



Supplement of

Elucidation of the myrcene ozonolysis mechanism from a Criegee Chemistry perspective

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Table S1 The characteristic infrared peaks of CIs were obtained using different computational methods.

CIs	Calculated band/(cm ⁻¹)				Experimental band/(cm ⁻¹) ^a	Assignment
	B3LYP-D3(BJ)/6-311++G(d,p)	B3LYP-D3(BJ)/aug-cc-pVTZ	B3LYP/6-311G++(d,2p)	B3LYP/6-311++G(2d,2p)		
Anti-CH ₃ CHOO	961	968	961	971	884	O-O stretch
Syn-CH ₃ CHOO	884	897	882	908.17	871.2	O-O stretch
(CH ₃) ₂ COO	912	925	909	928	887.4	O-O stretch
CH ₂ OO	899	912	901	923	909	O-O stretch
Syn-C7-CIs	883	893	882	900	\	O-O stretch
Anti-C7-CIs	912	923	910	928	\	O-O stretch

Note: ^a Data from references (Chhantyal-Pun et al., 2020).

As shown in Table S1, the table correspondingly list only the peak positions associated with this vibration because of the manuscript focused on the most intense O-O stretching vibration of CIs. Among the four computational methods, the B3LYP/6-311G++(d,2p) level demonstrated superior performance in predicting the O-O stretching vibrational frequencies of CIs. The results from this method were also in close agreement with the computational values reported previously by Li et al (Lin et al., 2015; Su et al., 2013; Wang et al., 2016). Thus, we have recalculated the infrared spectra of all relevant configurations in our manuscript using the B3LYP/6-311G++(d,2p) method. It could be observed that the calculated peak positions for alkyl-substituted CIs were systematically overestimated compared to the available experimental values. For example, a significant discrepancy of 77 cm⁻¹ was noted for anti-CH₃CHOO. In contrast, the deviation was much smaller for syn-CH₃CHOO being only 10.8 cm⁻¹. This was consistent with the trend previously observed by Lin et al (Lin et al., 2015). Therefore, the computational results provided strong support for the identification of syn-C7-CIs.

Table S2 The conformers, the Gibbs free energy and the Boltzmann distribution of anti-(CH₂=CH)-CH(CH₂)-CH₂CH₂CHOO obtained at DLPNO-CCSD(T)/CBS// B3LYP-D3(BJ)/aug-cc-pVTZ.

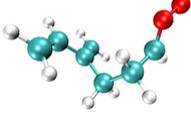
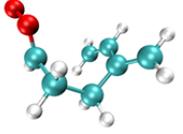
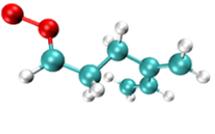
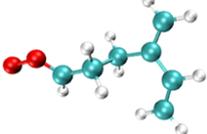
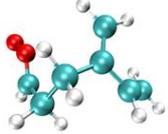
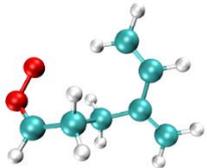
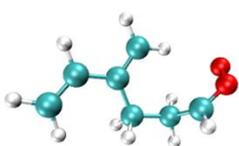
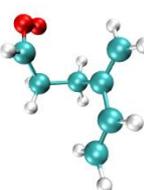
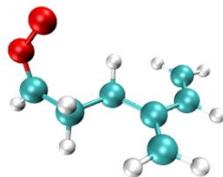
No.	Conformers	ΔG (kcal/mol)	Boltzmann distribution (%)		
			298 K	35 K	6 K
A1		0.55	11.03	0.02	0
A2		0	27.93	59.45	92.13
A3		1.04	4.86	0	0
A4		0.03	26.58	39	7.87
A5		0.59	10.24	0	0
A6		0.26	18.15	1.51	0
A7		1.86	1.20	0	0

Table S3 The conformers, the Gibbs free energy and the Boltzmann distribution of syn-(CH₂=CH)-CH(CH₂)-CH₂CH₂CHO obtained at DLPNO-CCSD(T)/CBS// B3LYP-D3(BJ)/aug-cc-pVTZ.

NO.	Conformers	ΔG (kcal/mol)	Boltzmann distribution (%)		
			298 K	35 K	6 K
S1		0.11	28.84	17.04	0.01
S2		0.48	15.44	0.08	0
S3		1.06	5.8	0	0
S4		0	34.72	82.87	99.99
S7		0.80	8.99	0	0
S10		1.44	3.05	0	0
S13		1.42	3.16	0	0

S15



1.20

4.58

0

0

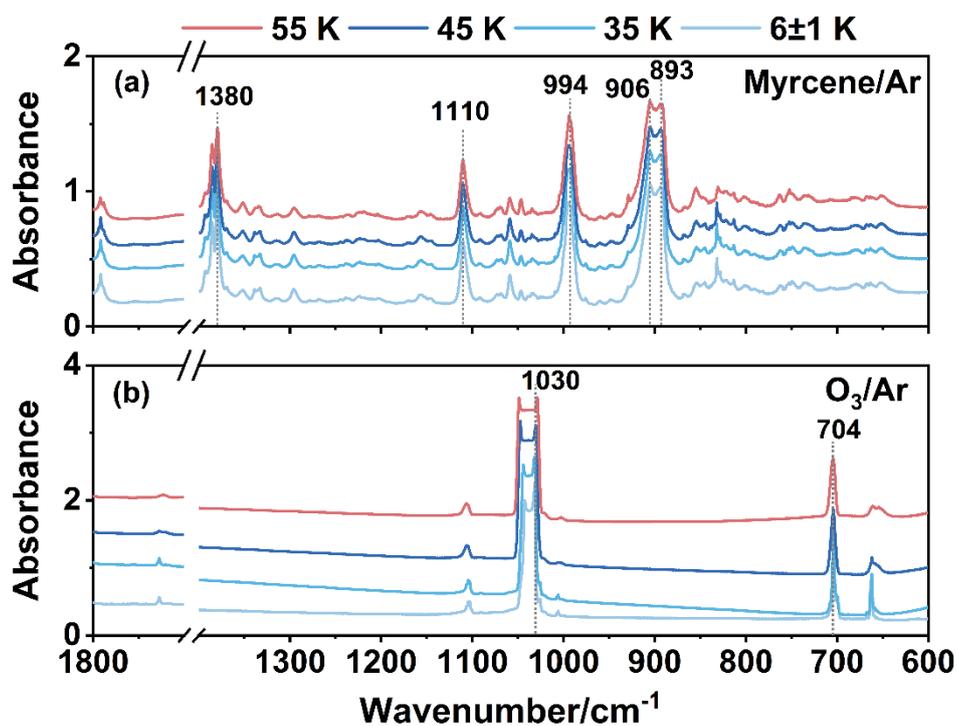


Figure S1 The IR spectra of precursor (myrcene/Ar and O_3 /Ar) in a low temperature after annealing to 35 K, 45 K and 55 K.

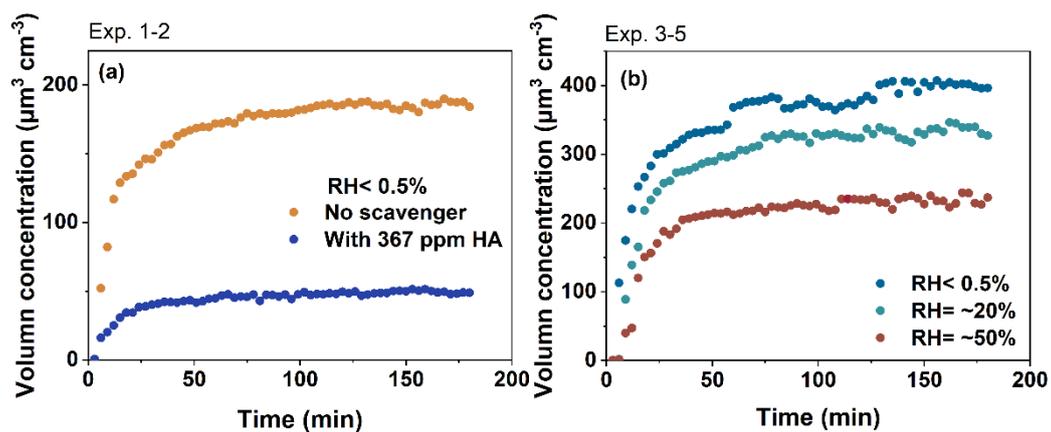


Figure S2 Time series of particle volume concentration in myrcene ozonolysis under different condition. (a) depict particle formation processes in Exp. 1-2 from Table 2, while (b) illustrate particle formation processes in Exp. 3-5 of Table 2.

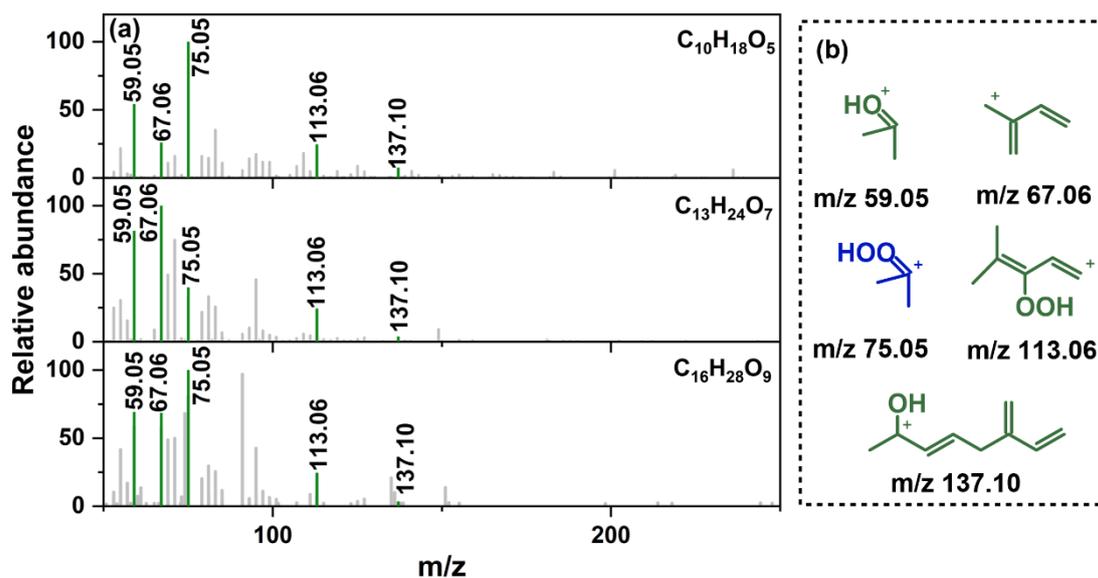


Figure S3 The MS/MS of $C_{10}H_{17}O_5$ + n-C3-SCIs + HO_2 sequence (a) and chemical structures of ions corresponding to major fragment peaks in MS/MS spectra (b).

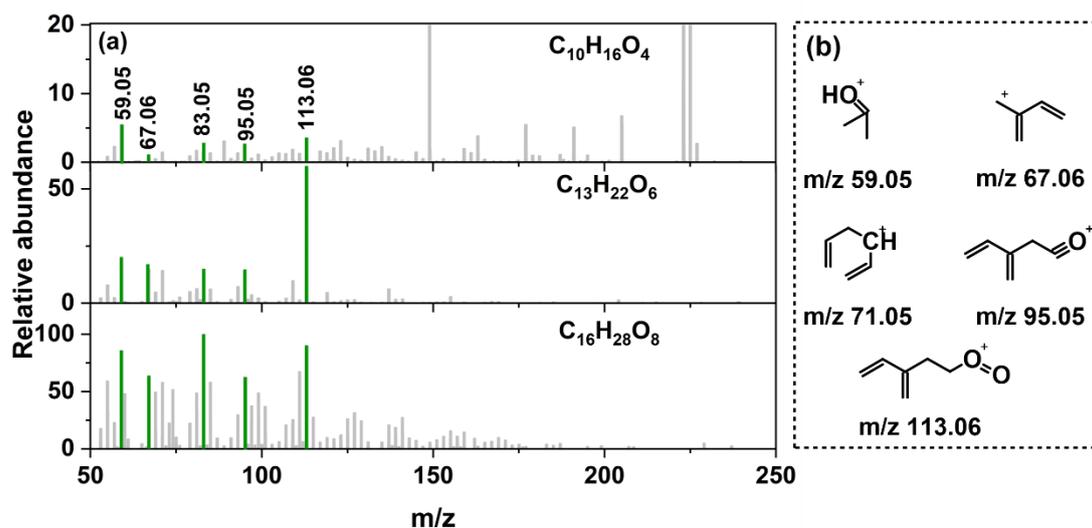
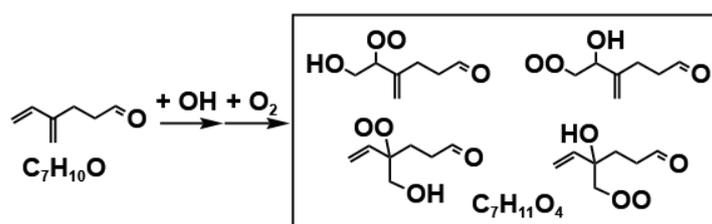


Figure S4 The MS/MS of $C_7H_9O_3$ + n-C3-SCIs + RO_2 sequence (a) and chemical structures of ions corresponding to major fragment peaks in MS/MS spectra (b).



Scheme S1 The formation pathway of $C_7H_{11}O_4$.

Table S4 The z-matrices of the optimized stationary points obtained by quantum chemistry calculations.

Compounds	Cartesian coordinates			
Myrcene	C	3.23845500	-1.39255200	0.10422100
	H	2.98891100	-2.44026800	0.00126900
	H	4.24995700	-1.15885700	0.41099600
	C	2.33972400	-0.43020300	-0.13837000
	C	2.73149100	0.97514000	0.00059400
	H	3.75046100	1.13758700	0.33808200
	C	1.97229300	2.04255700	-0.25387800
	H	0.94929100	1.96129900	-0.59524400
	H	2.36119300	3.04352100	-0.12961200
	C	0.92118700	-0.76539400	-0.52707100
	H	0.87785500	-1.79068500	-0.89804200
	H	0.59439300	-0.12522300	-1.34923900
	C	-0.07454800	-0.61383100	0.64658000
	H	0.01598300	0.38418700	1.07028200
	H	0.22744800	-1.30925800	1.43466100
	C	-1.48355000	-0.91083600	0.22937600
	H	-1.68168800	-1.95742500	0.01194300
	C	-2.48999500	-0.04965500	0.06315400
	C	-3.84843300	-0.51605100	-0.38765500
	H	-4.13911100	-0.02388900	-1.32052100
H	-3.87944900	-1.59329100	-0.54684400	
H	-4.61308900	-0.25758800	0.35089800	
C	-2.39461700	1.43428300	0.29323400	
H	-3.12307800	1.75286300	1.04428400	

	H	-1.41058400	1.76029400	0.62068200
	H	-2.64053300	1.97596900	-0.62470600
POZ1	C	3.62623400	-1.51978000	0.57737500
	H	3.23371800	-2.36286000	1.13008100
	H	4.66192300	-1.57804800	0.26896500
	C	2.86971700	-0.45420300	0.28767300
	C	3.45398400	0.66783600	-0.45013400
	H	4.48842900	0.52960200	-0.74808400
	C	2.85297700	1.81482400	-0.77049900
	H	1.82559300	2.02812500	-0.51240800
	H	3.38241100	2.58707100	-1.31050800
	C	1.41683900	-0.40610500	0.69958100
	H	1.19470100	0.56121700	1.15425700
	H	1.24523900	-1.15685600	1.47267000
	C	0.45840100	-0.67373600	-0.47347500
	H	0.72698000	-1.62967200	-0.92621000
	H	0.56862600	0.08005700	-1.24971100
	C	-0.99167000	-0.77557700	-0.03203200
	H	-1.07231900	-1.47937200	0.80270100
	C	-1.77381400	0.53071400	0.36560200
	C	-2.08944700	0.53907300	1.85590000
	H	-2.65602100	1.43096600	2.12113200
	H	-2.67782800	-0.33919400	2.11808100
	H	-1.16858800	0.52717600	2.44207100
	C	-1.16350400	1.84346600	-0.10255500
	H	-0.28345900	2.09533700	0.48659400
	H	-0.89623200	1.79879200	-1.15588200

	H	-1.89147300	2.64356600	0.02870300
	O	-3.08513100	-1.00383000	-0.70263000
	O	-1.74707600	-1.29130000	-1.12722000
	O	-2.99779300	0.40325700	-0.40353300
POZ2	C	3.62811600	-1.49217500	0.49599700
	H	3.24703800	-2.35770800	1.02134800
	H	4.66162700	-1.53079700	0.17734200
	C	2.86029400	-0.42365400	0.24990500
	C	3.42998600	0.72867100	-0.45164100
	H	4.46385700	0.61062000	-0.76013700
	C	2.81702700	1.88057500	-0.72843100
	H	1.78919600	2.07522800	-0.45719800
	H	3.33568800	2.67632100	-1.24420200
	C	1.40981100	-0.40234200	0.67201400
	H	1.18469400	0.54704400	1.16216600
	H	1.25116900	-1.18092300	1.42071000
	C	0.44310400	-0.63661000	-0.50152400
	H	0.75285500	-1.53993200	-1.02888700
	H	0.49422500	0.17527000	-1.22419000
	C	-0.99714000	-0.85159700	-0.05507800
	H	-1.03235400	-1.65222700	0.68931000
	C	-1.78997000	0.36848700	0.51073400
	C	-1.87830900	0.36390900	2.02827700
	H	-2.52047300	1.17425200	2.37125400
	H	-2.28509900	-0.58067000	2.38587300
	H	-0.88894200	0.50625600	2.46063700
	C	-1.35224200	1.72113100	-0.03961200

	H	-0.36362600	1.99265800	0.32543900
	H	-1.33697900	1.71369500	-1.12662800
	H	-2.05749000	2.48186400	0.29236600
	O	-2.86141100	-0.32667400	-1.30954400
	O	-1.78863200	-1.31161900	-1.16779400
	O	-3.11488800	0.05712800	0.03370800
Anti-C7-CIs-1	C	-0.57517100	1.93544400	0.20214600
	H	0.34115300	2.17522900	0.72250100
	H	-1.02776400	2.72447400	-0.38424500
	C	-1.12148100	0.71587100	0.26138900
	C	-2.35496800	0.43188300	-0.47605500
	H	-2.72807000	1.25595100	-1.07565200
	C	-3.04509000	-0.71053900	-0.47546200
	H	-2.74491300	-1.57662200	0.09929000
	H	-3.95246400	-0.81167700	-1.05382700
	C	-0.47543400	-0.39143100	1.06456700
	H	-1.23613200	-0.92970400	1.63112200
	H	0.21319300	0.03486300	1.79181100
	C	0.27399100	-1.40924500	0.18782800
	H	-0.34777000	-1.73649700	-0.64985900
	H	0.48843800	-2.32131400	0.76026600
	C	1.56591600	-0.93917200	-0.37081600
	H	2.10762000	-1.48003300	-1.14305900
	O	3.31212600	0.50118900	-0.44761700
	O	2.09789200	0.10737000	0.06512600
Anti-C7-CIs-2	C	0.98670800	2.00375400	0.22498500
	H	0.39380000	2.45370600	1.00995100

	H	1.31756900	2.65861300	-0.57005500
	C	1.29637500	0.70204400	0.23176500
	C	2.10906800	0.13687700	-0.84666700
	H	2.37075700	0.83308400	-1.63653800
	C	2.54882400	-1.11937200	-0.93800100
	H	2.33417400	-1.87164300	-0.19089500
	H	3.15246100	-1.43669900	-1.77632800
	C	0.78168000	-0.20790200	1.32223500
	H	0.46708000	0.39052900	2.17822100
	H	1.57317200	-0.86835100	1.67890000
	C	-0.40445700	-1.08590700	0.85385300
	H	-0.67524400	-1.77002800	1.66575500
	H	-0.13439200	-1.68596300	-0.01303500
	C	-1.59393300	-0.26745000	0.52470600
	H	-2.03257900	0.45317800	1.21091800
	O	-3.24805300	0.37190700	-0.87687800
	O	-2.14099600	-0.38799300	-0.59739200
Anti-C7-CIs-3	C	2.43361000	-0.41404400	1.16687000
	H	2.76858100	-1.44041500	1.23804300
	H	2.78367400	0.26747800	1.93071100
	C	1.62739200	-0.00314600	0.18070800
	C	1.20367000	1.39642400	0.11876000
	H	1.47944500	1.99593100	0.97979800
	C	0.53037100	1.98789300	-0.86960800
	H	0.23317600	1.46984800	-1.77072700
	H	0.25779000	3.03137800	-0.80882800
	C	1.10810300	-0.99003200	-0.83742800

	H	1.79808700	-1.82956100	-0.91593800
	H	1.05233700	-0.53989800	-1.82941900
	C	-0.27979600	-1.57285900	-0.45253100
	H	-0.22319400	-2.04259100	0.52862100
	H	-0.53928400	-2.34363100	-1.18560500
	C	-1.36817800	-0.57034100	-0.44378300
	H	-1.69463400	-0.02821700	-1.32633800
	O	-2.96605400	0.62320900	0.61710900
	O	-1.96482200	-0.31617100	0.63061000
Anti-C7-CIs-4	C	-2.38519300	-1.73757100	-0.08409400
	H	-1.83915400	-2.66467400	-0.19602700
	H	-3.44960400	-1.81591800	0.09470800
	C	-1.77805900	-0.54839700	-0.17279600
	C	-2.55932000	0.68287600	-0.03359100
	H	-3.60837700	0.53698400	0.20280800
	C	-2.11078100	1.93101600	-0.18023000
	H	-1.08251500	2.15863900	-0.42773300
	H	-2.77456600	2.77655900	-0.06848300
	C	-0.28762600	-0.45531000	-0.39691400
	H	-0.06223000	0.28597600	-1.16460200
	H	0.08998600	-1.40608900	-0.77084100
	C	0.45901200	-0.09335900	0.89444000
	H	0.28621000	-0.85948600	1.65931600
	H	0.06033400	0.82876200	1.33179000
	C	1.92254200	0.07503100	0.74864600
	H	2.57972500	0.29819100	1.58573000
	O	3.82048800	0.12915300	-0.48362400

	O	2.45910600	-0.03723500	-0.37880600
Anti-C7-CIs-5	C	-0.59810400	-1.47889900	0.66735300
	H	0.41897300	-1.41524000	1.02212800
	H	-1.03702100	-2.46763300	0.66366000
	C	-1.30281800	-0.42125400	0.24730200
	C	-2.68137100	-0.61539200	-0.21224400
	H	-3.03343700	-1.64121100	-0.18226000
	C	-3.51660000	0.32972400	-0.64693100
	H	-3.24287800	1.37435500	-0.70576700
	H	-4.51970900	0.07929700	-0.96197700
	C	-0.76030900	0.98880600	0.22531300
	H	-1.38536600	1.61438300	0.86718900
	H	-0.88305000	1.39600300	-0.78294400
	C	0.70113000	1.17302600	0.65733000
	H	0.88483000	0.78443900	1.65859400
	H	0.90677800	2.24941400	0.69059200
	C	1.66388900	0.56534800	-0.29252000
	H	1.58752700	0.67417000	-1.37194700
O	3.52766000	-0.63612000	-0.74395700	
O	2.63089700	-0.10089500	0.14759700	
Anti-C7-CIs-6	C	-2.29801600	1.84595100	-0.05353700
	H	-1.68854700	2.71188900	0.16719000
	H	-3.29429200	2.03320900	-0.43209300
	C	-1.84755000	0.60049700	0.13713100
	C	-2.71009600	-0.54425800	-0.16365000
	H	-3.67419500	-0.29106600	-0.59246300
	C	-2.42950400	-1.83166600	0.04573000

	H	-1.49451900	-2.16538100	0.47555400
	H	-3.14378200	-2.60376100	-0.20233700
	C	-0.44484400	0.35837900	0.64008700
	H	-0.45048200	-0.40405600	1.42213800
	H	-0.05242800	1.26919500	1.09071400
	C	0.50824900	-0.08066500	-0.50265600
	H	0.59994100	0.71513500	-1.24027900
	H	0.08467800	-0.95581900	-1.00254600
	C	1.84761300	-0.43428700	0.01312100
	H	2.02930100	-1.25643700	0.70161300
	O	4.07393900	-0.07223100	0.18535400
	O	2.84221300	0.25515400	-0.32096100
Anti-C7-ClIs-7	C	-0.99463500	-1.40299700	1.06884500
	H	-0.15224000	-1.66711600	1.69299800
	H	-1.67815400	-2.19595400	0.79832600
	C	-1.18340800	-0.15187700	0.64827200
	C	-2.29178600	0.22447300	-0.24751200
	H	-2.75105600	1.19041800	-0.05067400
	C	-2.73946800	-0.49756600	-1.27259000
	H	-2.28228800	-1.44129700	-1.54117500
	H	-3.57360300	-0.16378500	-1.87439000
	C	-0.27019400	0.97809900	1.07126300
	H	0.40099500	0.64549400	1.86133300
	H	-0.87383700	1.79063300	1.48382800
	C	0.54638900	1.55632500	-0.09502600
	H	1.02406300	2.49848500	0.20339500
	H	-0.10547300	1.81827000	-0.93424500

	C	1.61690800	0.67264500	-0.61969900
	H	2.14242500	0.86671400	-1.55158200
	O	2.99372400	-1.11663400	-0.45840500
	O	1.97456800	-0.33542500	0.03226400
Syn-C7-CIs-1	C	2.67271100	-1.30941400	-0.16096100
	H	2.46820900	-2.33750100	-0.42888100
	H	3.69214700	-1.06927000	0.11144600
	C	1.71566800	-0.37338800	-0.17570100
	C	2.03070700	1.01267100	0.17887100
	H	3.05940000	1.18578000	0.47886600
	C	1.18566200	2.04565000	0.15405900
	H	0.14499600	1.94860500	-0.12884700
	H	1.52481500	3.03556300	0.42696900
	C	0.29750100	-0.72968800	-0.54833800
	H	0.28217200	-1.69807900	-1.04725000
	H	-0.11532900	0.00818300	-1.23435800
	C	-0.62302400	-0.79671200	0.70836700
	H	-0.54469900	0.14904500	1.24824300
	H	-0.30894600	-1.61624300	1.35247000
	C	-2.03122000	-0.97393100	0.32803500
	H	-2.58009800	-1.90462300	0.42168800
	O	-2.15537900	1.18107300	-0.34527200
	O	-2.73345700	-0.05014700	-0.16801900
Syn-C7-CIs-2	C	2.78620900	-0.75159500	0.13903600
	H	2.94442900	-1.79517400	-0.09933300
	H	3.60544100	-0.23072900	0.61733400
	C	1.63741700	-0.12931100	-0.15463800

	C	1.47133200	1.29005300	0.16615000
	H	2.29533700	1.73660300	0.71399800
	C	0.43141700	2.06019100	-0.16271200
	H	-0.42289900	1.69763600	-0.72010100
	H	0.41216900	3.10382700	0.11953700
	C	0.49772900	-0.88255700	-0.79656600
	H	0.89074500	-1.74666000	-1.33082200
	H	-0.03474000	-0.26876100	-1.51833800
	C	-0.53643500	-1.43529400	0.22820700
	H	-0.03137400	-2.09756900	0.92995300
	H	-1.28601800	-1.99329900	-0.34235900
	C	-1.28457800	-0.42206200	0.99177000
	H	-1.14193600	-0.22902600	2.04846600
	O	-2.45100200	0.15103900	-0.85324200
	O	-2.20521000	0.27978700	0.49251500
Syn-C7-CIs-3	C	-0.37795500	1.52331200	-0.18594600
	H	0.67848600	1.49240800	-0.42148600
	H	-0.79536100	2.50551000	-0.00508300
	C	-1.16398300	0.44063300	-0.12743900
	C	-2.59093900	0.59821500	0.16708900
	H	-2.91272500	1.62070100	0.33555500
	C	-3.50333400	-0.37316600	0.23661700
	H	-3.26406000	-1.41577400	0.07670000
	H	-4.53729700	-0.14722800	0.45618800
	C	-0.65823700	-0.96385300	-0.36451600
	H	-1.16402100	-1.38288500	-1.23787100
	H	-0.95970600	-1.59506200	0.47731300

	C	0.85779100	-1.09555500	-0.58099400
	H	1.21739200	-0.48110100	-1.40119700
	H	1.08020800	-2.14134500	-0.82176900
	C	1.62265300	-0.76180800	0.63740900
	H	1.41220700	-1.22636700	1.59582400
	O	2.94389200	0.75766100	-0.42142600
	O	2.57222100	0.06289900	0.70298900
Syn-C7-CIs-4	C	-0.81357700	1.97730600	-0.03077400
	H	0.12131500	2.38963100	0.32450500
	H	-1.46306100	2.63911300	-0.58928200
	C	-1.15581900	0.70599100	0.21375400
	C	-2.43475300	0.18665200	-0.27510300
	H	-3.02567800	0.88957300	-0.85388300
	C	-2.92882200	-1.03596100	-0.06988900
	H	-2.40468700	-1.78903900	0.50301000
	H	-3.89346800	-1.31971400	-0.46637300
	C	-0.21574700	-0.20582300	0.96559700
	H	-0.76002400	-0.80291600	1.69812800
	H	0.52402400	0.37985500	1.50469500
	C	0.54711700	-1.19155700	0.03503600
	H	-0.14843400	-1.83590400	-0.49856400
	H	1.21400900	-1.79247400	0.65937800
	C	1.39070600	-0.48492500	-0.94533600
	H	1.17081100	-0.41973800	-2.00440800
	O	2.83860400	0.12409700	0.68048000
	O	2.45271600	0.11984200	-0.63509400
Syn-C7-CIs-5	C	-0.86035000	1.53319000	-1.32255400

	H	-0.27038900	2.43517200	-1.22686900
	H	-1.27238800	1.32155600	-2.30001200
	C	-1.06719900	0.71323900	-0.28631500
	C	-1.88596100	-0.48884800	-0.44760400
	H	-2.20699100	-0.69061000	-1.46362500
	C	-2.26362800	-1.32812500	0.51652300
	H	-1.97793100	-1.19911500	1.55189500
	H	-2.87571800	-2.19033000	0.29362800
	C	-0.43796200	1.00230300	1.05483800
	H	-1.15649100	0.84799300	1.86094900
	H	-0.13779000	2.04984800	1.09977500
	C	0.79549800	0.10182700	1.35284800
	H	0.52482400	-0.94894800	1.27843800
	H	1.15363300	0.32718000	2.35990200
	C	1.89577500	0.36309500	0.40526800
	H	2.55941500	1.21705300	0.48969700
	O	1.40900800	-1.46291200	-0.85288800
	O	2.16634000	-0.35582400	-0.59483700
Syn-C7-CIs-6	C	2.21198000	-0.77787200	0.97947100
	H	2.40406900	-1.84248700	0.98264600
	H	2.68810000	-0.19291700	1.75490700
	C	1.41503800	-0.20915900	0.06957500
	C	1.18713300	1.23665700	0.08884500
	H	1.51315200	1.74265100	0.99037200
	C	0.63882500	1.96444100	-0.88545500
	H	0.30856400	1.53565900	-1.82225100
	H	0.51045900	3.03199900	-0.77759500

	C	0.71870900	-1.04882900	-0.97100900
	H	1.22056700	-2.01221000	-1.05457600
	H	0.77776800	-0.58070000	-1.95495300
	C	-0.77170800	-1.35530100	-0.63573500
	H	-0.82277200	-1.81957000	0.34925600
	H	-1.14633100	-2.04597000	-1.39465000
	C	-1.68155200	-0.19295100	-0.61931600
	H	-2.18761100	0.17893100	-1.50319200
	O	-1.42893400	0.10436400	1.61098500
	O	-2.01813000	0.43347300	0.42298700
Syn-C7-CIs-7	C	1.58169200	2.00106400	0.10393100
	H	0.75377900	2.67515000	-0.06854000
	H	2.50328400	2.43591000	0.46880800
	C	1.47354700	0.68635100	-0.12163300
	C	2.61726700	-0.19489000	0.12215300
	H	3.49777400	0.29713400	0.52294100
	C	2.67613200	-1.50850200	-0.10484100
	H	1.84389300	-2.06902100	-0.50927100
	H	3.57660500	-2.06929400	0.10194000
	C	0.16963400	0.09916200	-0.60249600
	H	0.34956100	-0.63330500	-1.39100100
	H	-0.46452200	0.88109300	-1.01202100
	C	-0.60777000	-0.58061200	0.56441800
	H	-0.79980500	0.18324600	1.32154200
	H	-0.02366600	-1.39167100	0.99408400
	C	-1.91116700	-1.09073400	0.11468400
	H	-2.13650300	-2.13804400	-0.05397800

	O	-2.74102000	1.01046300	0.02948100
	O	-2.89603100	-0.34074100	-0.13345600
Syn-C7-CIs-8	C	-0.65125800	-1.13928000	-0.58473800
	H	0.40897300	-1.27789600	-0.75654400
	H	-1.26982500	-2.02153500	-0.67737100
	C	-1.20497100	0.04284900	-0.30363500
	C	-2.65350000	0.20319600	-0.07639800
	H	-3.08319900	1.13841900	-0.42649500
	C	-3.44798900	-0.66852300	0.54023200
	H	-3.06468200	-1.59257300	0.95369000
	H	-4.50624500	-0.47917200	0.65548400
	C	-0.42479100	1.33773700	-0.22087000
	H	-0.67068700	1.83871000	0.72165400
	H	-0.77819800	2.01266300	-1.00594500
	C	1.09971300	1.20553800	-0.35197700
	H	1.53597200	2.21095900	-0.35950100
	H	1.39556800	0.70620100	-1.27026900
	C	1.69162500	0.48545600	0.79374800
	H	1.49361900	0.77417100	1.82139200
	O	2.79444900	-1.00985400	-0.51879900
	O	2.46626800	-0.50411900	0.71451500
Syn-C7-CIs-9	C	-0.65348100	-1.21561700	-0.08755300
	H	0.36946000	-1.40047200	-0.39156200
	H	-1.23951700	-2.08553200	0.17574200
	C	-1.19622000	0.00329400	-0.02742500
	C	-2.60869100	0.21984600	0.33724800
	H	-2.81585700	1.11667900	0.91553400

	C	-3.62962500	-0.56004100	-0.01111600
	H	-3.48872000	-1.43644000	-0.63050800
	H	-4.63892500	-0.33896200	0.30756500
	C	-0.42959600	1.27740800	-0.31073300
	H	-0.57664600	1.96636000	0.52875500
	H	-0.87496200	1.77885800	-1.17427700
	C	1.07330200	1.10450000	-0.57706200
	H	1.49475100	2.08316500	-0.83353500
	H	1.27259100	0.42943100	-1.40445100
	C	1.79577700	0.61983200	0.61620200
	H	1.70947200	1.10843200	1.58180700
	O	2.76507200	-1.11659300	-0.48815400
	O	2.56987200	-0.37301300	0.64909900
Syn-C7-CIs-10	C	-1.17504700	-1.74681600	-0.33375400
	H	-0.33213400	-2.42467500	-0.31688800
	H	-2.03763200	-2.04199300	-0.91562800
	C	-1.15620400	-0.60264400	0.35331900
	C	-2.27359200	0.35784400	0.32567700
	H	-2.47516400	0.87027100	1.26315800
	C	-3.01135900	0.66390100	-0.73962000
	H	-2.81931200	0.21842900	-1.70756300
	H	-3.82798000	1.36977500	-0.67539100
	C	0.02796100	-0.21913600	1.20820200
	H	0.74392500	-1.03457000	1.26603000
	H	-0.30583000	0.00848200	2.22380100
	C	0.76657600	1.04284000	0.68032900
	H	1.61867800	1.23581900	1.33709800

	H	0.09690200	1.90180500	0.67216400
	C	1.29673800	0.83794100	-0.67904600
	H	0.87404500	1.28367600	-1.57186300
	O	2.90935000	-0.52943300	0.11933900
	O	2.29240800	0.10560700	-0.92753300
Syn-C7-CIs-11	C	-2.42988400	-1.42924000	-0.32789500
	H	-2.18697600	-2.48110500	-0.40172900
	H	-3.47845200	-1.16851700	-0.28590100
	C	-1.47727100	-0.49411200	-0.31826200
	C	-1.76780400	0.94579500	-0.19767300
	H	-1.09022300	1.60388400	-0.73408600
	C	-2.74249000	1.48216800	0.53344000
	H	-3.40542800	0.87168300	1.13344500
	H	-2.89993000	2.55154700	0.55926100
	C	-0.01888600	-0.85028100	-0.46316100
	H	0.41288000	-0.28915100	-1.29304200
	H	0.09288300	-1.91334500	-0.67398400
	C	0.78518900	-0.48740700	0.82006700
	H	0.47083800	-1.11840700	1.64999100
	H	0.59322700	0.56200200	1.05914600
	C	2.23115100	-0.62706400	0.60114600
	H	2.83875800	-1.43537800	0.99263700
	O	2.24513300	1.25759400	-0.64610500
	O	2.90141600	0.18961000	-0.09035900
Syn-C7-CIs-12	C	-2.68616700	0.64787000	0.60481000
	H	-3.05266400	1.66414400	0.67441200
	H	-3.33542800	-0.13758400	0.96558900

	C	-1.47956100	0.37061900	0.10851300
	C	-0.98243700	-1.01523300	0.00918800
	H	0.00029900	-1.21296700	0.43190200
	C	-1.66393600	-2.01838000	-0.53860800
	H	-2.63990100	-1.86500900	-0.98211400
	H	-1.26053800	-3.02165500	-0.56133600
	C	-0.57622900	1.48094500	-0.38525900
	H	-0.98211400	2.44191500	-0.07198400
	H	-0.58075800	1.48251300	-1.48041900
	C	0.89184200	1.39273700	0.10872400
	H	0.95189300	1.10499200	1.15470600
	H	1.34267000	2.38406100	-0.00767700
	C	1.71460200	0.46901100	-0.69640200
	H	1.86249700	0.61388500	-1.76203000
	O	2.21612400	-0.88716900	1.05948100
	O	2.33204500	-0.54029400	-0.26283700
Syn-C7-CIs-13	C	1.20010800	1.83124500	-0.33747300
	H	0.33149600	2.42723400	-0.09922800
	H	1.99146400	2.34014600	-0.87115400
	C	1.31968400	0.54259100	0.00423300
	C	2.55141400	-0.17333600	-0.34515400
	H	3.29833000	0.42158700	-0.86055100
	C	2.82445100	-1.45325000	-0.08793600
	H	2.13009300	-2.11112100	0.41610100
	H	3.76827100	-1.88752700	-0.38640400
	C	0.26294200	-0.23451300	0.75093900
	H	0.68319600	-0.56897000	1.70252100

	H	0.01314500	-1.14041100	0.19877000
	C	-1.05779100	0.50603100	1.05549300
	H	-0.87242000	1.45132700	1.56305700
	H	-1.65083800	-0.14729000	1.70147200
	C	-1.87237400	0.74331400	-0.15018600
	H	-2.02050700	1.71062800	-0.61522000
	O	-2.38928100	-1.45557000	-0.26143400
	O	-2.49107400	-0.17794100	-0.74967400
Syn-C7-ClIs-14	C	1.17606900	1.74685700	-0.33620300
	H	0.33383500	2.42557000	-0.32022500
	H	2.03898500	2.04043700	-0.91839000
	C	1.15605200	0.60356900	0.35233000
	C	2.27242500	-0.35810700	0.32578500
	H	2.47357800	-0.86962400	1.26385400
	C	3.00972300	-0.66628900	-0.73924200
	H	2.81792400	-0.22187300	-1.70771900
	H	3.82563400	-1.37290600	-0.67423900
	C	-0.02827600	0.22263300	1.20812500
	H	-0.74417800	1.03829300	1.26336100
	H	0.30537000	-0.00189400	2.22447600
	C	-0.76696100	-1.04083800	0.68399700
	H	-1.61961800	-1.23124500	1.34080100
	H	-0.09762400	-1.90007700	0.67915100
	C	-1.29605500	-0.84023100	-0.67643600
	H	-0.87287400	-1.28919000	-1.56741800
	O	-2.90864400	0.53047500	0.11637100
	O	-2.29121800	-0.10835800	-0.92809600

Syn-C7-CIs-15	C	-1.68147000	-1.79253400	-0.45334700
	H	-0.86779500	-2.50184000	-0.47936700
	H	-2.64928800	-2.16448700	-0.76204300
	C	-1.52783300	-0.51805500	-0.07691400
	C	-2.68997200	0.37672300	-0.08335700
	H	-3.62409300	-0.08835900	-0.38114500
	C	-2.69665200	1.67321600	0.22959100
	H	-1.80554300	2.20912600	0.52627500
	H	-3.61150400	2.24743800	0.18824000
	C	-0.20939000	0.07338900	0.35856300
	H	-0.33635000	0.50609700	1.35443500
	H	0.05497100	0.89440700	-0.30910000
	C	0.97310700	-0.91810700	0.38352000
	H	1.13571100	-1.29441100	-0.63025600
	H	0.76904200	-1.74584400	1.06164000
	C	2.21772600	-0.25045200	0.79858400
	H	2.68061400	-0.36891400	1.77197000
	O	2.37908900	0.77238800	-1.20921400
O	2.86355400	0.53282400	0.04915300	

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