₂O₅, all reactions at 10 °C, nr= no reaction.

^1H and ^{13}C NMR spectra

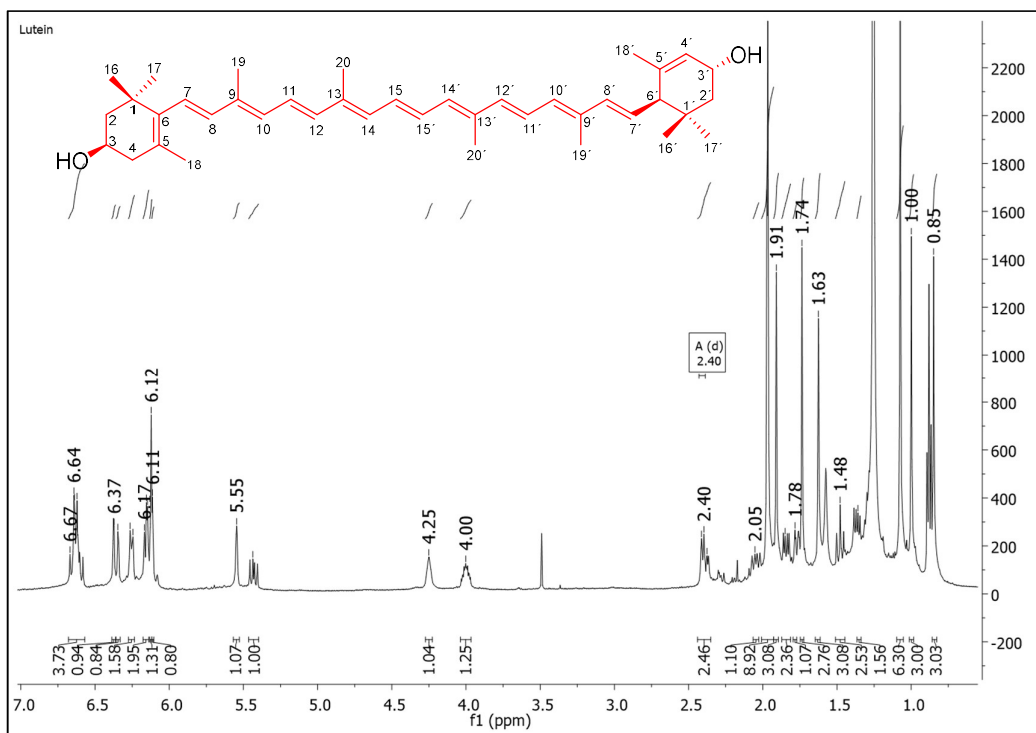


Figure S6. ^1H NMR spectrum of (3*R*,3'*R*,6'*R*)-lutein.

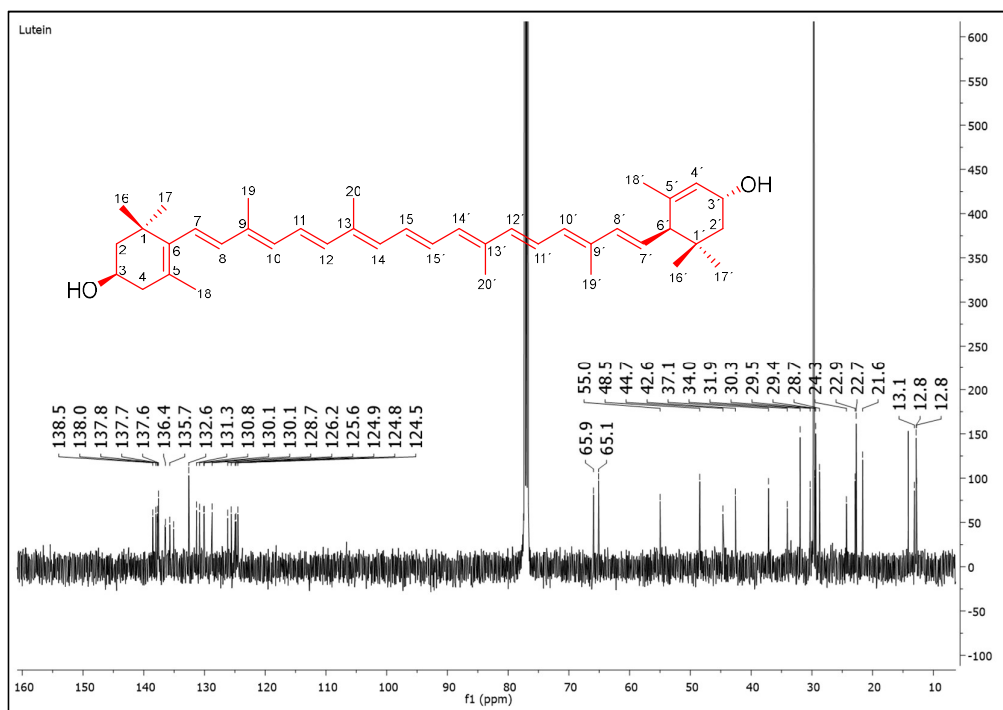


Figure S7. ^{13}C NMR spectrum of (3*R*,3'*R*,6'*R*)-lutein.

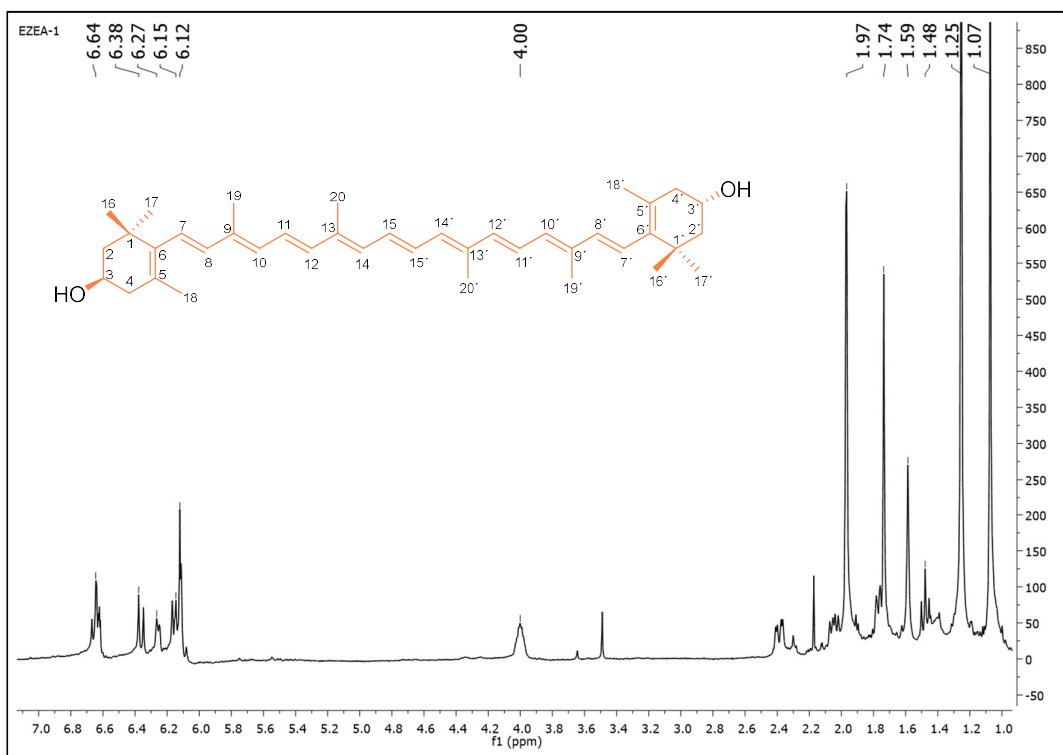


Figure S8. ^1H NMR spectrum of of $(3R,3'S)$ -zeaxanthin.

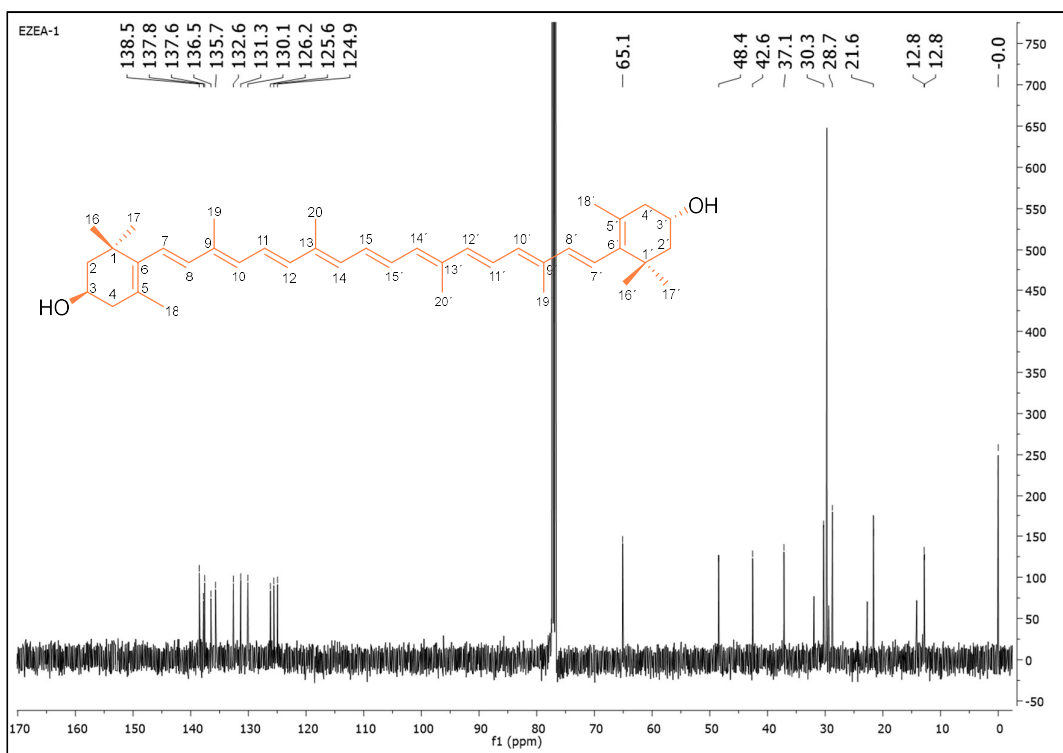


Figure S9. ^{13}C NMR spectrum of $(3R,3'S)$ -zeaxanthin.

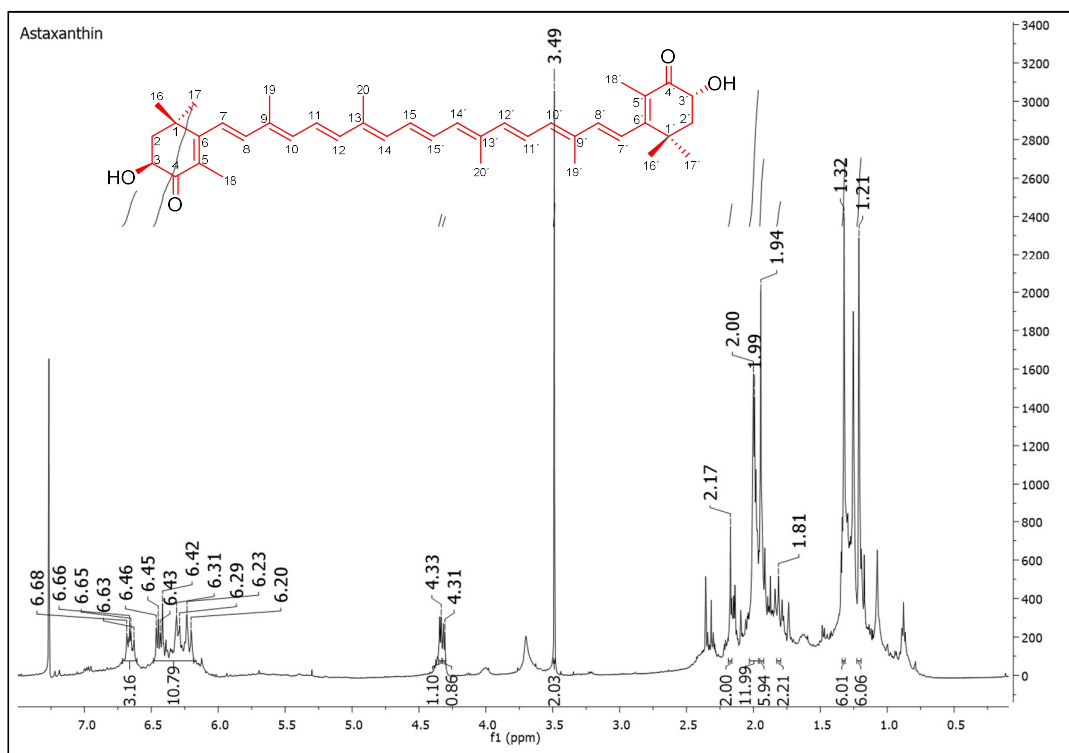


Figure S10. ¹H NMR spectrum of (3*R*,3'*S*)-astaxanthin.

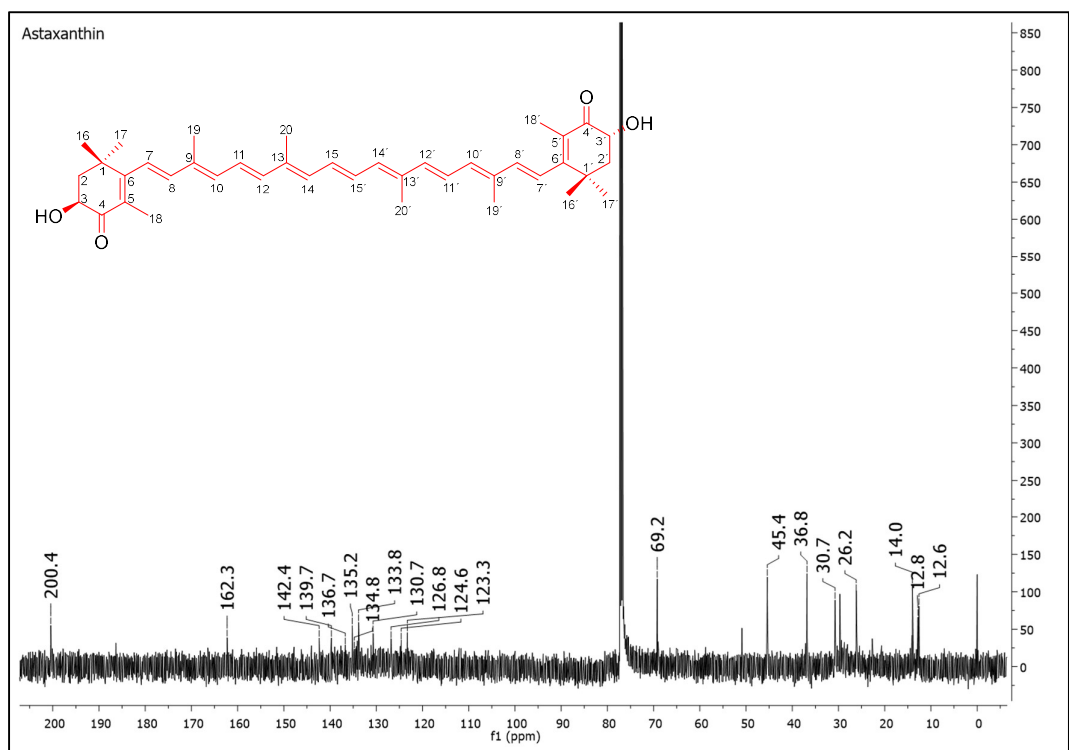


Figure S11. ¹³C NMR spectrum of (3*R*,3'*S*)-astaxanthin.

Calculated reaction mechanisms

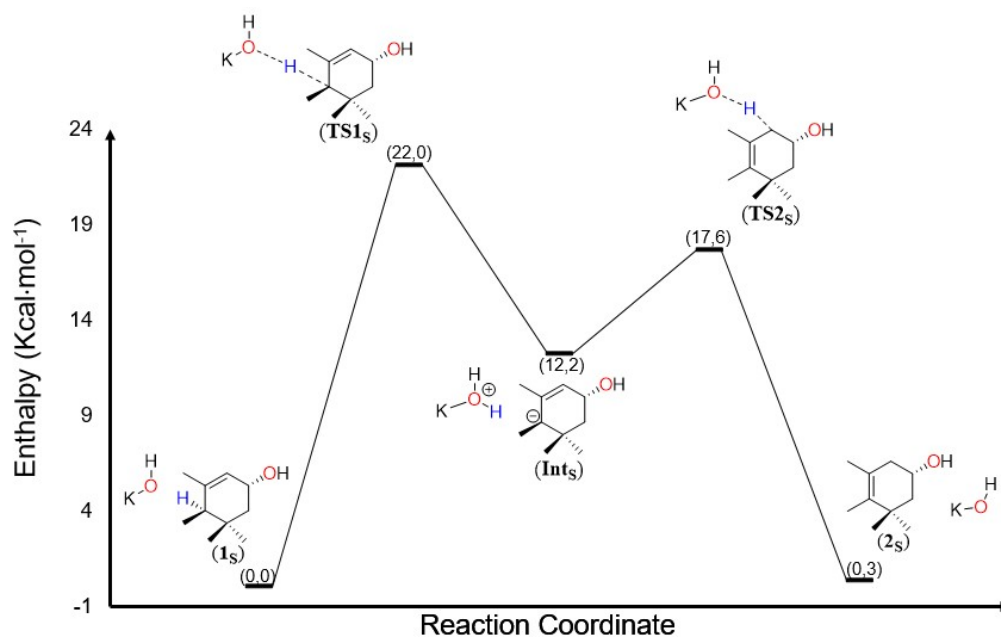


Figure S12. Energy profile for the conversion reaction of lutein (1) to zeaxanthin (2) calculated at the (PCM:*n*-butanol) M06-L/6-311+G(2d)//M06-L/6-31G(d) level, using sodium hydroxide as the base. Energy values are expressed as enthalpies in $\text{kcal}\cdot\text{mol}^{-1}$.

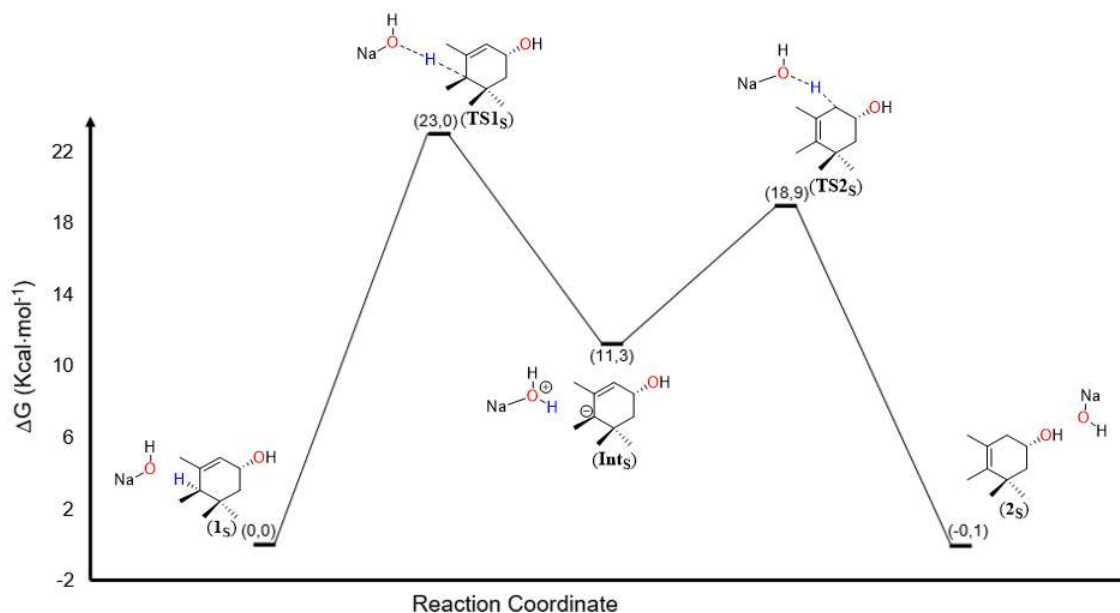


Figure S13. Energy profile for the conversion reaction of lutein (1) to zeaxanthin (2) calculated at the (PCM:*n*-butanol) M06-L/6-311+G(2d)//M06-L/6-31G(d) level, using sodium hydroxide as the base. Energy values are expressed as free energies in $\text{kcal}\cdot\text{mol}^{-1}$.

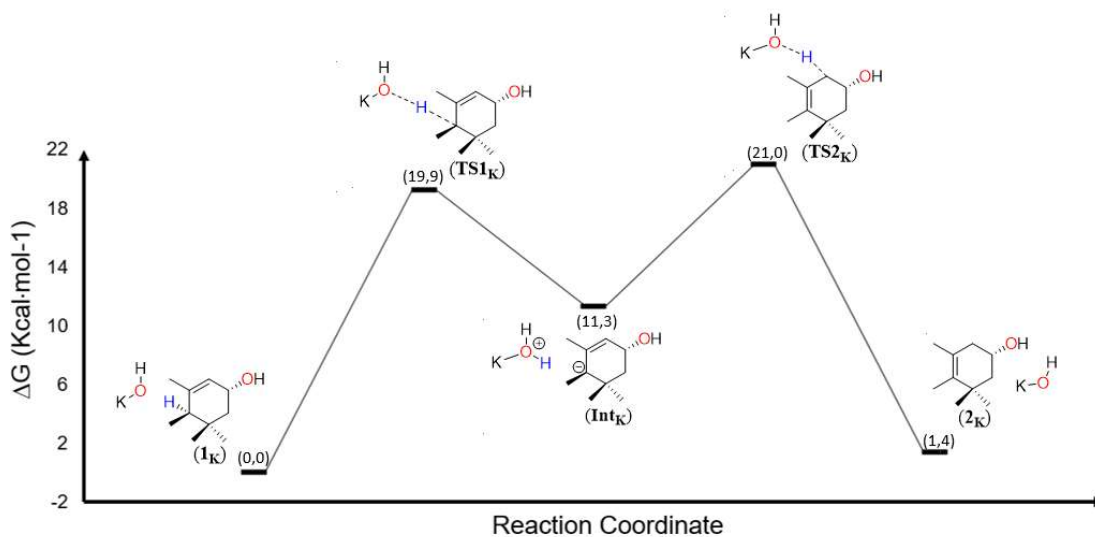


Figure S14. Energy profile for the conversion reaction of lutein (**1**) to zeaxanthin (**2**) calculated at the (PCM:*n*-butanol) M06-L/6-311+G(2d)//M06-L/6-31G(d) level, using potassium hydroxide as the base. Energy values are expressed as free energies in $\text{kcal}\cdot\text{mol}^{-1}$.

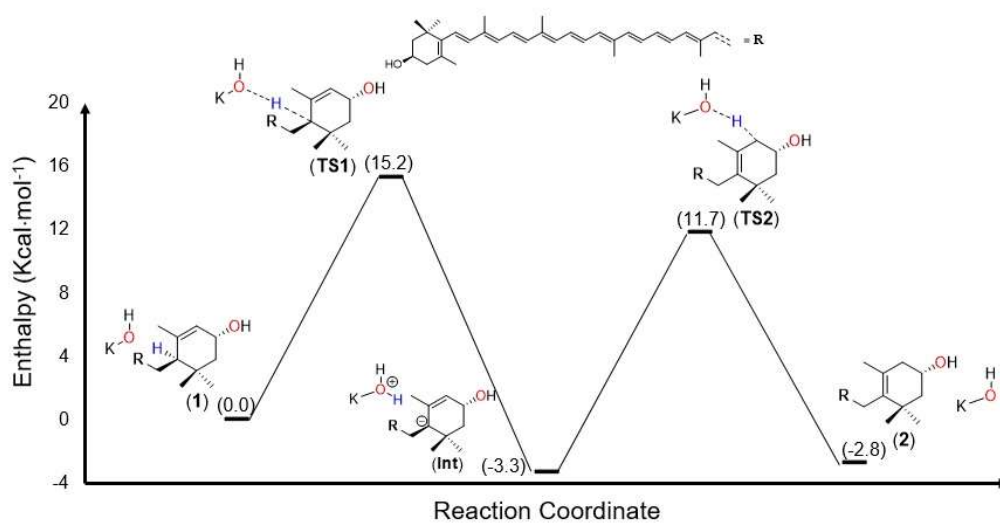


Figure S15. Energy profile for the conversion reaction of lutein (**1**) to zeaxanthin (**2**) calculated at the (PCM:*n*-butanol) M06-L/6-311+G(2d)//M06-L/6-31G(d) level, using potassium hydroxide as the base. Energy values are expressed as enthalpies in $\text{Kcal}\cdot\text{mol}^{-1}$. **Note:** The real system is shown here for comparison with Figure 2.

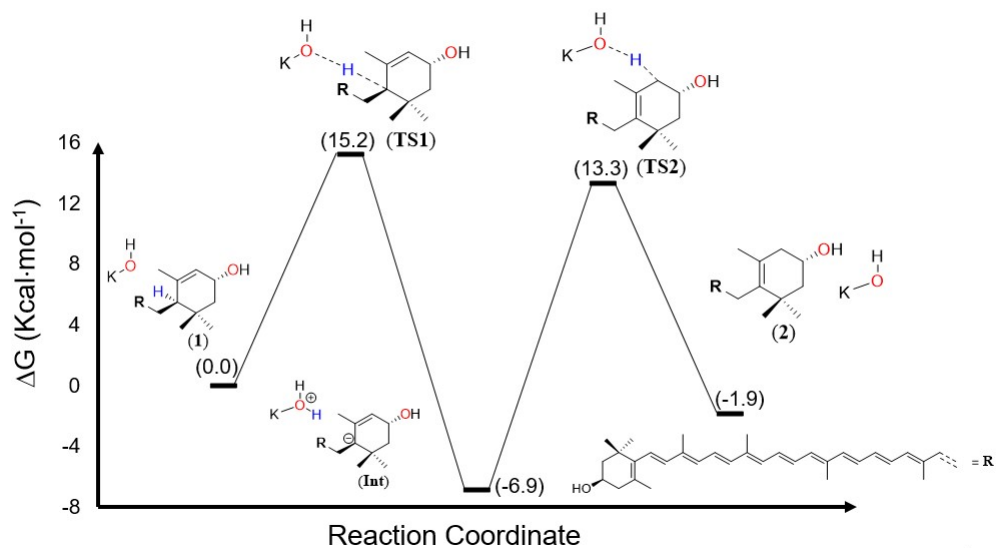


Figure S16. Energy profile for the conversion reaction from lutein (**1**) to zeaxanthin (**2**) with potassium hydroxide as base and calculated at the (PCM:*n*-butanol) M06-L/6-311+G(2d)/M06-L/6-31G(d) level. Energy values are expressed as free energies in Kcal·mol⁻¹. **Note:** The complete system is shown here for comparison with Figure S1.

Table S5. Cartesian coordinates (xyz) for the optimized geometries involved in the conversion reaction mechanism of lutein (**1**) to zeaxanthin (**2**), calculated at the (PCM:1-butanol)M06-L/6-311+G(2d)/M06-L/6-31G(d) level.

- With sodium hydroxide:

I_s				TS1_s			
E(scf) = -743.286248060 a.u.				E(scf) = -743.257407875 a.u.			
				v _{min} = -1188.20 cm ⁻¹			
C	-2.288121000	0.018338000	-0.4511860	C	-2.01612500	0.568590000	0.878233000
C	-0.9063280	0.301398000	-1.052594000	C	-0.85050500	1.134301000	0.046747000
C	0.015676000	0.861882000	0.060124000	C	0.348123000	0.162257000	0.171328000
C	-0.040749000	0.020098000	1.319115000	C	-0.05275300	-1.24722500	-0.086716000
C	-1.076681000	-0.787234000	1.59470400	C	-1.330865000	-1.673380000	-0.00260300
C	-2.28306900	-0.951620000	0.729551000	C	-2.470405000	-0.82780400	0.455634000
H	-2.72304400	0.975336000	-0.115291000	H	-1.68524300	0.527794000	1.931006000
H	-2.96796800	-0.366484000	-1.229960000	H	-2.88597300	1.249775000	0.851181000
H	-1.05667200	-1.391862000	2.508188000	H	-1.58405600	-2.695882000	-0.305312000
C	1.129218000	0.161997000	2.239446000	C	1.000768000	-2.189619000	-0.60559200
H	1.055356000	-0.49652600	3.113911000	H	0.626275000	-3.21767800	-0.697694000
H	2.064280000	-0.06100400	1.698676000	H	1.339926000	-1.861581000	-1.600994000
H	1.231568000	1.198690000	2.596167000	H	1.901034000	-2.21795800	0.025152000
C	-1.04618800	1.313497000	-2.187275000	C	-0.529727000	2.536334000	0.56024000
H	-1.544294000	2.233141000	-1.85402100	H	-0.36367300	2.555229000	1.645205000
H	-0.06228300	1.597084000	-2.58689200	H	0.368337000	2.946712000	0.075199000
H	-1.635465000	0.891232000	-3.01284000	H	-1.36274700	3.219619000	0.343302000
C	-0.28075800	-0.972317000	-1.625102000	C	-1.25351900	1.270084000	-1.427229000
H	-0.954426000	-1.44839800	-2.350678000	H	-2.172032000	1.864808000	-1.53535800
H	0.660486000	-0.73436600	-2.141432000	H	-0.45310900	1.766065000	-1.992360000
H	-0.065103000	-1.711053000	-0.84493700	H	-1.442398000	0.293243000	-1.88551800
C	-0.275326000	2.292762000	0.419892000	C	1.237611000	0.380187000	1.306875000
H	-1.30965200	2.517952000	0.713418000	H	1.498083000	1.433769000	1.479097000

C	0.634895000	3.267543000	0.446092000	C	1.874492000	-0.508526000	2.11206600
H	1.673493000	3.073612000	0.167423000	H	1.667736000	-1.578789000	2.08226400
H	0.388036000	4.287198000	0.740561000	H	2.579594000	-0.172581000	2.87199700
H	1.111036000	0.821773000	-0.32703200	H	1.257114000	0.504292000	-0.87036100
O	-2.32528300	-2.330999000	0.322629000	O	-3.443493000	-0.795606000	-0.60914200
H	-3.217072000	-0.73859500	1.367208000	H	-2.966180000	-1.331763000	1.36311500
H	-3.19893300	-2.455139000	-0.124273000	H	-4.232249000	-0.330005000	-0.23704600
O	3.526371000	0.017561000	-0.56629200	O	2.152121000	0.767931000	-1.682186000
H	3.438925000	0.462091000	0.296266000	H	1.899571000	0.238713000	-2.46057700
Na	3.273421000	-2.11865800	-0.51106800	Na	3.690764000	-0.054870000	-0.29141600

Ints

E(scf) = -743.274536505 a.u.

C	-2.334410000	0.591868000	0.61191700
C	-1.025215000	1.146533000	0.018076000
C	0.152322000	0.313854000	0.559538000
C	-0.100039000	-1.106738000	0.65366900
C	-1.337100000	-1.669540000	0.46829200
C	-2.589557000	-0.885537000	0.34140900
H	-2.298526000	0.741518000	1.71434800
H	-3.196594000	1.188976000	0.23896700
H	-1.428233000	-2.759651000	0.49403600
C	1.039160000	-2.049185000	0.93892900
H	0.737058000	-3.090856000	0.76601300
H	1.919065000	-1.836646000	0.31376000
H	1.385074000	-1.977383000	1.98047000
C	-0.962696000	2.628141000	0.39694200
H	-0.853449000	2.767000000	1.48194700
H	-0.132051000	3.154104000	-0.09308000
H	-1.888245000	3.133002000	0.08354900
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H	-1.980516000	1.553632000	-1.91775200
H	-0.202141000	1.570272000	-1.95699300
H	-1.088340000	0.026574000	-1.86083300
C	1.355379000	0.954766000	0.927461000
H	1.332690000	2.031557000	0.720392000
C	2.585079000	0.562035000	1.455728000
H	2.769390000	-0.421998000	1.89167400
H	3.273156000	1.351290000	1.775524000
H	1.272971000	-0.123971000	-1.25159500
O	-3.181065000	-1.120867000	-0.96386200
H	-3.350313000	-1.255235000	1.11694900
H	-4.046645000	-0.643948000	-0.95222200
O	1.905646000	-0.384785000	-1.95980900
H	1.571812000	-1.261895000	-2.24324400
Na	3.833604000	-0.129414000	-0.73092100

2s

E(scf) = -743.295128858 a.u.

C	0.734695000	-1.815980000	-0.90817600
C	1.456339000	-0.914457000	0.10695100
C	1.007874000	0.547727000	-0.02294300
C	-0.086915000	0.917578000	-0.73548400
C	-0.934702000	-0.070475000	-1.49486900
C	-0.737615000	-1.519885000	-1.10555200
H	1.219627000	-1.693001000	-1.90352000
H	0.882471000	-2.880935000	-0.61957100
H	-0.732423000	0.044551000	-2.57852200
C	-0.592304000	2.324387000	-0.86020600
H	-1.687625000	2.323599000	-0.73466000

TS2s

E(scf) = -743.257407875.u.

$v_{\min} = -1188.2010^{-1}$

C	-2.016125000	0.568590000	0.878233000
C	-0.850505000	1.134301000	0.046747000
C	0.348123000	0.162257000	0.171328000
C	-0.052753000	-1.247225000	-0.08671600
C	-1.330865000	-1.673380000	-0.00260300
C	-2.470405000	-0.827804000	0.45563400
H	-1.685243000	0.527794000	1.93100600
H	-2.885973000	1.249775000	0.851181000
H	-1.584056000	-2.695882000	-0.30531200
C	1.000768000	-2.189619000	-0.60559200
H	0.626275000	-3.217678000	-0.69769400
H	1.339926000	-1.861581000	-1.60099400
H	1.901034000	-2.217958000	0.02515200
C	-0.529727000	2.536334000	0.560240000
H	-0.363673000	2.555229000	1.64520500
H	0.368337000	2.946712000	0.075199000
H	-1.362747000	3.219619000	0.34330200
C	-1.253519000	1.270084000	-1.42722900
H	-2.172032000	1.864808000	-1.53535800
H	-0.453109000	1.766065000	-1.99236000
H	-1.442398000	0.293243000	-1.88551800
C	1.237611000	0.380187000	1.306875000
H	1.498083000	1.433769000	1.479097000
C	1.874492000	-0.508526000	2.112066000
H	1.667736000	-1.578789000	2.08226400
H	2.579594000	-0.172581000	2.87199700
H	1.257114000	0.504292000	-0.87036100
O	-3.443493000	-0.795606000	-0.60914200
H	-2.966180000	-1.331763000	1.36311500
H	-4.232249000	-0.330005000	-0.23704600
O	2.152121000	0.767931000	-1.68218600
H	1.899571000	0.238713000	-2.46577000
Na	3.690764000	-0.054870000	-0.29141600

H	-0.155118000	3.010633000	-0.12851500
H	-0.390632000	2.737547000	-1.86124200
C	1.864410000	1.500237000	0.698736000
H	2.234990000	1.151916000	1.672879000
C	2.302831000	2.692011000	0.272149000
H	2.042354000	3.089705000	-0.70862500
H	2.958681000	3.306332000	0.887715000
C	2.960263000	-1.021911000	-0.18682300
H	3.201641000	-0.613405000	-1.17781000
H	3.563117000	-0.482401000	0.55565200
H	3.273124000	-2.075732000	-0.16972400
C	1.229443000	-1.411323000	1.54558200
H	1.535076000	-2.464093000	1.63387700
H	1.826988000	-0.838070000	2.26735400
H	0.176165000	-1.340431000	1.841893000
H	-2.000836000	0.199463000	-1.36527900
H	-1.138353000	-2.176459000	-1.91088600
O	-1.514850000	-1.745488000	0.08770800
O	-3.823656000	0.949499000	0.39436600
H	-3.899150000	0.274757000	-0.30575100
Na	-2.195236000	0.006892000	1.49723400
H	-1.280351000	-2.649315000	0.42236700

- With potassium hydroxide:

I_k			TS1_k			
E(scf) = -1180.88449886 a.u.			E(scf) = -1180.86344412 a.u.			
C	-2.439383000	-0.272665000	v_{\min}	= -1333.3081	cm ⁻¹	
C	-1.235113000	0.276655000	C	2.295470000	-0.492942000	0.88491100
C	-0.264615000	0.957663000	C	1.126906000	-1.124172000	0.10882100
C	0.003088000	0.094973000	C	-0.090376000	-0.169986000	0.20681800
C	-0.809224000	-0.914736000	C	0.284774000	1.228784000	-0.14396400
C	-2.079436000	-1.273020000	C	1.556811000	1.679159000	-0.11791000
H	-2.974352000	0.575084000	C	2.719043000	0.882925000	0.371588000
H	-3.155120000	-0.741768000	H	1.981571000	-0.393975000	1.93920200
H	-0.554654000	-1.523864000	H	3.176085000	-1.160794000	0.884629000
C	1.214403000	0.463850000	H	1.787671000	2.682785000	-0.49349100
H	1.424615000	-0.268560000	C	-0.801766000	2.120452000	-0.68275100
H	2.094249000	0.568329000	H	-0.423294000	3.113981000	-0.95757400
H	1.081131000	1.447150000	H	-1.25069100	1.661639000	-1.578245000
C	-1.712554000	1.286612000	H	-1.624083000	2.268391000	0.03299100
H	-2.294030000	2.097955000	C	0.837627000	-2.500229000	0.70142600
H	-0.862718000	1.745639000	H	0.683268000	-2.461540000	1.787701000
H	-2.347700000	0.798203000	H	-0.060990000	-2.946636000	0.25089600
C	-0.51386700	-0.856161000	H	1.677968000	-3.182863000	0.511595000
H	-1.189787000	-1.345954000	C	1.504559000	-1.331836000	-1.36349400
H	0.345091000	-0.466612000	H	2.425662000	-1.925036000	-1.45708900
H	-0.171550000	-1.634783000	H	0.695478000	-1.859995000	-1.88457800
C	-0.736797000	2.308620000	H	1.678561000	-0.378159000	-1.87400800
H	-1.740907000	2.339885000	C	-0.928762000	-0.314098000	1.39713300
C	-0.014268000	3.428076000	H	-1.269530000	-1.365497000	1.63205200
H	0.990855000	3.430252000	C	-1.456320000	0.646337000	2.19849000
H	-0.388617000	4.379351000	H	-1.186792000	1.699630000	2.10419900
H	0.762600000	1.113171000	H	-2.147080000	0.395560000	3.00403500
O	-1.940519000	-2.620686000	H	-0.96083000	-0.601223000	-0.80894100
H	-2.926644000	-1.261931000	O	3.676469000	0.804187000	-0.70447100
H	-2.835299000	-2.884835000	H	3.218899000	1.447064000	1.239938000
O	3.329273000	0.859795000	H	4.475347000	0.366083000	-0.32090800
H	3.032108000	1.698767000	O	-1.786550000	-0.969014000	-1.68068200
K	2.743542000	-1.525134000	H	-1.361686000	-0.654317000	-2.49793800
			K	-3.627510000	0.045640000	-0.19998100
Int_k			TS2_k			
E(scf) = -1180.87785427 a.u.			E(scf) = -1180.86765647a.u.			
C	2.696351000	0.610310000	v_{\min}	= -1513.1702	cm ⁻¹	
C	1.341857000	1.152243000	C	-1.229004000	-1.829910000	0.61925000
C	0.211585000	0.338164000	C	-1.745727000	-0.551832000	-0.06255900
C	0.471357000	-1.075842000	C	-0.902912000	0.668861000	0.34718100
C	1.689194000	-1.651095000	C	0.186611000	0.518113000	1.185191000
C	2.927304000	-0.876429000	C	0.883849000	-0.742020000	1.38791900
H	2.755560000	0.797493000	C	0.285216000	-1.939564000	0.69567700
H	3.524138000	1.191772000	H	-1.600714000	-1.856483000	1.65764800
H	1.781690000	-2.739542000	H	-1.668834000	-2.708358000	0.11320100
C	-0.639332000	-2.004202000	H	1.121754000	-0.933897000	2.455107000
H	-0.340148000	-3.053206000	C	0.839098000	1.685072000	1.875566000
H	-1.557922000	-1.834243000	H	1.253257000	1.355926000	2.839622000
H	-0.917116000	-1.869321000	H	1.693159000	2.082937000	1.303249000
C	1.313451000	2.643738000	H	0.150241000	2.520150000	2.050382000
H	1.280258000	2.811427000	C	-1.355447000	1.938324000	-0.19194600
H	0.453822000	3.162875000	H	-2.38256700	1.928387000	-0.57791100
H	2.217705000	3.134350000	C	-0.699840000	3.109397000	-0.36929400
C	1.264225000	1.033630000	H	0.337478000	3.271417000	-0.08031800
H	2.123199000	1.520494000	H	-1.207171000	3.960695000	-0.82055900
H	0.347107000	1.512146000	C	-3.199778000	-0.36228900	0.405383000

H	1.260583000	-0.015408000	1.87954600	H	-3.244619000	-0.160468000	1.48347200
C	-0.966736000	0.995586000	-1.05800200	H	-3.705124000	0.461330000	-0.11415300
H	-0.953540000	2.066731000	-0.82331000	H	-3.782674000	-1.272932000	0.20763800
C	-2.150758000	0.628940000	-1.68411200	C	-1.785125000	-0.727820000	-1.58915800
H	-2.347890000	-0.357487000	-2.10677200	H	-2.435819000	-1.570358000	-1.86638000
H	-2.844209000	1.420857000	-1.98372300	H	-2.183503000	0.170959000	-2.07954100
H	-1.029886000	-0.232629000	1.05104400	H	-0.793534000	-0.935905000	-2.00583100
O	3.416788000	-1.152858000	1.11675700	H	2.139290000	-0.531376000	0.89724900
H	3.747338000	-1.222629000	-0.94766600	H	0.550796000	-2.864086000	1.24445500
H	4.280245000	-0.677167000	1.18552500	O	0.865050000	-2.031724000	-0.63657900
O	-1.640850000	-0.560950000	1.74866900	O	3.303380000	-0.282440000	0.37390200
H	-1.194688000	-1.373768000	2.06286000	H	3.551838000	-1.182975000	0.097105000
K	-3.986565000	-0.068554000	0.57441300	H	0.377628000	-2.753572000	-1.10734000
				K	1.622107000	0.470206000	-1.54815500

2_k

E(scf) = -1180.89235949 a.u.

C	-1.251753000	-1.747781000	0.91526300
C	-1.795545000	-0.734692000	-0.10536500
C	-1.125070000	0.636972000	0.052926000
C	0.001380000	0.818022000	0.789135000
C	0.664130000	-0.299775000	1.552644000
C	0.246455000	-1.694568000	1.138235000
H	-1.730375000	-1.553638000	1.90211900
H	-1.565951000	-2.772042000	0.61245100
H	0.454267000	-0.165315000	2.63260300
C	0.743170000	2.115394000	0.91907500
H	1.825236000	1.916568000	0.81324500
H	0.435759000	2.864449000	0.18197900
H	0.599914000	2.562321000	1.91613600
C	-1.797003000	1.717977000	-0.68286100
H	-2.211592000	1.432962000	-1.65982000
C	-2.029175000	2.971572000	-0.27002900
H	-1.715197000	3.328688000	0.71068200
H	-2.563775000	3.683037000	-0.89853600
C	-3.305507000	-0.606928000	0.14370200
H	-3.510709000	-0.186414000	1.13795700
H	-3.789086000	0.039435000	-0.60095300
H	-3.783518000	-1.595781000	0.08975400
C	-1.602702000	-1.247628000	-1.54320000
H	-2.072672000	-2.235402000	-1.65874200
H	-2.072629000	-0.577420000	-2.27567900
H	-0.541738000	-1.346601000	-1.79715100
H	1.761326000	-0.194354000	1.44929900
H	0.522084000	-2.415541000	1.94188000
O	0.993884000	-2.022964000	-0.04713400
O	3.774373000	0.658529000	0.501475000
H	3.592124000	0.930174000	1.416309000
H	0.638211000	-2.883963000	-0.38399800
K	2.373262000	-0.078266000	-1.40112700

- With potassium hydroxide (Real system):

I			TS1					
E(scf) = -2383.87582120 a.u.			E(scf) = -2383.85609406 a.u.					
C	-13.55839700	0.72053600	0.92315900	$v_{\min} = -1670.2610\text{cm}^{-1}$	C	-13.78647100	0.80383700	0.68569400
C	-14.62653200	-0.271854000	1.39764100	C	-14.87162500	-0.12715100	1.2409470	
C	-15.19212000	-1.10692300	0.26857500	C	-15.33625500	-1.15250700	0.2287040	
C	-14.08312000	-1.93101500	-0.34890100	C	-14.17052900	-2.03494300	-0.1592490	
C	-12.80779500	-1.17116000	-0.59182300	C	-12.89842300	-1.2852610	-0.4478410	
C	-12.54061400	0.02231000	0.00682700	C	-12.69507500	-0.00145100	-0.0404110	
H	-14.18123000	-0.96383500	2.14885100	H	-14.47430600	-0.67339100	2.1269620	
H	-15.44026900	0.28710900	1.91257000	H	-15.73060700	0.48555900	1.59634200	
H	-13.87353000	-2.78702800	0.32778300	H	-13.99409100	-2.75497400	0.6683220	
H	-14.42732100	-2.38983400	-1.2940680	H	-14.4382040	-2.65979400	-1.0312560	
C	-12.86412500	1.28175300	2.17117900	C	-13.18921900	1.57427300	1.87042400	
H	-12.15381200	2.08277100	1.92717200	H	-12.46643900	2.33618100	1.54923400	
H	-13.61235000	1.69983200	2.85959800	H	-13.98780200	2.08644100	2.42603200	
H	-12.31446900	0.49594100	2.70738100	H	-12.67552200	0.89661100	2.56621700	
C	-14.21384900	1.88776500	0.16919600	C	-14.40651000	1.81849900	-0.2874540	
H	-14.91508200	2.42109000	0.82733500	H	-15.16106200	2.43036700	0.22790700	
H	-13.46539000	2.61638800	-0.17206200	H	-13.64844300	2.50321200	-0.6922600	
H	-14.76853500	1.54398800	-0.71301100	H	-14.89310300	1.32202200	-1.1368930	
C	-11.88038900	-1.85206300	-1.55326800	H	-11.89647300	-2.08327000	-1.2280540	
H	-11.28975100	-2.64228800	-1.0625020	C	-11.28166800	-2.7261260	-0.5777020	
H	-12.45464300	-2.35036400	-2.3474020	H	-12.4090360	-2.75800800	-1.9282260	
H	-11.16716200	-1.16363900	-2.0201340	H	-11.2030190	-1.453034000	-1.796793	
C	-11.30594900	0.77110200	-0.1905480	C	-11.4705410	0.74754700	-0.2903270	
H	-11.41884200	1.86104000	-0.18247000	H	-11.61103000	1.82381000	-0.4386620	
C	-10.03925300	0.28378400	-0.27021300	C	-10.18738200	0.29500700	-0.2650430	
H	-9.88220800	-0.79595400	-0.18936100	H	-10.00131100	-0.7574410	-0.0316310	
C	-8.84379400	1.07745800	-0.39352200	C	-9.01113000	1.09882400	-0.46867700	
C	-7.62900600	0.4346690	-0.39008400	C	-7.77814800	0.4974650	-0.36472200	
H	-7.65439200	-0.65855200	-0.30826600	H	-7.77789900	-0.5754500	-0.1363150	
C	-6.33514900	1.01759700	-0.46525100	C	-6.4981990	1.09466500	-0.51032900	
H	-6.25977900	2.10575300	-0.54426700	H	-6.44747200	2.16293100	-0.7388930	
C	-5.17748300	0.28463900	-0.43091300	C	-5.32244700	0.39987900	-0.37184000	
H	-5.26547600	-0.80520200	-0.35057300	H	-5.38956300	-0.67050500	-0.1421110	
C	-8.97859500	2.56583900	-0.49799500	C	-9.18159800	2.55693900	-0.77000800	
H	-9.60698900	2.84739100	-1.35536400	H	-9.78614100	2.70970400	-1.67615500	
H	-9.47277700	2.98182600	0.39316400	H	-9.71667700	3.06990600	0.04372700	
H	-8.01477000	3.07210000	-0.60977300	H	-8.22733400	3.07305200	-0.91543000	
C	-3.84997900	0.81060000	-0.47940100	C	-4.00729700	0.93684600	-0.49063500	
C	-2.78855400	-0.06963900	-0.42031100	C	-2.92589100	0.09382500	-0.31031800	
H	-3.04162600	-1.13393200	-0.34532200	H	-3.16131300	-0.95413500	-0.0874520	
C	-1.40704500	0.23616500	-0.43667500	C	-1.55213400	0.4140940	-0.37113500	
H	-1.09909300	1.28470800	-0.50749800	H	-1.25952200	1.44692800	-0.5874380	
C	-0.41530700	-0.71273900	-0.35890100	C	-0.54365100	-0.50465600	-0.1677430	
H	-0.72189900	-1.76163100	-0.28631400	H	-0.8430790	-1.53609500	0.0481050	
C	-3.67007600	2.29532500	-0.58610900	C	-3.8522120	2.39609000	-0.8016110	
H	-4.13249600	2.68443400	-1.50510100	H	-4.31950800	2.65013300	-1.76468700	
H	-4.16197600	2.81458300	0.24914600	H	-4.35188800	3.01886800	-0.0449080	
H	-2.61810400	2.59641600	-0.59071400	H	-2.80449800	2.70912900	-0.84934100	
C	0.96573400	-0.40330100	-0.36128800	C	0.83118000	-0.19389400	-0.2140800	
H	1.21603200	0.66149800	-0.43803400	H	1.07836600	0.85251200	-0.42960000	
C	2.02902900	-1.27761800	-0.26930300	C	1.90461900	-1.04759400	-0.01358800	
C	3.35499200	-0.74282200	-0.27603600	C	3.22514100	-0.52552200	-0.08963300	
H	3.43795800	0.34623000	-0.37106400	H	3.31279300	0.54446300	-0.31252400	
C	4.51468600	-1.46214300	-0.16515500	C	4.39017200	-1.23604000	0.09832300	
H	4.44756400	-2.54914600	-0.06176300	H	4.30754100	-2.30349500	0.3245320	
C	1.85452500	-2.76205500	-0.15368900					

H	2.28706600	-3.13930000	0.78462300	C	1.72279500	-2.50661400	0.2880880
H	0.80470400	-3.06956300	-0.18274700	H	2.15263600	-2.76654700	1.26644900
H	2.37885200	-3.28587300	-0.96600100	H	0.67158000	-2.81030200	0.29701500
C	5.80548500	-0.86245700	-0.16881200	H	2.24329200	-3.13150000	-0.45201200
H	5.82392100	0.22787100	-0.28558200	C	5.68190500	-0.66989000	0.01970700
C	7.02128700	-1.48236600	-0.03133800	H	5.72149600	0.40162600	-0.21078900
C	8.21392300	-0.66772000	-0.05243600	C	6.90112400	-1.29991900	0.20430300
H	8.06941400	0.41132900	-0.20953900	C	8.10216000	-0.53272800	0.10689100
C	9.48234900	-1.10142000	0.11438600	H	7.96928800	0.52899800	-0.13356900
C	7.17545100	-2.96085800	0.14741200	C	9.37188200	-0.9995500	0.33609800
H	7.64717900	-3.19336400	1.11396900	C	7.0022670	-2.76276600	0.5239400
H	6.22307300	-3.49884500	0.10293700	H	7.5101030	-2.92245500	1.48674600
H	7.83822900	-3.38192800	-0.62317600	H	6.0267800	-3.25561100	0.5794500
O	-16.19478500	-2.01671300	0.71852400	H	7.60309300	-3.29316600	-0.22873200
H	-16.92356800	-1.46317500	1.09472600	O	-16.35781100	-2.00218400	0.7492600
H	-15.62065800	-0.43287900	-0.5129610	H	-17.12071800	-1.41374300	0.9737510
C	12.56753500	-1.78476200	-0.24930500	H	-15.71314700	-0.6300990	-0.6843490
C	11.79328300	-0.61345900	-0.86675000	C	11.26482800	0.7029900	2.36872600
C	10.671049000	-0.18668200	0.11541100	C	11.61753500	-0.4186700	1.37763400
C	11.18622700	-0.03197800	1.53384800	C	10.6332110	-0.29858400	0.17827000
C	12.32913400	-0.600499000	1.94781700	C	10.54968800	1.09738200	-0.35093300
C	13.19800400	-1.47840500	1.10822800	C	10.95702400	2.16762400	3.605110
H	11.87241500	-2.63374500	-0.12884900	C	11.3794710	2.11334700	1.79035300
H	13.35224900	-2.12987800	-0.94380900	H	10.22390200	0.5424300	2.69934900
H	12.672366000	-0.42516000	2.97362400	H	11.89604300	0.6332270	3.27217700
C	10.32318900	0.78384200	2.44477500	H	10.97085500	3.15801400	-0.10882600
H	10.82958300	1.02758100	3.38732300	C	10.08832800	1.2652510	-1.7736800
H	10.00080800	1.70987100	1.94026200	H	10.28840900	2.27758400	-2.14950200
H	9.39291700	0.24728700	2.69107200	H	10.59464700	0.53397300	-2.42139600
C	11.19564500	-1.04821800	-2.20308700	H	9.0127400	1.0752220	-1.89403500
H	10.57060700	-1.94491600	-2.09959800	C	11.50254100	-1.76417300	2.0905200
H	10.56557500	-0.25531400	-2.63100200	H	10.53030500	-1.89262200	2.58342700
H	11.98974200	-1.27404200	-2.92831700	H	11.6381470	-2.60056100	1.38961400
C	12.71379500	0.58181300	-1.12193800	H	12.27887400	-1.8499190	2.86312300
H	13.57073100	0.29332000	-1.74594000	C	13.06861200	-0.27399500	0.90772900
H	12.16574800	1.37556600	-1.65014700	H	13.75556900	-0.25914700	1.76504900
H	13.11279500	0.99651900	-0.19001600	H	13.34689100	-1.11626000	0.26088800
O	14.48118800	-0.83711400	0.99857800	H	13.21996700	0.66836500	0.36926400
H	15.07928900	-1.49950600	0.57226200	O	12.715460	2.64787200	1.87354500
O	8.74160900	2.84339000	0.1337150	H	12.91445000	2.72854400	2.8389250
H	8.34562300	2.23977700	0.78383100	O	11.93187000	-1.51695700	-1.7967680
H	10.27337300	0.85381700	-0.20618400	H	11.19046700	-1.7112240	-2.39905200
K	10.61129300	4.30155300	-0.47890800	H	11.24636400	-0.96089300	-0.7942000
H	9.67803600	-2.16676300	0.29648600	K	13.63402600	0.30796200	-2.44309400
H	13.34454300	-2.47463500	1.66513200	H	9.4585900	-2.04759800	0.64383300
				H	10.6889280	2.80193400	2.40151200

Int

E(scf) = -2383.88980483 a.u.

C	13.75578300	0.10640400	-0.5825390
C	14.77327800	-1.02108700	-0.36522200
C	15.01547600	-1.31521000	1.09987000
C	13.72378900	-1.78340900	1.73094800
C	12.53259700	-0.93074100	1.38260500
C	12.51749500	-0.08961600	0.30981100
H	14.40197100	-1.95480900	-0.8467800
H	15.72814800	-0.75331000	-0.87135100
H	13.54449100	-2.83152300	1.40868100
H	13.8341600	-1.83504100	2.82979300
C	13.36088700	0.09155600	-2.06472100
H	12.71212200	0.93653800	-2.33003200

TS2

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C	-13.27344500	-0.38955200	0.07664100
C	-11.98683300	-1.1786590	0.3788130
C	-10.77398000	-0.58230000	-0.3627420
C	-10.94184100	0.52058000	-1.1947490
C	-12.04713800	1.44698900	-1.0717410
C	-13.08020200	1.11375100	-0.0239840
H	-13.6853090	-0.72577700	-0.9009260
H	-14.03976900	-0.64396300	0.8437500
H	-12.48775400	1.72934400	-2.043750
C	-9.93617200	0.91930300	-2.23676200
H	-9.27347300	1.72041200	-1.86990500

H	14.2605800	0.15193200	-2.69416100	H	-9.30353500	0.0893120	-2.5702980
H	12.82881100	-0.83407800	-2.32464500	H	-10.45789100	1.34083400	-3.1087560
C	14.40237100	1.46554900	-0.27032000	C	-12.22563500	-2.61840500	-0.1091590
H	15.26278800	1.64084000	-0.93249800	H	-12.34763200	-2.6512060	-1.2003860
H	13.69476500	2.29206800	-0.42388700	H	-11.40373900	-3.29459700	0.1615950
H	14.75547400	1.51946600	0.76754600	H	-13.14188100	-3.02300800	0.3453070
C	11.38511800	-1.0903520	2.33557400	C	-11.7352200	-1.24735000	1.89350600
H	10.75481400	-1.9607410	2.0908200	H	-12.59004900	-1.71543700	2.4043830
H	11.75835300	-1.26246400	3.35565700	H	-10.84468700	-1.85155700	2.1181190
H	10.72367500	-0.21615300	2.34915500	H	-11.59348100	-0.25287200	2.3327100
C	11.3722800	0.73049000	-0.06599900	H	-11.45601800	2.59081900	-0.7619150
H	11.61991800	1.6999940	-0.5125300	H	-14.05064700	1.59290400	-0.2844930
C	10.05206100	0.3934950	-0.01515600	O	-12.62905200	1.66579800	1.24039400
H	9.78291100	-0.6075970	0.33610600	O	-10.76434000	3.68191800	-0.4128250
C	8.94782700	1.21548500	-0.42036600	H	-10.28909000	3.86073200	-1.2435680
C	7.67175000	0.69888600	-0.3311980	H	-13.24203500	1.31640500	1.93482200
H	7.59942600	-0.32814600	0.05010400	C	-9.53529700	-1.27528800	-0.1789580
C	6.43615900	1.30864300	-0.65524200	C	-8.24581600	-0.82470600	-0.3625360
H	6.43969700	2.33413600	-1.03632900	H	-8.07934300	0.20576900	-0.6880040
C	5.22295400	0.66686500	-0.50534000	C	-7.06149100	-1.58239200	-0.1245770
H	5.24996700	-0.36048400	-0.11963200	C	-5.83128600	-0.96794700	-0.2944360
C	9.23062200	2.59932300	-0.92228700	H	-5.85528900	0.08182000	-0.61155100
H	9.77246300	3.19561700	-0.17218500	C	-4.5462260	-1.52217400	-0.10641700
H	9.87646900	2.57837600	-1.81434800	H	-4.47309600	-2.57014900	0.19936100
H	8.31944300	3.14623300	-1.18709600	C	-3.37826000	-0.8134900	-0.28346600
C	3.93838600	1.18784500	-0.79313900	H	-3.46484200	0.23761300	-0.58354100
C	2.82080500	0.38788400	-0.56832400	C	-7.18592500	-3.01353600	0.30817800
H	3.03055000	-0.61584600	-0.17568600	H	-7.72870000	-3.09458700	1.26177100
C	1.46566400	0.68363100	-0.76973700	H	-7.76068900	-3.60143400	-0.4217000
H	1.18589100	1.66894400	-1.15823800	H	-6.21536400	-3.50177400	0.43917900
C	0.43900400	-0.21616900	-0.49362900	C	-2.05765300	-1.3102590	-0.1093580
H	0.74769200	-1.19318700	-0.10377600	C	-0.98910300	-0.45053700	-0.3082890
C	3.82746100	2.58637200	-1.32726500	H	-1.24221700	0.57790800	-0.5924880
H	4.25187600	3.32175500	-0.62653900	C	0.38714800	-0.73230500	-0.18300700
H	4.38828300	2.70443400	-2.26710900	H	0.69499600	-1.74661100	0.09367000
H	2.79047300	2.87939600	-1.52370900	C	1.38458300	0.19865200	-0.38439100
C	-0.92416500	0.03070200	-0.66654400	H	1.07959000	1.21473200	-0.65629900
H	-1.19271900	1.02092900	-1.05509400	C	-1.87157600	-2.74439500	0.29089100
C	-2.00034100	-0.82829700	-0.3915710	H	-2.32464000	-2.94483000	1.27296800
C	-3.31542900	-0.39111600	-0.6090040	H	-2.36660000	-3.42170000	-0.4197750
H	-3.43781000	0.62500000	-1.00309900	H	-0.81801400	-3.03501400	0.34759600
C	-4.48098500	-1.12279700	-0.3568580	C	2.76125500	-0.08757500	-0.25665200
H	-4.35703900	-2.13433000	0.04202500	H	3.01067600	-1.12125800	0.01224000
C	-1.77326600	-2.21452900	0.14744200	C	3.82974000	0.77353500	-0.42788600
H	-2.26910200	-2.97144300	-0.4766270	C	5.15102900	0.26832900	-0.25050500
H	-0.71308400	-2.47976700	0.20265700	H	5.23203600	-0.79370600	0.01088300
H	-2.19370500	-2.32662900	1.15774800	C	6.31669900	0.98164300	-0.37713400
C	-5.77282800	-0.65379900	-0.5631990	H	6.25380400	2.04266100	-0.63465200
H	-5.86268800	0.36725900	-0.95542300	C	3.65517200	2.21812600	-0.79132300
C	-6.99598500	-1.31913700	-0.3169690	H	2.60537300	2.49632100	-0.92772100
C	-8.19810200	-0.65087700	-0.5564120	H	4.07638700	2.87687700	-0.01734100
H	-8.09772800	0.35987800	-0.94757300	H	4.18797200	2.46078200	-1.72259100
C	-9.47827300	-1.21940300	-0.3461040	C	7.60268500	0.40818600	-0.19452500
C	-7.00730300	-2.72789600	0.21322900	H	7.61457500	-0.65976700	0.05526100
H	-7.60196500	-3.39268800	-0.4292640	C	8.82830000	1.02448500	-0.29790700
H	-6.00381500	-3.15817400	0.28621300	C	10.01239200	0.23685700	-0.07793300
H	-7.46151400	-2.7814800	1.21328400	H	9.83567000	-0.81308800	0.17317500
O	15.98518300	-2.34455100	1.29200300	C	11.29191100	0.6984010	-0.11740300
H	16.82420700	-2.01383400	0.88553300	H	11.42419100	1.77288400	-0.28353900
H	15.35141000	-0.38251400	1.61574100	C	8.98254200	2.47895400	-0.62346500

C	-13.14172200	-1.38007300	-1.0359450	H	8.02239700	2.98385900	-0.76937000
C	-11.92868300	-1.72756400	-0.1575200	H	9.51867800	3.00859000	0.17864000
C	-10.77733000	-0.75272200	-0.4647360	H	9.579339000	2.62322600	-1.5360830
C	-11.16757600	0.6232400	-0.7317930	C	12.52009000	-0.04342100	0.1390490
C	-12.47076300	0.99610800	-0.8787750	C	13.61293200	0.77718200	0.84333200
C	-13.62093700	0.05864400	-0.9337140	C	13.97208600	-2.09492800	0.08857200
H	-12.86544300	-1.5769980	-2.0963280	C	14.74416800	-0.11936800	1.37321300
H	-13.98109200	-2.0694270	-0.7953780	C	15.17387600	-1.23582200	0.44781900
H	-12.69773100	2.0601200	-1.0004450	H	15.61629700	0.51697700	1.6394000
C	-10.13531200	1.71478700	-0.8164410	H	14.40043600	-0.59971400	2.31608200
H	-10.62112200	2.70022900	-0.8374700	C	14.16077900	1.83816700	-0.12534100
H	-9.43731500	1.68708700	0.03154800	H	13.37628200	2.54453100	-0.43051400
H	-9.52171900	1.63524700	-1.7250320	H	14.95293600	2.42237400	0.36497800
C	-11.58186500	-3.19096200	-0.4519040	H	14.58442800	1.37811000	-1.02298400
H	-11.18825400	-3.3169940	-1.4701340	C	13.02110200	1.50908100	2.05734000
H	-10.84389800	-3.60438200	0.2480640	H	12.26527200	2.24958700	1.76305900
H	-12.48690300	-3.8078310	-0.3603950	H	12.54851600	0.80527800	2.75660700
C	-12.29625200	-1.62275900	1.3310080	H	13.81555200	2.04116700	2.60048600
H	-13.15743100	-2.26512400	1.5695080	C	12.71660300	-1.33527900	-0.2430990
H	-11.45029200	-1.94258700	1.9572530	H	13.75762800	-2.78784900	0.92906300
H	-12.56701600	-0.59819300	1.6081460	C	11.71881900	-2.14193500	-1.0199200
O	-14.45808400	0.30502400	0.2167030	H	11.10618800	-2.78555200	-0.3680340
H	-15.26393300	-0.25423200	0.0870400	H	11.02402500	-1.52000900	-1.5957940
O	-10.78810600	1.42585600	2.4364410	H	12.23777000	-2.81864300	-1.7140550
H	-11.55468600	1.36273100	1.8269210	H	14.23676700	-2.75619000	-0.7586140
K	-9.55809300	3.81027800	2.1981170	H	-9.62460400	-2.28288000	0.24083500
H	-9.42028200	-2.26170900	-0.0279230	K	-9.93609700	2.07637000	1.46336400
H	-10.25852800	0.63737700	2.1932120	O	15.77955700	-0.66390200	-0.7145440
H	-14.24011500	0.29584700	-1.8725130	H	16.03068300	-1.42176900	-1.2984500
				H	15.92356200	-1.87201900	0.97493500

2

E(scf) = -2383.88567346 a.u.

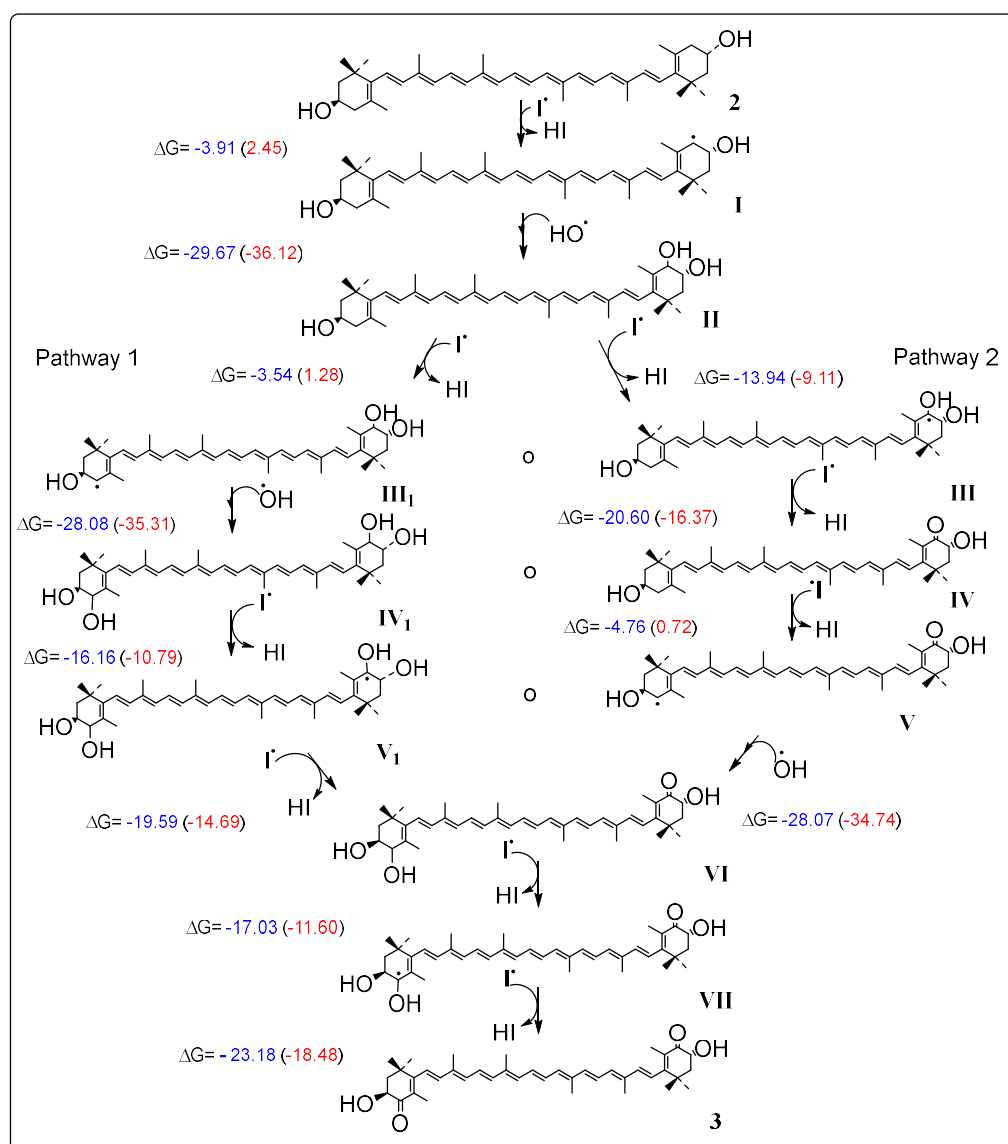
C	-13.29884700	-0.36503000	0.0722740
C	-12.01503000	-1.17088700	0.3426670
C	-10.80820700	-0.59958800	-0.4202900
C	-10.91086800	0.51565000	-1.1989300
C	-12.12136800	1.40552800	-1.1845070
C	-13.09466500	1.13058500	-0.0589810
H	-13.74979200	-0.7121390	-0.8848640
H	-14.04208300	-0.59304700	0.8684770
H	-12.64941900	1.34232400	-2.1561930
C	-9.85777400	1.03082700	-2.1271690
H	-9.38602700	1.92958600	-1.6805360
H	-9.08938700	0.29371600	-2.3812090
H	-10.33491000	1.37427300	-3.0590330
C	-12.29450100	-2.60882000	-0.1275890
H	-12.4150780	-2.65494300	-1.2186070
H	-11.50077900	-3.31081400	0.1594090
H	-13.22694500	-2.97064600	0.3289840
C	-11.71116900	-1.22598700	1.8480500
H	-12.55312800	-1.67713900	2.3930070
H	-10.81969300	-1.83752000	2.0475160
H	-11.5398040	-0.22632700	2.2655140
H	-11.75280400	2.45092800	-1.1142570
H	-14.06977900	1.62031600	-0.2830910
O	-12.54726800	1.71860000	1.1350190
O	-9.48402000	3.77416000	-0.4308020
H	-9.92706800	3.92154400	-1.2832340
H	-13.13804100	1.44798100	1.8831490
C	-9.57391600	-1.35659800	-0.2605660

C	-8.30029800	-0.87311900	-0.2524750
H	-8.13477700	0.20138900	-0.3828530
C	-7.10667600	-1.65573200	-0.0727100
C	-5.89275500	-1.00957800	-0.1073940
H	-5.92183100	0.07577800	-0.2630430
C	-4.59791400	-1.58005400	0.0117050
H	-4.51733800	-2.66041600	0.1625720
C	-3.44421000	-0.84337800	-0.0701050
H	-3.54015300	0.23777100	-0.2253070
C	-7.23747200	-3.13450400	0.1286680
H	-7.84943500	-3.36064900	1.0146770
H	-7.74693900	-3.60831300	-0.7232150
H	-6.27079700	-3.63126400	0.2573920
C	-2.11374100	-1.35376200	0.0167140
C	-1.05954800	-0.47020400	-0.1054120
H	-1.32191400	0.58309700	-0.2607500
C	0.32383000	-0.76073600	-0.0619360
H	0.64178400	-1.79737500	0.0920590
C	1.30634100	0.19118300	-0.2074600
H	0.98809100	1.22744900	-0.3632580
C	-1.92023200	-2.82541700	0.22891600
H	-2.37941900	-3.15337000	1.17291700
H	-2.40675100	-3.40617600	-0.5681370
H	-0.86531700	-3.11508900	0.25424200
C	2.68995200	-0.09939000	-0.16978500
H	2.95319700	-1.15166400	-0.00902600
C	3.74304100	0.78218800	-0.31210200
C	5.07463800	0.27139100	-0.24027100
H	5.17197800	-0.80718100	-0.06877000
C	6.22674400	1.00377500	-0.36365500
H	6.14418900	2.08062200	-0.53714100
C	3.54787000	2.25145500	-0.53826600
H	2.49303500	2.54220200	-0.55040000
H	4.04778600	2.84078200	0.24405600
H	3.99228200	2.56779600	-1.49325600
C	7.52426400	0.43294900	-0.27057800
H	7.55623300	-0.64804600	-0.08872000
C	8.73685400	1.07263300	-0.37486700
C	9.93662800	0.29109400	-0.22330900
H	9.78088500	-0.77255000	-0.02139500
C	11.20629300	0.77768900	-0.25813900
H	11.31699700	1.86137600	-0.37488300
C	8.86297300	2.54445200	-0.62376900
H	7.89341800	3.0403380	-0.73235400
H	9.40099600	3.03971100	0.1986490
H	9.44567000	2.74494800	-1.5346590
C	12.45232200	0.0520350	-0.0528630
C	13.53965000	0.86244300	0.6730000
C	13.97097100	-1.94089100	-0.2524490
C	14.64862100	-0.05749400	1.19967900
C	15.12992400	-1.05183200	0.16452200
H	15.49841000	0.56143500	1.56215800
H	14.26353400	-0.62794500	2.07773000
C	14.13051300	1.89960000	-0.29414300
H	13.35471100	2.57356300	-0.68323000
H	14.87864600	2.51972300	0.22048800
H	14.61734100	1.42235500	-1.15447200
C	12.94734000	1.60609900	1.87723800
H	12.21398600	2.36645300	1.57735500
H	12.44834300	0.91179400	2.5673790

H	13.74714200	2.11681800	2.43213100
C	12.67726800	-1.21379200	-0.5028080
H	13.80622500	-2.69573900	0.54780200
C	11.68331300	-2.01193100	-1.2930470
H	11.09363800	-2.68736800	-0.6526240
H	10.96715200	-1.38363100	-1.8352660
H	12.20219800	-2.65407900	-2.0185710
O	16.24231600	-1.81977600	0.62141000
H	15.51431700	-0.50991600	-0.7271350
H	15.93164700	-2.29504700	1.43347500
H	14.24540800	-2.53024900	-1.1468610
H	-9.69378500	-2.42336400	-0.0479190
K	-9.86606400	2.16552400	1.41741900

Table S6. Oxidation reaction mechanism enthalpy and free energy values (Scheme S1).

Pathway 1	ΔH	ΔG	Pathway 2	ΔH	ΔG
I	2,45	-3,91	I	2,45	-3,91
II	-36,12	-29,67	II	-36,12	-29,67
III₁	1,28	-3,54	III	-9,11	-13,94
IV₁	-35,31	-28,08	IV	-16,37	-20,60
V₁	-10,79	-16,16	V	0,72	-4,76
VI₁	-14,69	-19,59	VI	-34,75	-28,07
VII	-11,60	-17,03	VII	-11,60	-17,03
3	-18,48	-23,18	3	-18,48	-23,18
Total =	-123,26	-141,16	Total =	-123,26	-141,16



Scheme S1. Possible pathways for the allylic oxidation of 2 to 3.

Table S7. Cartesian coordinates (xyz) for the optimized geometries involved in the oxidation reaction mechanism calculated at the (PCM:1-butanol)M06-L/6-311+G(2d)//M06-L/6-31G(d) level.

2			I				
E(scf) = -1708.05727324 a.u.			E(scf) = -1707.43842737a.u.				
C	14.065214000	-0.457466000	0.520507000	C	13.876730000	0.098320000	-1.02193900
C	12.78997600	0.354519000	0.796002000	C	12.954400000	0.800519000	-0.01266300
C	11.67304100	0.004001000	-0.195403000	C	11.652642000	-0.004086000	0.06951600
C	11.78000400	-1.032307000	-1.068227000	C	11.826628000	-1.447943000	0.20246000
C	12.95014600	-1.973330000	-1.081155000	C	13.014566000	-2.036528000	-0.08166800
C	13.83242200	-1.909352000	0.146241000	C	14.192274000	-1.350388000	-0.67622400
H	14.61454900	0.008322000	-0.312911000	H	13.393952000	0.131202000	-2.01084600
H	14.73196600	-0.382906000	1.395057000	H	14.816713000	0.663985000	-1.11743200
H	13.56073900	-1.784514000	-1.980270000	C	10.727278000	-2.324502000	0.73534200
C	10.78866500	-1.334764000	-2.149322000	H	10.168532000	-1.838533000	1.54332000
H	10.12728200	-2.171486000	-1.879010000	H	9.998707000	-2.596855000	-0.03943200
H	10.15230300	-0.480955000	-2.399883000	H	11.142972000	-3.262119000	1.12022000
H	11.31514600	-1.653158000	-3.060989000	C	12.761357000	2.236998000	-0.49946500
C	13.18545000	1.835104000	0.679111000	H	12.212921000	2.280003000	-1.44931800
H	13.42021600	2.109364000	-0.357352000	H	12.227943000	2.858930000	0.22974400
H	12.40349400	2.511417000	1.042889000	H	13.741629000	2.704884000	-0.65609100
H	14.07941900	2.028373000	1.287001000	C	13.608116000	0.852763000	1.37788600
C	12.28158200	0.109827000	2.224908000	H	14.578205000	1.365929000	1.32669500
H	13.06378300	0.344762000	2.961344000	H	12.968223000	1.408792000	2.07537900
H	11.41780400	0.750911000	2.442719000	H	13.785876000	-0.145255000	1.78743700
H	11.97040200	-0.929969000	2.361738000	H	13.143072000	-3.099595000	0.12708900
H	12.58297800	-3.004618000	-1.195753000	H	14.468487000	-1.882031000	-1.60780100
H	14.80516100	-2.38129800	-0.085371000	O	15.270736000	-1.486388000	0.25615800
O	13.17744400	-2.65648600	1.167228000	H	16.064607000	-1.148976000	-0.18280900
H	13.68368200	-2.53208300	1.982581000	C	10.446942000	0.663403000	0.09673100
C	10.48956600	0.84953900	-0.107928000	C	9.112682000	0.190038000	0.06330300
C	9.19572100	0.44880900	-0.215161000	H	8.919754000	-0.871825000	-0.06823000
H	8.99059200	-0.61187900	-0.375668000	C	7.989114000	1.006013000	0.13637600
C	8.03944900	1.29490100	-0.097344000	C	6.714306000	0.403680000	0.03554700
C	6.79523200	0.72104500	-0.189438000	H	6.715687000	-0.681567000	-0.10634800
H	6.77054100	-0.36123400	-0.349412000	C	5.470798000	1.012654000	0.09568700
C	5.52796300	1.35372500	-0.102582000	H	5.418857000	2.092163000	0.24681900
H	5.49628300	2.43376300	0.050656000	C	4.263349000	0.318931000	-0.02640100
C	4.34241500	0.67542600	-0.200411000	H	4.324414000	-0.761325000	-0.18689600
H	4.39161300	-0.40732100	-0.349248000	C	8.137341000	2.490167000	0.31740500
C	8.24643200	2.76060100	0.127775000	H	8.713201000	2.729203000	1.22002600
H	8.78849700	2.94339400	1.066166000	H	8.673187000	2.944031000	-0.52663300
H	8.85597700	3.20235200	-0.671751000	H	7.175972000	3.002768000	0.40078300
H	7.30867300	3.31981700	0.176678000	C	2.980938000	0.877331000	0.04027300
C	3.03498100	1.24066800	-0.123723000	C	1.870370000	0.035422000	-0.11016600
C	1.94571100	0.40210500	-0.231914000	H	2.093734000	-1.021055000	-0.28765000
H	2.16588000	-0.66033000	-0.374217000	C	0.519794000	0.377945000	-0.06133200
C	0.57442100	0.73861000	-0.179964000	H	0.241548000	1.417544000	0.12722600
H	0.29186400	1.78473000	-0.040020000	C	-0.519172000	-0.528739000	-0.23697800
C	-0.43819000	-0.18284000	-0.292095000	H	-0.245469000	-1.567932000	-0.43366700
H	-0.14829000	-1.22716600	-0.429693000	C	2.831306000	2.353349000	0.27001900
C	2.90344900	2.72012400	0.074262000	H	3.273017000	2.655252000	1.22853500
H	3.36934700	3.03715900	1.016942000	H	3.345974000	2.929945000	-0.50935500
H	3.41280700	3.27249700	-0.726467000	H	1.787794000	2.677009000	0.27545700
H	1.86341200	3.05482300	0.093130000	C	-1.872891000	-0.180228000	-0.17681600
C	-1.81311100	0.13762500	-0.237813000	H	-2.086785000	0.872149000	0.03397900
H	-2.05020100	1.19724600	-0.102352000	C	-2.980871000	-1.003631000	-0.35084800
C	-2.88655700	-0.72331400	-0.330381000	C	-4.273757000	-0.436719000	-0.23491900
C	-4.20757800	-0.19052700	-0.246175000	H	-4.316738000	0.630997000	-0.00010700

H	-4.286796000	0.89265200	-0.11521500	C	-5.471300000	-1.099691000	-0.38513400
C	-5.36994400	-0.91159000	-0.30912400	H	-5.445163000	-2.163579000	-0.62613300
H	-5.29698000	-1.99266200	-0.43701600	C	-2.853960000	-2.465610000	-0.65623300
C	-2.72487900	-2.20219000	-0.51306600	H	-1.814919000	-2.801319000	-0.69788800
H	-1.67885900	-2.51559500	-0.54456000	H	-3.366583000	-3.074477000	0.10018200
H	-3.20915400	-2.75589700	0.30216500	H	-3.316761000	-2.711244000	-1.62147100
H	-3.19882000	-2.54042900	-1.444201000	C	-6.729755000	-0.473585000	-0.23953100
C	-6.66319100	-0.33579200	-0.209908000	H	-6.702303000	0.591257000	0.01158700
H	-6.69049000	0.75103100	-0.085244000	C	-7.980904000	-1.037106000	-0.36874800
C	-7.87615600	-0.97846100	-0.244818000	C	-9.132041000	-0.207473000	-0.15369600
C	-9.07714000	-0.19782200	-0.109040000	H	-8.921333000	0.829320000	0.11622300
H	-8.9321000	0.87786100	0.011484000	C	-10.428051000	-0.619258000	-0.20684800
C	-10.34024800	-0.696248000	-0.07250600	H	-10.599897000	-1.682980000	-0.39122300
H	-10.44189300	-1.784088000	-0.10186800	C	-8.189437000	-2.480128000	-0.70960000
C	-8.00691400	-2.461618000	-0.40630500	H	-7.251665000	-3.019289000	-0.86557500
H	-7.04381900	-2.963194000	-0.527637000	H	-8.739360000	-2.999105000	0.08787400
H	-8.5049700	-2.912312000	0.463660000	H	-8.790239000	-2.590633000	-1.62204900
H	-8.62367900	-2.712610000	-1.279352000	C	-11.625121000	0.162259000	0.06512500
C	-11.5876200	0.032806000	0.112352000	C	-12.733829000	-0.622567000	0.78175300
C	-12.6148410	-0.702735000	0.984399000	C	-13.000479000	2.261041000	0.04006500
C	-13.1267240	1.984890000	-0.218261000	C	-13.823891000	0.311917000	1.32908300
C	-13.78157500	0.214878000	1.382770000	C	-14.226563000	1.438600000	0.40480800
C	-14.27885200	1.130907000	0.287701000	H	-14.707490000	-0.282854000	1.59993700
H	-14.61100800	-0.398914000	1.761002000	H	-13.460420000	0.773798000	2.25962600
H	-13.46241100	0.857018000	2.217991000	C	-13.339828000	-1.656138000	-0.18096000
C	-13.13816800	-1.942342000	0.240747000	H	-12.589157000	-2.388204000	-0.50517100
H	-12.33370500	-2.661553000	0.040726000	H	-14.138850000	-2.216076000	0.32339500
H	-13.88571300	-2.460595000	0.856470000	H	-13.768840000	-1.177583000	-1.06414200
H	-13.61065600	-1.670377000	-0.705803000	C	-12.149703000	-1.374024000	1.98665400
C	-11.95213700	-1.169959000	2.288181000	H	-11.424248000	-2.138041000	1.68218100
H	-11.16582100	-1.912553000	2.106819000	H	-11.640182000	-0.689931000	2.67735100
H	-11.49669600	-0.330604000	2.829229000	H	-12.950832000	-1.880515000	2.54170100
H	-12.69890800	-1.632262000	2.947868000	C	-11.776886000	1.460419000	-0.31065200
C	-11.84474600	1.237297000	-0.462586000	H	-12.761322000	2.940041000	0.87792700
H	-12.94316500	2.801361000	0.502658000	C	-10.762490000	2.229717000	-1.10078200
C	-10.90276300	1.944542000	-1.388167000	H	-10.135792000	2.871821000	-0.46269400
H	-10.33498800	2.737362000	-0.877076000	H	-10.086764000	1.581189000	-1.66676800
H	-10.17259100	1.271211000	-1.847371000	H	-11.263106000	2.905698000	-1.80776600
H	-11.46093900	2.445596000	-2.191394000	H	-13.247664000	2.937830000	-0.79496300
H	-13.43093200	2.503072000	-1.143403000	H	10.523023000	1.749667000	0.10670400
H	10.66437900	1.898799000	0.140190000	O	-14.848825000	0.869512000	-0.74115800
O	-14.84083000	0.325565000	-0.741496000	H	-15.051575000	1.594373000	-1.34805600
H	-15.08150600	0.914644000	-1.469368000	H	-14.949863000	2.089287000	0.93054700
H	-15.05964000	1.794638000	0.704035000				

II

E(scf) = -1783.25802236 a.u.

C	13.751843000	-0.253161000	0.47745200
C	12.489284000	0.579604000	0.74091600
C	11.326391000	0.130101000	-0.15073600
C	11.400531000	-0.965515000	-0.95117900
C	12.575921000	-1.901413000	-0.93766600
C	13.495253000	-1.728422000	0.26198600
H	14.239559000	0.109940000	-0.43920300
H	14.471358000	-0.090580000	1.29595900
C	10.373704000	-1.356264000	-1.96853000
H	9.713917000	-2.159580000	-1.60694800
H	9.735564000	-0.520060000	-2.26849000
H	10.881789000	-1.744491000	-2.86021500
C	12.864806000	2.040207000	0.44431300

III₁

E(scf) = -1782.64060457a.u.

C	13.776713000	-0.159677000	0.3163750
C	12.511186000	0.673853000	0.5649990
C	11.312609000	0.119289000	-0.2141070
C	11.370478000	-1.048251000	-0.9089170
C	12.568576000	-1.955302000	-0.8707620
C	13.542090000	-1.652853000	0.2582680
H	14.207843000	0.119640000	-0.6562430
H	14.533195000	0.094936000	1.0757220
C	10.303624000	-1.556905000	-1.8281370
H	9.680092000	-2.329450000	-1.3530420
H	9.633217000	-0.766950000	-2.1790290
H	10.775637000	-2.026416000	-2.7003250
C	12.840560000	2.104232000	0.1081230
H	12.967879000	2.158594000	-0.9802290

H	13.054851000	2.195922000	-0.62502100	H	12.072722000	2.829742000	0.4004600
H	12.091308000	2.748975000	0.76176300	H	13.780028000	2.432118000	0.5726440
H	13.780884000	2.303824000	0.98954100	C	12.160587000	0.718614000	2.0596010
C	12.057765000	0.485245000	2.21217500	H	13.008291000	1.102317000	2.6452250
H	12.880972000	0.781919000	2.87800200	H	11.306968000	1.385213000	2.2374900
H	11.212064000	1.155554000	2.41212600	H	11.892437000	-0.273480000	2.4351200
H	11.744173000	-0.530998000	2.46935400	H	14.498147000	-2.160176000	0.0219210
H	14.453560000	-2.231397000	0.02541400	O	12.983616000	-2.206196000	1.4417700
O	12.868052000	-2.380133000	1.35775100	H	13.53358700	-1.915036000	2.18230900
H	13.374710000	-2.159123000	2.15146400	C	10.113015000	0.940592000	-0.1499340
C	10.135441000	0.965724000	-0.06972300	C	8.824316000	0.503482000	-0.1069310
C	8.846264000	0.537859000	-0.09703500	H	8.637727000	-0.572102000	-0.1014600
H	8.655473000	-0.534501000	-0.17542500	C	7.660110000	1.337711000	-0.0407530
C	7.679357000	1.371737000	-0.00225500	C	6.421845000	0.734901000	0.0199420
C	6.444580000	0.771275000	-0.01344400	H	6.416714000	-0.359397000	0.0282740
H	6.436672000	-0.320675000	-0.08365100	C	5.151781000	1.352315000	0.0595920
C	5.167784000	1.387714000	0.04602300	H	5.100934000	2.442208000	0.0361500
H	5.118098000	2.476491000	0.10103800	C	3.969335000	0.648060000	0.1148490
C	3.993397000	0.683567000	0.03079400	H	4.035353000	-0.443558000	0.1428400
H	4.059313000	-0.407261000	-0.01892700	C	7.841586000	2.823782000	-0.0486110
C	7.866302000	2.853683000	0.09806700	H	8.437450000	3.152141000	0.8143130
H	8.450330000	3.118548000	0.99038000	H	8.386949000	3.151912000	-0.9434180
H	8.426052000	3.241329000	-0.76356900	H	6.894629000	3.368521000	-0.0187150
H	6.920612000	3.398946000	0.15195400	C	2.665896000	1.201879000	0.1304830
C	2.677903000	1.233904000	0.07007600	C	1.574509000	0.340037000	0.1841050
C	1.600778000	0.372993000	0.05506700	H	1.809805000	-0.727942000	0.2244360
H	1.836205000	-0.695001000	0.02031300	C	0.214666000	0.667514000	0.1859300
C	0.225327000	0.694649000	0.07672300	H	-0.079866000	1.718358000	0.1357210
H	-0.070404000	1.746000000	0.10171200	C	-0.807469000	-0.273288000	0.2436210
C	-0.777030000	-0.244338000	0.06416300	H	-0.510466000	-1.323182000	0.3004950
H	-0.477398000	-1.294619000	0.04222800	C	2.510981000	2.691906000	0.0786340
C	2.526180000	2.723519000	0.12557900	H	3.031036000	3.174506000	0.9166090
H	2.998249000	3.135705000	1.02760700	H	2.949395000	3.104371000	-0.8399460
H	3.018059000	3.204016000	-0.73055700	H	1.466828000	3.011671000	0.1155620
H	1.481734000	3.044477000	0.12669500	C	-2.163397000	0.049030000	0.2256320
C	-2.154410000	0.069238000	0.07411000	H	-2.404452000	1.114166000	0.1556340
H	-2.398859000	1.135607000	0.08855800	C	-3.260607000	-0.821780000	0.2799640
C	-3.223100000	-0.802290000	0.06224900	C	-4.550987000	-0.281637000	0.2236520
C	-4.546024000	-0.267737000	0.06015900	H	-4.628251000	0.805502000	0.1321640
H	-4.627998000	0.823121000	0.06928300	C	-5.748609000	-1.001724000	0.2670060
C	-5.707964000	-0.992066000	0.04189000	H	-5.682243000	-2.086234000	0.3686870
H	-5.636165000	-2.080934000	0.03323800	C	-3.088825000	-2.308584000	0.3957770
C	-3.055342000	-2.291303000	0.04579000	H	-2.040429000	-2.615954000	0.3862480
H	-2.008157000	-2.602315000	0.05977300	H	-3.531009000	-2.688130000	1.3262680
H	-3.547333000	-2.754169000	0.91160300	H	-3.590119000	-2.833106000	-0.4275670
H	-3.518196000	-2.731783000	-0.84748900	C	-6.998788000	-0.410371000	0.1793390
C	-6.999302000	-0.403531000	0.02647600	H	-7.011384000	0.678019000	0.0646780
H	-7.020126000	0.690583000	0.02978900	C	-8.267662000	-1.033385000	0.2077190
C	-8.216866000	-1.037556000	0.00031200	C	-9.395823000	-0.233977000	0.0625020
C	-9.411066000	-0.235931000	-0.02397400	H	-9.207575000	0.830316000	-0.0541290
H	-9.255090000	0.844573000	-0.00355800	C	-10.728406000	-0.711262000	0.1012570
C	-10.682870000	-0.713679000	-0.03074200	H	-10.804848000	-1.771226000	0.3402110
H	-10.804102000	-1.797594000	0.03995600	C	-8.401875000	-2.519438000	0.3820160
C	-8.360472000	-2.527748000	-0.00223500	H	-7.436312000	-3.018625000	0.4938930
H	-7.399964000	-3.048864000	0.00630800	H	-8.996273000	-2.764812000	1.2716480
H	-8.928996000	-2.869220000	0.87404700	H	-8.911373000	-2.981114000	-0.4730920
H	-8.917671000	-2.870834000	-0.88408400	C	-11.934163000	-0.063722000	-0.0634920
C	-11.926582000	0.043880000	-0.02091400	C	-13.240881000	-0.833939000	0.1562400
C	-13.041211000	-0.601885000	0.81442800	C	-13.295031000	1.944527000	-0.4021450
C	-13.393892000	1.978205000	-0.65302700	C	-14.200963000	0.067358000	0.9510110

C	-14.213236000	0.367659000	1.04032000	C	-14.495015000	1.400529000	0.2938820
C	-14.601344000	1.192930000	-0.16548000	H	-15.153246000	-0.454709000	1.1148200
H	-15.083905000	-0.195924000	1.40339000	H	-13.761594000	0.251395000	1.9421980
H	-13.941702000	1.073723000	1.83971900	C	-13.841270000	-1.203597000	-1.2099510
C	-13.529280000	-1.886215000	0.12457300	H	-13.179889000	-1.904541000	-1.7359430
H	-12.726336000	-2.630920000	0.05089900	H	-14.820083000	-1.683561000	-1.0825240
H	-14.338481000	-2.342575000	0.71043900	H	-13.990669000	-0.324404000	-1.8421270
H	-13.912666000	-1.681304000	-0.87748600	C	-13.068919000	-2.121914000	0.9611490
C	-12.502448000	-0.978683000	2.20199300	H	-12.513102000	-2.890466000	0.4103310
H	-11.720922000	-1.746133000	2.14375200	H	-12.553486000	-1.945658000	1.9140590
H	-12.074671000	-0.108443000	2.71636600	H	-14.055531000	-2.546271000	1.1859410
H	-13.312183000	-1.377579000	2.82797700	C	-12.101039000	1.312157000	-0.5257970
C	-12.111353000	1.195410000	-0.71884300	C	-10.989738000	2.051914000	-1.2182620
H	-13.250971000	2.857450000	-0.00003800	H	-10.273336000	2.487836000	-0.5101590
C	-11.081581000	1.807296000	-1.61918400	H	-10.419637000	1.402941000	-1.8930330
H	-10.531759000	2.624920000	-1.12805800	H	-11.395694000	2.883530000	-1.8052070
H	-10.337712000	1.083926000	-1.96691600	H	-13.393468000	2.948938000	-0.8247750
H	-11.562737000	2.255678000	-2.99607000	H	10.273259000	2.016992000	-0.0626170
H	-13.611334000	2.409052000	-1.64492100	O	-15.595039000	1.208825000	-0.6093130
H	10.303891000	2.031719000	0.09679900	H	-15.654826000	2.001678000	-1.1606460
O	-15.104230000	0.310384000	-1.16141800	H	-14.810944000	2.120452000	1.0732090
H	-15.295878000	0.841317000	-1.94634300	O	13.227114000	-1.845263000	-2.1356530
H	-15.394682000	1.904542000	0.12956900	H	13.823288000	-2.603776000	-2.2122180
O	13.301511000	-1.693902000	-2.15286800	H	12.201170000	-2.989141000	-0.7264710
H	13.882446000	-2.459020000	-2.27049300				
H	12.181255000	-2.934724000	-0.90775400				

IV₁

E(scf) = -1858.45883268 a.u.

C	13.981261000	-0.096850000	1.00384000
C	12.706879000	0.758837000	0.94772300
C	11.650215000	0.132602000	0.03000600
C	11.816280000	-1.084226000	-0.55142100
C	12.975427000	-1.983915000	-0.22841000
C	13.731021000	-1.588263000	1.03100300
H	14.587184000	0.095440000	0.10624800
H	14.592739000	0.219639000	1.86392100
C	10.913969000	-1.664485000	-1.59557800
H	10.216595000	-2.406770000	-1.17822900
H	10.315642000	-0.904532000	-2.10702500
H	11.521704000	-2.190097000	-2.34295400
C	13.133257000	2.136900000	0.41720900
H	13.454586000	2.081264000	-0.63015300
H	12.335586000	2.884852000	0.49147900
H	13.978674000	2.513679000	1.00820100
C	12.106102000	0.949178000	2.34856200
H	12.850543000	1.375193000	3.03621500
H	11.253222000	1.639223000	2.31505000
H	11.747517000	0.000243000	2.75856600
H	14.703291000	-2.119106000	1.02104200
O	12.950543000	-2.031190000	2.13240900
H	13.355022000	-1.673430000	2.93499700
C	10.454412000	0.944351000	-0.15172400
C	9.174800000	0.497786000	-0.25089100
H	8.991173000	-0.577704000	-0.21077800
C	8.002893000	1.324276000	-0.34862300
C	6.773260000	0.713998000	-0.38944800
H	6.772791000	-0.379921000	-0.36306400
C	5.493546000	1.324138000	-0.44866500
H	5.437812000	2.413978000	-0.45791000
C	4.322435000	0.614999000	-0.48155200

V₁

E(scf) = -1857.86172744 a.u.

C	13.997507000	0.008034000	0.84497000
C	12.712027000	0.848248000	0.81169200
C	11.630506000	0.188692000	-0.05251600
C	11.792068000	-1.040183000	-0.61149500
C	12.976295000	-1.915273000	-0.31321800
C	13.765882000	-1.484927000	0.91321300
H	14.571898000	0.185794000	-0.07609200
H	14.632659000	0.350611000	1.67747300
C	10.862150000	-1.657423000	-1.60922600
H	10.189715000	-2.397955000	-1.14996800
H	10.236375000	-0.918829000	-2.11905600
H	11.451436000	-2.193985000	-2.36366700
C	13.103622000	2.218005000	0.23504500
H	13.389283000	2.141118000	-0.82127700
H	12.299901000	2.958319000	0.31971000
H	13.964203000	2.618516000	0.78747000
C	12.158341000	1.065337000	2.22813500
H	12.921866000	1.514044000	2.87954800
H	11.297572000	1.745975000	2.20889200
H	11.824168000	0.122679000	2.67209300
H	14.743747000	-2.005095000	0.88476700
O	13.024625000	-1.911934000	2.04727400
H	13.445780000	-1.527183000	2.82845400
C	10.419324000	0.980074000	-0.21025000
C	9.141284000	0.513145000	-0.26052400
H	8.976031000	-0.563665000	-0.18890200
C	7.958452000	1.318598000	-0.34630100
C	6.731930000	0.689154000	-0.33299700
H	6.750337000	-0.403273000	-0.27073700
C	5.448491000	1.277073000	-0.38087400
H	5.375156000	2.364654000	-0.43460700
C	4.279525000	0.548236000	-0.35460900

H	4.391707000	-0.476762000	-0.475860000	H	4.367344000	-0.541070000	-0.304022000
C	8.176831000	2.810881000	-0.383984000	C	8.106779000	2.806219000	-0.430874000
H	8.676889000	3.172725000	0.525253000	H	8.615057000	3.204991000	0.458300000
H	8.810834000	3.114880000	-1.227469000	H	8.721455000	3.094721000	-1.293822000
H	7.228956000	3.347438000	-0.473889000	H	7.148457000	3.323922000	-0.520829000
C	3.005893000	1.163441000	-0.511327000	C	2.965465000	1.074738000	-0.380444000
C	1.930002000	0.301210000	-0.538758000	C	1.889510000	0.192010000	-0.347368000
H	2.166613000	-0.767006000	-0.550405000	H	2.144587000	-0.871594000	-0.310850000
C	0.554422000	0.622776000	-0.544415000	C	0.524314000	0.494239000	-0.351870000
H	0.258627000	1.674027000	-0.516512000	H	0.211431000	1.540596000	-0.380620000
C	-0.448750000	-0.314987000	-0.575095000	C	-0.482550000	-0.464839000	-0.316717000
H	-0.150708000	-1.365432000	-0.608890000	H	-0.168422000	-1.511027000	-0.291079000
C	2.851610000	2.653842000	-0.502009000	C	2.782760000	2.561389000	-0.441055000
H	3.307503000	3.093358000	0.395322000	H	3.275857000	3.057165000	0.405550000
H	3.358059000	3.109456000	-1.363393000	H	3.232187000	2.979072000	-1.352042000
H	1.807123000	2.973335000	-0.530247000	H	1.732177000	2.861336000	-0.428553000
C	-1.825535000	0.000783000	-0.555484000	C	-1.842848000	-0.163535000	-0.309314000
H	-2.067546000	1.066480000	-0.501402000	H	-2.100290000	0.899852000	-0.329357000
C	-2.896289000	-0.867763000	-0.587325000	C	-2.927760000	-1.051432000	-0.273919000
C	-4.217373000	-0.332280000	-0.527705000	C	-4.225129000	-0.527594000	-0.255812000
H	-4.295872000	0.755957000	-0.449079000	H	-4.318091000	0.562193000	-0.270590000
C	-5.381471000	-1.053176000	-0.546857000	C	-5.413373000	-1.264389000	-0.214194000
H	-5.313564000	-2.139088000	-0.629933000	H	-5.333162000	-2.352924000	-0.199668000
C	-2.731845000	-2.354639000	-0.676384000	C	-2.734590000	-2.539850000	-0.247355000
H	-1.685068000	-2.667213000	-0.688748000	H	-1.682903000	-2.832093000	-0.297828000
H	-3.216749000	-2.858438000	0.170186000	H	-3.152053000	-2.978699000	0.668428000
H	-3.203582000	-2.750073000	-1.586024000	H	-3.247451000	-3.022975000	-1.088996000
C	-6.669380000	-0.465666000	-0.447985000	C	-6.670171000	-0.682877000	-0.182983000
H	-6.685107000	0.623710000	-0.346007000	H	-6.696800000	0.411304000	-0.189594000
C	-7.888918000	-1.096510000	-0.448078000	C	-7.931471000	-1.320130000	-0.135686000
C	-9.075711000	-0.299768000	-0.287541000	C	-9.069981000	-0.526259000	-0.085965000
H	-8.911850000	0.773070000	-0.166724000	H	-8.904293000	0.549867000	-0.084095000
C	-10.345343000	-0.776801000	-0.214471000	C	-10.395757000	-1.008010000	0.033455000
H	-10.469331000	-1.862430000	-0.248093000	H	-10.481668000	-2.086595000	0.159643000
C	-8.038776000	-2.580022000	-0.585812000	C	-8.048894000	-2.817587000	-0.128429000
H	-7.083217000	-3.092732000	-0.721050000	H	-7.087278000	-3.315109000	-0.277926000
H	-8.523820000	-3.012852000	0.300378000	H	-8.459926000	-3.183478000	0.822123000
H	-8.675709000	-2.836038000	-1.442838000	H	-8.722884000	-3.170042000	-0.918923000
C	-11.564504000	-0.017788000	0.027437000	C	-11.573207000	-0.292882000	0.080209000
C	-12.579777000	-0.740699000	0.922810000	C	-12.890344000	-0.997581000	0.424115000
C	-13.041069000	1.992234000	-0.179631000	C	-12.786275000	1.809554000	0.186443000
C	-13.682138000	0.207517000	1.426122000	C	-13.585289000	-0.163572000	1.513485000
C	-14.198665000	1.177136000	0.370867000	C	-13.819261000	1.288807000	1.133197000
H	-14.521780000	-0.417597000	1.783414000	H	-14.550608000	-0.612687000	1.786819000
C	-13.218727000	-1.898303000	0.137799000	C	-13.777505000	-1.087721000	-0.829176000
H	-12.457025000	-2.630421000	-0.157542000	H	-13.335293000	-1.764672000	-1.570122000
H	-13.946590000	-2.428249000	0.766981000	H	-14.774179000	-1.477560000	-0.577014000
H	-13.733984000	-1.547707000	-0.758397000	H	-13.892295000	-0.114402000	-1.323225000
C	-11.882298000	-1.338634000	2.154921000	C	-12.714276000	-2.410445000	0.973903000
H	-11.207994000	-2.152641000	1.863590000	H	-12.313838000	-3.100709000	0.221964000
H	-11.303404000	-0.588798000	2.700308000	H	-12.044712000	-2.429654000	1.842449000
H	-12.627751000	-1.755394000	2.844715000	H	-13.686608000	-2.809052000	1.290547000
C	-11.812150000	1.199105000	-0.522581000	C	-11.694936000	1.120240000	-0.244475000
H	-12.771550000	2.760566000	0.563530000	C	-10.731020000	1.827815000	-1.154391000
C	-10.899034000	1.890545000	-1.487407000	H	-9.939723000	2.358165000	-0.607343000
H	-10.291096000	2.667494000	-0.998712000	H	-10.241772000	1.128764000	-1.840289000
H	-10.206902000	1.204002000	-1.984082000	H	-11.260384000	2.585925000	-1.741088000
H	-11.483033000	2.408922000	-2.261044000	H	10.549134000	2.064161000	-0.195434000
H	-13.380783000	2.558357000	-1.063052000	O	-15.127221000	1.569350000	0.597847000
H	10.599155000	2.025882000	-0.112145000	H	-15.232981000	1.017803000	-0.193304000

O	-14.880530000	0.434710000	-0.62519900	H	-13.806253000	1.910791000	2.04066100
H	-15.092202000	1.043744000	-1.34544100	O	13.815135000	-1.914198000	-1.47187500
H	-14.912002000	1.866107000	0.86923600	H	14.416416000	-2.667997000	-1.38812800
O	13.852696000	-1.980172000	-1.35798000	H	12.597308000	-2.937757000	-0.12518000
H	14.434118000	-2.748714000	-1.26880500	H	-12.958904000	-0.195635000	2.41632900
H	12.572714000	-3.002310000	-0.06935700	O	-13.005045000	3.091781000	-0.21162800
O	-13.145399000	0.976857000	2.49732800	H	-13.938290000	3.274806000	0.00511100
H	-13.867200000	1.516198000	2.84933200				

VI

E(scf) = -1857.27296088a.u.

C	14.173573000	-0.039620000	0.55000200
C	12.892842000	0.807157000	0.59799100
C	11.724443000	0.113583000	-0.11453800
C	11.830013000	-1.156325000	-0.63533900
C	12.980186000	-2.015705000	-0.32920100
C	13.949243000	-1.524029000	0.73526700
H	14.660651000	0.097717000	-0.42865600
H	14.887388000	0.347334000	1.29501700
C	10.824273000	-1.789585000	-1.54472600
H	10.105742000	-2.418163000	-0.99988100
H	10.252924000	-1.048546000	-2.11294300
H	11.345830000	-2.462936000	-2.23222100
C	13.226772000	2.137978000	-0.09647300
H	13.388377000	2.000420000	-1.17294300
H	12.449260000	2.898297000	0.03763500
H	14.151386000	2.548686000	0.33046000
C	12.492853000	1.106236000	2.05124200
H	13.317174000	1.606266000	2.57849000
H	11.622588000	1.773860000	2.08849600
H	12.240703000	0.186934000	2.58702600
H	14.890296000	-2.079241000	0.59307800
O	13.361624000	-1.857599000	1.99064300
H	14.000187000	-1.609309000	2.67470300
C	10.524488000	0.915214000	-0.19699900
C	9.232239000	0.481099000	-0.26217300
H	9.032916000	-0.590283000	-0.27648900
C	8.074733000	1.324799000	-0.25071900
C	6.835793000	0.726420000	-0.27698800
H	6.826058000	-0.367040000	-0.31326000
C	5.563015000	1.347862000	-0.26158900
H	5.514251000	2.436773000	-0.21432900
C	4.387125000	0.643996000	-0.30105100
H	4.453463000	-0.446659000	-0.35155200
C	8.262450000	2.809575000	-0.20435800
H	8.810526000	3.110869000	0.69910100
H	8.856006000	3.160687000	-1.05880700
H	7.317055000	3.357607000	-0.21267100
C	3.073664000	1.195767000	-0.28091800
C	1.997227000	0.333851000	-0.33304000
H	2.234337000	-0.732592000	-0.39276800
C	0.622317000	0.653797000	-0.31679300
H	0.323746000	1.702352000	-0.24930700
C	-0.376307000	-0.288131000	-0.37996100
H	-0.071241000	-1.334667000	-0.45102100
C	2.920372000	2.684016000	-0.20015900
H	3.376308000	3.079602000	0.71729300
H	3.425641000	3.180499000	-1.03908200
H	1.875876000	3.004372000	-0.21214100
C	-1.754602000	0.016963000	-0.35247400
H	-2.006278000	1.078169000	-0.26690400

VII

E(scf) = -1856.67665269 a.u.

C	14.170726000	0.078747000	0.48800700
C	12.877594000	0.907082000	0.52890500
C	11.710438000	0.174818000	-0.14733800
C	11.832414000	-1.108948000	-0.63423100
C	12.997437000	-1.941036000	-0.31604400
C	13.971668000	-1.402808000	0.72093800
H	14.642505000	0.193750000	-0.50092000
H	14.888358000	0.498962000	1.21117700
C	10.829674000	-1.781458000	-1.51839700
H	10.126849000	-2.408956000	-0.95222500
H	10.240759000	-1.064403000	-2.09921000
H	11.357174000	-2.462348000	-2.19393800
C	13.180417000	2.222023000	-0.20809400
H	13.331937000	2.055443000	-1.28191300
H	12.391438000	2.972662000	-0.08697900
H	14.102627000	2.660504000	0.19574000
C	12.493392000	1.241159000	1.97873400
H	13.315662000	1.771711000	2.47876000
H	11.611088000	1.892940000	2.00984600
H	12.266844000	0.333011000	2.54433000
H	14.919786000	-1.947448000	0.58398000
O	13.405383000	-1.706756000	1.99364900
H	14.042847000	-1.415066000	2.66135000
C	10.497771000	0.951359000	-0.23886800
C	9.209938000	0.491058000	-0.28435900
H	9.032451000	-0.584059000	-0.26410500
C	8.040632000	1.309926000	-0.29437500
C	6.807097000	0.685966000	-0.28448700
H	6.820621000	-0.408144000	-0.27505700
C	5.529936000	1.281169000	-0.28295800
H	5.459541000	2.370131000	-0.28837100
C	4.357797000	0.552769000	-0.27226700
H	4.444739000	-0.537661000	-0.26793400
C	8.196334000	2.799271000	-0.30733800
H	8.731601000	3.148992000	0.58637500
H	8.787593000	3.128750000	-1.17182800
H	7.239276000	3.325718000	-0.34281000
C	3.047188000	1.081832000	-0.26429900
C	1.970266000	0.197167000	-0.25405200
H	2.225739000	-0.866800000	-0.25576100
C	0.606821000	0.499658000	-0.24080600
H	0.293317000	1.546076000	-0.23573700
C	-0.399593000	-0.461976000	-0.23237900
H	-0.084404000	-1.507973000	-0.24010200
C	2.864650000	2.569680000	-0.26622400
H	3.341519000	3.029315000	0.60964400
H	3.330038000	3.025223000	-1.15038200
H	1.813916000	2.868994000	-0.26033400
C	-1.758843000	-0.161775000	-0.21360500
H	-2.017544000	0.901341000	-0.20331500

C	-2.816481000	-0.861640000	-0.414950000	C	-2.843053000	-1.052436000	-0.204937000
C	-4.142939000	-0.340595000	-0.350278000	C	-4.139791000	-0.529272000	-0.179880000
H	-4.233868000	0.744484000	-0.247686000	H	-4.233196000	0.560422000	-0.166183000
C	-5.297989000	-1.074910000	-0.394794000	C	-5.328287000	-1.267440000	-0.168211000
H	-5.216094000	-2.157873000	-0.499461000	H	-5.248447000	-2.355888000	-0.181854000
C	-2.636158000	-2.343581000	-0.544871000	C	-2.648465000	-2.540585000	-0.224260000
H	-1.586661000	-2.646219000	-0.556849000	H	-1.595352000	-2.831332000	-0.214224000
H	-3.122690000	-2.875258000	0.283251000	H	-3.125964000	-3.016044000	0.642111000
H	-3.096513000	-2.717205000	-1.469191000	H	-3.101556000	-2.988726000	-1.118236000
C	-6.594450000	-0.506540000	-0.299474000	C	-6.584333000	-0.685576000	-0.136277000
H	-6.628447000	0.580897000	-0.184476000	H	-6.610223000	0.408467000	-0.120249000
C	-7.803124000	-1.157878000	-0.321577000	C	-7.846502000	-1.322905000	-0.116732000
C	-9.005255000	-0.380700000	-0.175416000	C	-8.983986000	-0.527723000	-0.070923000
H	-8.862104000	0.694461000	-0.052946000	H	-8.817313000	0.548151000	-0.051289000
C	-10.265414000	-0.883578000	-0.121758000	C	-10.311938000	-1.008696000	0.023033000
H	-10.367256000	-1.971235000	-0.153779000	H	-10.402374000	-2.087960000	0.139256000
C	-7.927074000	-2.641911000	-0.476426000	C	-7.966600000	-2.819845000	-0.136556000
H	-6.962476000	-3.138626000	-0.605348000	H	-7.002453000	-3.317525000	-0.267601000
H	-8.415319000	-3.092212000	0.399129000	H	-8.403546000	-3.199352000	0.796847000
H	-8.549744000	-2.898375000	-1.343554000	H	-8.619973000	-3.157909000	-0.950267000
C	-11.508042000	-0.153620000	0.094578000	C	-11.487190000	-0.289145000	0.057080000
C	-12.509206000	-0.888258000	0.994659000	C	-12.811389000	-0.990062000	0.380899000
C	-13.043714000	1.804516000	-0.194492000	C	-12.693158000	1.816921000	0.151496000
C	-13.652605000	0.037934000	1.431710000	C	-13.516796000	-0.156374000	1.463717000
C	-14.180184000	0.940389000	0.344740000	C	-13.739488000	1.298360000	1.085216000
C	-13.058346000	-2.127154000	0.269228000	C	-13.682250000	-1.072372000	-0.884191000
H	-12.263258000	-2.851697000	0.051302000	H	-13.232023000	-1.746361000	-1.622979000
H	-13.791333000	-2.638503000	0.907428000	H	-14.682244000	-1.462183000	-0.646067000
H	-13.554515000	-1.857239000	-0.665552000	H	-13.789927000	-0.096558000	-1.374890000
C	-11.803016000	-1.355361000	2.275994000	C	-12.647453000	-2.405317000	0.928282000
H	-11.024224000	-2.099125000	2.068473000	H	-12.240732000	-3.094804000	0.179032000
H	-11.330588000	-0.515577000	2.800795000	H	-11.988980000	-2.430155000	1.805095000
H	-12.528664000	-1.816987000	2.958907000	H	-13.625061000	-2.801152000	1.231578000
C	-11.769513000	1.054374000	-0.468752000	C	-11.598059000	1.124638000	-0.266064000
C	-10.838205000	1.788027000	-1.383131000	C	-10.619876000	1.829728000	-1.162715000
H	-10.252006000	2.544452000	-0.842185000	H	-9.839260000	2.364664000	-0.604939000
H	-10.132036000	1.124940000	-1.892672000	H	-10.117987000	1.128220000	-1.836803000
H	-11.406434000	2.337228000	-2.146552000	H	-11.140147000	2.583792000	-1.762581000
H	-13.384570000	2.256282000	-1.151224000	H	10.621380000	2.032373000	-0.162217000
H	10.668303000	1.991368000	-0.093717000	O	-15.039102000	1.588135000	0.536602000
O	-14.761878000	0.147471000	-0.677633000	H	-15.142178000	1.037148000	-0.255311000
H	-15.005048000	0.739260000	-1.403602000	H	-13.732076000	1.917537000	1.994588000
H	-14.943526000	1.618341000	0.779209000	O	13.176771000	-3.046744000	-0.818316000
O	13.148233000	-3.107946000	-0.862519000	H	-12.902873000	-0.194221000	2.374777000
H	-13.289391000	0.701028000	2.230021000	H	-14.487482000	-0.602152000	1.722740000
H	-14.468214000	-0.562930000	1.857034000	O	-12.901983000	3.098743000	-0.248717000
O	-12.708430000	2.847021000	0.723367000	H	-13.835681000	3.288358000	-0.038977000
H	-13.480870000	3.427150000	0.794094000				

3

E(scf) = -1856.09491320 a.u.

C	14.123510000	-0.154434000	0.422137000
C	12.854326000	0.665913000	0.694623000
C	11.672710000	0.179670000	-0.152127000
C	11.742616000	-0.942142000	-0.944839000
C	12.884337000	-1.863374000	-0.868540000
C	13.888000000	-1.639808000	0.253011000
H	14.593679000	0.210184000	-0.504888000
H	14.855110000	0.038595000	1.223334000
C	10.715295000	-1.337316000	-1.959242000
H	10.014556000	-2.089334000	-1.570589000

III

E(scf) = -1782.65811824 a.u.

C	13.482304000	0.279479000	-1.018788000
C	12.658004000	0.890954000	0.124640000
C	11.304790000	0.170566000	0.145215000
C	11.376745000	-1.281159000	0.175115000
C	12.515801000	-1.899770000	-0.237216000
C	13.655988000	-1.227927000	-0.925084000
H	12.983438000	0.517010000	-1.969926000
H	14.474832000	0.753474000	-1.061242000
C	10.296122000	-2.134068000	0.775694000
H	9.732752000	-1.586123000	1.537798000

H	10.126603000	-0.484067000	-2.3093100	H	9.574282000	-2.494114000	0.02985300
H	11.220430000	-1.813776000	-2.80546400	H	10.736368000	-3.025071000	1.23497700
C	13.198264000	2.124710000	0.35053300	C	12.554407000	2.391071000	-0.13970800
H	13.341790000	2.262591000	-0.72851100	H	11.988281000	2.610161000	-1.05377200
H	12.435190000	2.834897000	0.68840100	H	12.076787000	2.924423000	0.69077500
H	14.135230000	2.403141000	0.85037500	H	13.559754000	2.815846000	-0.25592200
C	12.465042000	0.599873000	2.17979900	C	13.381574000	0.690063000	1.46553800
H	13.294855000	0.953857000	2.80708300	H	14.367534000	1.174042000	1.44474900
H	11.598045000	1.240953000	2.38410500	H	12.803385000	1.136979000	2.28378700
H	12.213193000	-0.422000000	2.47656700	H	13.537356000	-0.368623000	1.69383100
H	14.819262000	-2.148437000	-0.04343000	H	13.728137000	-1.648380000	-1.94654700
O	13.329844000	-2.263136000	1.40728500	O	14.825493000	-1.649949000	-0.19773200
H	13.980856000	-2.174340000	2.11818700	H	15.598068000	-1.420096000	-0.73247200
C	10.486353000	1.004896000	-0.06275500	C	10.137009000	0.900792000	0.21302100
C	9.193334000	0.583451000	-0.15295200	C	8.795987000	0.464337000	0.09669000
H	8.998305000	-0.479323000	-0.30100100	H	8.600773000	-0.582547000	-0.12942300
C	8.031905000	1.413586000	-0.02430500	C	7.679811000	1.286290000	0.19793600
C	6.797480000	0.810152000	-0.08779700	C	6.401106000	0.707934000	0.03222900
H	6.795055000	-0.275983000	-0.21865700	H	6.394314000	-0.366677000	-0.17579400
C	5.519919000	1.418040000	-0.01257200	C	5.162043000	1.323726000	0.11105700
H	5.462273000	2.502170000	0.09663800	H	5.116732000	2.394045000	0.31987400
C	4.351468000	0.704451000	-0.07641300	C	3.951871000	0.643117000	-0.05385700
H	4.429110000	-0.381829000	-0.17679600	H	4.011172000	-0.430792000	-0.25378400
C	8.213021000	2.887234000	0.16655000	C	7.841237000	2.751275000	0.48911300
H	8.775805000	3.100639000	1.08572300	H	8.296199000	2.918199000	1.47408700
H	8.788157000	3.326915000	-0.65882500	H	8.498247000	3.234202000	-0.24574100
H	7.264429000	3.425934000	0.23256700	H	6.891057000	3.291174000	0.47446700
C	3.031863000	1.240134000	-0.02569100	C	2.669890000	1.200306000	0.02032300
C	1.966368000	0.365089000	-0.08452500	C	1.560642000	0.360468000	-0.15142800
H	2.216161000	-0.697285000	-0.15990100	H	1.787765000	-0.693675000	-0.33841500
C	0.588121000	0.668472000	-0.05804300	C	0.208257000	0.695621000	-0.10719700
H	0.277376000	1.713831000	0.00359000	H	-0.078340000	1.734273000	0.07468300
C	-0.399214000	-0.286421000	-0.10676500	C	-0.820276000	-0.225118000	-0.27386700
H	-0.082868000	-1.330249000	-0.16354100	H	-0.529262000	-1.263354000	-0.44995100
C	2.861477000	2.723851000	0.09094400	C	2.517540000	2.669503000	0.28803500
H	3.309622000	3.101219000	1.01974800	H	2.940454000	2.943245000	1.26359600
H	3.364646000	3.245511000	-0.73350600	H	3.048284000	3.267684000	-0.46385200
H	1.813754000	3.033378000	0.08391500	H	1.473914000	2.993540000	0.28337900
C	-1.779868000	0.005576000	-0.08573500	C	-2.180239000	0.098849000	-0.22400500
H	-2.042202000	1.066407000	-0.03667800	H	-2.417014000	1.153432000	-0.05176300
C	-2.833338000	-0.885565000	-0.11997900	C	-3.269128000	-0.757351100	-0.35879200
C	-4.162318000	-0.371530000	-0.09349400	C	-4.577503000	-0.221531000	-0.27058400
H	-4.261928000	0.716837000	-0.05132400	H	-4.65345700	0.857936000	-0.10907100
C	-5.313638000	-1.115446000	-0.11417400	C	-5.751630000	-0.935419000	-0.36257700
H	-5.226485000	-2.202145000	-0.15365500	H	-5.683403000	-2.013441000	-0.51717400
C	-2.640741000	-2.370059000	-0.18418300	C	-3.106162000	-2.230124000	-0.58802000
H	-1.588982000	-2.664677000	-0.17682300	H	-2.059421000	-2.541375000	-0.62100200
H	-3.126565000	-2.868640000	0.66476800	H	-3.595365000	-2.810651000	0.20542100
H	-3.093363000	-2.788163000	-1.09307000	H	-3.571460000	-2.539517000	-1.53341800
C	-6.609907000	-0.545273000	-0.08379500	C	-7.035569000	-0.354215000	-0.25922000
H	-6.647325000	0.547639000	-0.05209600	H	-7.056908000	0.730271000	-0.11296100
C	-7.820206000	-1.199765000	-0.08780500	C	-8.258429000	-0.987512000	-0.31286800
C	-9.017214000	-0.412505000	-0.05266500	C	-9.450956000	-0.201357000	-0.17018500
H	-8.872879000	0.668244000	-0.02724300	H	-9.299208000	0.871974000	-0.03656400
C	-10.285011000	-0.912138000	0.01580100	C	-10.720081000	-0.691283000	-0.13961600
H	-10.383826000	-1.996295000	0.08549300	H	-10.828952000	-1.778194000	-0.17742000
C	-7.941644000	-2.691694000	-0.12266800	C	-8.397175000	-2.467169000	-0.49916300
H	-6.974354000	-3.195814000	-0.18554500	H	-7.436330000	-2.971341000	-0.62797100
H	-8.451004000	-3.068004000	0.77520500	H	-8.897378000	-2.930150000	0.36324100
H	-8.542110000	-3.019633000	-0.98112800	H	-9.014737000	-2.701362000	-1.37634300

C	-11.523398000	-0.177136000	0.09191300	C	-11.960955000	0.045180000	0.05229900
C	-12.698584000	-0.890599000	0.77954500	C	-12.995608000	-0.691931000	0.91433500
C	-13.070587000	1.616281000	-0.51416700	C	-13.483774000	2.014842000	-0.25484800
C	-13.550855000	0.155706000	1.50643600	C	-14.153803000	0.231193000	1.32472600
C	-14.023232000	1.293679000	0.62771000	C	-14.643437000	1.165411000	0.24164400
C	-13.529481000	-1.621492000	-0.28394500	H	-14.988610000	-0.379657000	1.69588900
H	-12.914794000	-2.346050000	-0.83485700	H	-13.828347000	0.860013000	2.16765700
H	-14.355353000	-2.168896000	0.18880100	C	-13.529999000	1.916386000	0.15412200
H	-13.968278000	-0.924853000	-1.00612800	H	-12.731114000	-2.638369000	-0.05794500
C	-12.237674000	-1.905196000	1.83082000	H	-14.280582000	-2.437906000	0.76343100
H	-11.782007000	-2.799599000	1.38994100	H	-14.001776000	-1.626160000	-0.78731500
H	-11.514941000	-1.468580000	2.53163700	C	-12.338455000	-1.182018000	2.21263200
H	-13.103344000	-2.245902000	2.41262700	H	-11.559748000	-1.930302000	2.02257500
C	-11.728412000	1.033459000	-0.53250600	H	-11.874654000	-0.353966000	2.76390500
C	-10.748363000	1.718025000	-1.43139600	H	-13.090565000	-1.644427000	2.86624100
H	-10.097464000	2.415572000	-0.88597500	C	-12.208360000	1.259164000	-0.50820700
H	-10.094425000	1.007048000	-1.94926800	H	-13.293466000	2.821597000	0.47532200
H	-11.299323000	2.307311000	-2.17096600	C	-11.260616000	1.968735000	-1.42605000
H	10.647301000	2.054917000	0.18672900	H	-10.686841000	2.752275000	-0.90728200
O	-15.301866000	1.009662000	0.09346400	H	-10.535566000	1.294490000	-1.89194400
H	-15.383636000	1.615923000	-0.66504700	H	-11.814731000	2.481949000	-2.22452200
H	-14.0718300	2.220253000	1.23442300	H	-13.783752000	2.546270000	-1.17397300
O	13.018693000	-2.806585000	-1.64076900	H	10.255096000	1.976844000	0.33105400
H	-12.954819000	0.565135000	2.33422200	O	-15.214440000	0.378122000	-0.79678300
H	-14.429081000	-0.324487000	1.95841100	H	-15.447317000	0.978152000	-1.51822600
O	-13.488916000	2.367204000	-1.39857200	H	-15.417649000	1.831260000	0.66688600
				O	12.675460000	-3.242690000	-0.09161700
				H	13.635041000	-3.399591000	-0.15519900

IV

E(scf) = -1782.07233750 a.u.

C	-13.867200000	0.016382000	0.52087300
C	-12.581750000	-0.823850000	0.56031900
C	-11.413644000	-0.111077000	-0.13396400
C	-11.525748000	1.165540000	-0.63682700
C	-12.682482000	2.012622000	-0.32253700
C	-13.651145000	1.498718000	0.73182900
H	-14.349605000	-0.107228000	-0.46187400
H	-14.581837000	-0.386933000	1.25639600
C	-10.520500000	1.818727000	-1.53240500
H	-9.808645000	2.444174000	-0.97531700
H	-9.941729000	1.089806000	-2.10871600
H	-11.043887000	2.498355000	-2.21231700
C	-12.903494000	-2.143619000	-0.16029800
H	-13.061807000	-1.986838000	-1.23461900
H	-12.121173000	-2.900901000	-0.03740600
H	-13.826889000	-2.568534000	0.25515600
C	-12.188465000	-1.146540000	2.01032300
H	-13.011975000	-1.662892000	2.52287600
H	-11.313020000	-1.807607000	2.04118600
H	-11.947329000	-0.235038000	2.56426200
H	-14.594805000	2.051440000	0.59754600
O	-13.067290000	1.813698000	1.99377500
H	-13.703802000	1.546337000	2.67253800
C	-10.207666000	-0.902820000	-0.22121900
C	-8.917943000	-0.459325000	-0.27671300
H	-8.725550000	0.613383000	-0.27957400
C	-7.755237000	-1.295614000	-0.26688000
C	-6.519602000	-0.689690000	-0.28124200
H	-6.515886000	0.403974000	-0.31209800
C	-5.244150000	-1.304893000	-0.25671400

V

E(scf) = -1781.45521977 a.u.

C	-13.867603000	0.013867000	0.46475400
C	-12.585190000	-0.831427000	0.49388300
C	-11.408891000	-0.104801000	-0.17243000
C	-11.513368000	1.186496000	-0.64150900
C	-12.669867000	2.028384000	-0.31414100
C	-13.648970000	1.489452000	0.71776200
H	-14.340923000	-0.081665000	-0.52544900
H	-14.590511000	-0.406757000	1.18229300
C	-10.500750000	1.859119000	-1.51400300
H	-9.792073000	2.469943000	-0.93702200
H	-9.919059000	1.143396000	-2.10356700
H	-11.018336000	2.555757000	-2.18104000
C	-12.904674000	-2.132265000	-0.26090100
H	-13.054781000	-1.949323000	-1.33226000
H	-12.125054000	-2.894224000	-0.15047900
H	-13.832005000	-2.564623000	0.13760700
C	-12.204941000	-1.189750000	1.93901000
H	-13.033313000	-1.717490000	2.43177300
H	-11.330414000	-1.852320000	1.96119600
H	-11.968093000	-0.291986000	2.51680000
H	-14.589991000	2.048369000	0.59087100
O	-13.074481000	1.768760000	1.99237100
H	-13.713472000	1.477379000	2.65876900
C	-10.206014000	-0.896111000	-0.27496000
C	-8.912248000	-0.453362000	-0.31089300
H	-8.718364000	0.618444000	-0.27388500
C	-7.755234000	-1.290544000	-0.32988400
C	-6.512395000	-0.686800000	-0.30383800
H	-6.507342000	0.407024000	-0.27704600
C	-5.245335000	-1.304471000	-0.30348200

H	-5.191704000	-2.393502000	-0.20722000	H	-5.194476000	-2.394163000	-0.32605600
C	-4.069791000	-0.597686000	-0.28719100	C	-4.060871000	-0.598182000	-0.27194900
H	-4.137750000	0.492631000	-0.34241200	H	-4.127352000	0.493418000	-0.25089200
C	-7.934182000	-2.781885000	-0.23376100	C	-7.934684000	-2.776800000	-0.36692900
H	-8.482435000	-3.094589000	0.66570300	H	-8.480509000	-3.131151000	0.51846400
H	-8.523914000	-3.128582000	-1.09264500	H	-8.526260000	-3.083279000	-1.23953300
H	-6.985644000	-3.324390000	-0.24559600	H	-6.986219000	-3.318167000	-0.40530500
C	-2.756145000	-1.147709000	-0.24945800	C	-2.759915000	-1.152492000	-0.26129100
C	-1.678409000	-0.286786000	-0.29774400	C	-1.667489000	-0.288502000	-0.22912200
H	-1.913126000	0.779062000	-0.37514200	H	-1.902565000	0.780079000	-0.21835300
C	-0.304993000	-0.610142000	-0.25665500	C	-0.309698000	-0.617707000	-0.20810700
H	-0.012348000	-1.658150000	-0.15999900	H	-0.016548000	-1.669925000	-0.21288000
C	0.701538000	0.322936000	-0.32964600	C	0.714371000	0.323674000	-0.18017500
H	0.408100000	1.370035000	-0.43494800	H	0.420054000	1.375651000	-0.17951000
C	-2.603780000	-2.635456000	-0.15531100	C	-2.604838000	-2.643202000	-0.28619600
H	-3.066968000	-3.024209000	0.76141000	H	-3.107066000	-3.109559000	0.57156500
H	-3.102614000	-3.137961000	-0.99451500	H	-3.060843000	-3.073751000	-1.18760500
H	-1.559494000	-2.956494000	-0.15770600	H	-1.559999000	-2.961767000	-0.26554000
C	2.075554000	0.003355000	-0.27339500	C	2.067771000	-0.004165000	-0.15376000
H	2.311563000	-1.057281000	-0.14531300	H	2.304953000	-1.072325000	-0.15067000
C	3.151262000	0.863375000	-0.35757500	C	3.168606000	0.864566000	-0.13105200
C	4.467435000	0.323702000	-0.25783300	C	4.454867000	0.314355000	-0.10116800
H	4.536759000	-0.756354000	-0.09893000	H	4.526057000	-0.776995000	-0.09167900
C	5.638785000	1.029054000	-0.33794700	C	5.656920000	1.028839000	-0.08297200
H	5.583383000	2.105781000	-0.50689500	H	5.597803000	2.118346000	-0.09794300
C	2.995107000	2.341172000	-0.54961200	C	3.003804000	2.356318000	-0.14032300
H	1.950164000	2.658786000	-0.57674600	H	1.956524000	2.667314000	-0.14354700
H	3.488808000	2.898539000	0.25707100	H	3.477307000	2.814441000	0.73747400
H	3.462685000	2.669232000	-1.48753400	H	3.478944000	2.803248000	-1.02325400
C	6.918957000	0.432970000	-0.20522500	C	6.901887000	0.422693000	-0.04778400
H	6.919882000	-0.643959000	-0.01137300	H	6.906192000	-0.671602000	-0.03035000
C	8.148648000	1.040197000	-0.28323000	C	8.175646000	1.036535000	-0.03219400
C	9.323504000	0.235278000	-0.08352600	C	9.298013000	0.216932000	0.00678900
H	9.138359000	-0.815185000	0.14876600	H	9.100934000	-0.851344000	0.03402000
C	10.605688000	0.684769000	-0.10750900	C	10.631096000	0.692159000	0.05466000
H	10.749799000	1.757606000	-0.25994100	H	10.701542000	1.777342000	0.10378800
C	8.319025000	2.502551000	-0.55498500	C	8.321993000	2.530993000	-0.05950000
H	7.367717000	3.022811000	-0.69119800	H	7.360057000	3.048254000	-0.09348600
H	8.851989000	2.998189000	0.26817400	H	8.856262000	2.896150000	0.82705800
H	8.919864000	2.671011000	-1.45846200	H	8.899769000	2.860192000	-0.93217700
C	11.821907000	-0.071156000	0.15431800	C	11.840433000	0.031525000	0.09467200
C	12.907142000	0.726833000	0.89152600	C	13.133662000	0.842006000	0.23344800
C	13.249987000	-2.133259000	0.09386700	C	13.210208000	-1.991401000	0.25739700
C	14.014159000	-0.192122000	1.43138800	C	14.046440000	0.129626000	1.24592300
C	14.452609000	-1.290721000	0.48990000	C	14.371986000	-1.307008000	0.89249300
C	13.493372000	1.788365000	-0.05272200	C	13.812016000	0.935909000	-1.14343400
H	12.728227000	2.511391000	-0.36348000	H	13.182083000	1.508403000	-1.83677100
H	14.282234000	2.354667000	0.46027700	H	14.781014000	1.444816000	-1.05965500
H	13.929811000	1.333516000	-0.94465000	H	13.999274000	-0.050635000	-1.57599300
C	12.299852000	1.446234000	2.10459400	C	12.918993000	2.264622000	0.75130300
H	11.561241000	2.200831000	1.80809900	H	12.396685000	2.901284000	0.02677200
H	11.800566000	0.740873000	2.78124000	H	12.351250000	2.280003000	1.69067800
H	13.087006000	1.960065000	2.67255200	H	13.892452000	2.733952000	0.94040200
C	12.009267000	-1.355947000	-0.24933100	C	12.028994000	-1.408011000	-0.06573200
C	11.020566000	-2.134716000	-1.06239800	C	10.955443000	-2.286206000	-0.64565400
H	10.40018900	-2.798491000	-0.44061900	H	10.191304000	-2.553016000	0.09575200
H	10.337864000	-1.492729000	-1.62743600	H	10.436820000	-1.806919000	-1.48391000
H	11.543380000	-2.790052000	-1.77247300	H	11.386965000	-3.227164000	-1.00464400
H	13.520924000	-2.784327000	-0.75396600	H	-10.344266000	-1.976434000	-0.21617200
H	-10.344198000	-1.981015000	-0.1303200	O	15.519179000	-1.296233000	0.02955100

O	15.074889000	-0.684703000	-0.63670200	H	15.620034000	-2.190433000	-0.32615200
H	15.314555000	-1.393384000	-1.24929200	H	14.640999000	-1.850296000	1.81856400
H	15.184150000	-1.935345000	1.01141600	O	-12.836657000	3.140725000	-0.80502900
O	-12.856508000	3.111239000	-0.84070000	H	13.552619000	0.148041000	2.22844300
H	13.652609000	-0.680002000	2.34925300	H	14.989496000	0.682499000	1.35124200
H	14.880684000	0.418037000	1.72210100	H	13.327081000	-3.061615000	0.06188000
H	13.018661000	-2.837029000	0.91321500				