Supplement of

Elucidation of the myrcene ozonolysis mechanism from a Criegee Chemistry perspective

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Table S1 The conformers, the Gibbs free energy and the Boltzmann distribution of anti-(CH_2=CH)-CH(CH_2)-CH_2CH_2CHOO obtained at DLPNO-CCSD(T)/CBS// B3LYP-D3(BJ)/aug-cc-pVTZ.

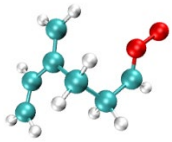
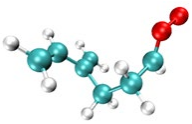
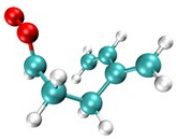
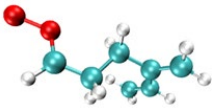
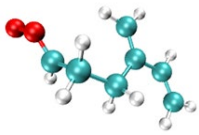
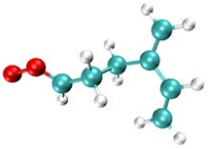
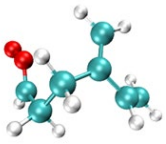
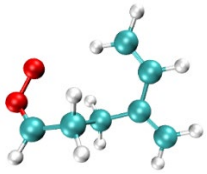
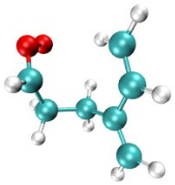
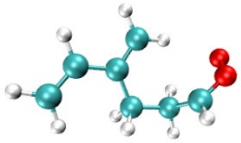
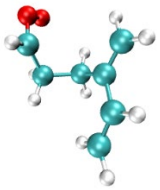
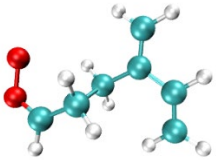
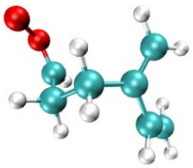
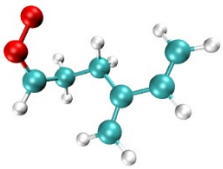
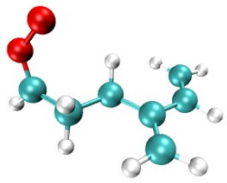
No.	Conformers	ΔG (kcal/mol)	Boltzmann distribution (%)		
			298 K	35 K	6 K
A1		0.55	11.03	0.02	0
A2		0	27.93	59.45	92.13
A3		1.04	4.86	0	0
A4		0.03	26.58	39	7.87
A5		0.59	10.24	0	0
A6		0.26	18.15	1.51	0
A7		1.86	1.20	0	0

Table S2 The conformers, the Gibbs free energy and the Boltzmann distribution of syn-(CH_2=CH)-CH(CH_2)-CH_2CH_2CHOO 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

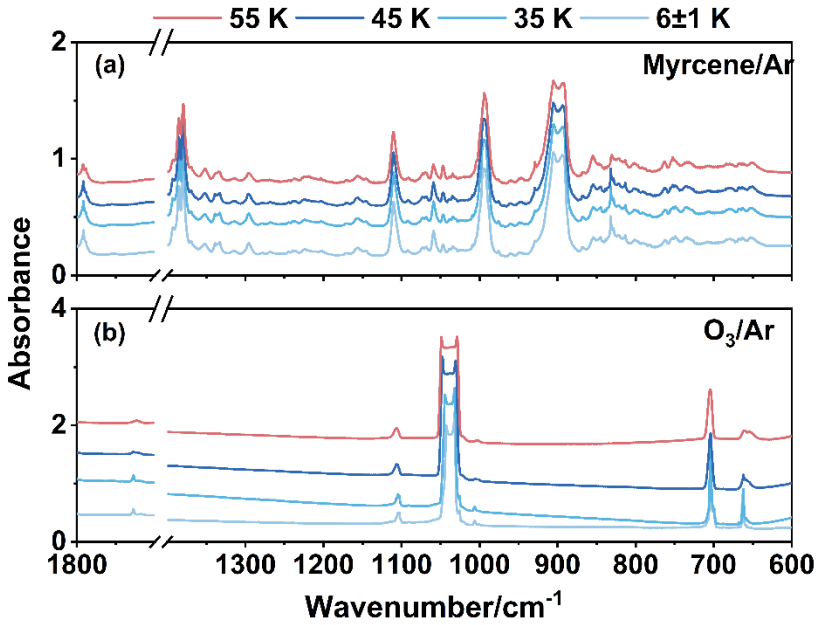


Figure S1 The IR spectra of precursor (myrcene/Ar and O_3/Ar) in a low temperature after annealing to 35 K, 45 K and 55 K.

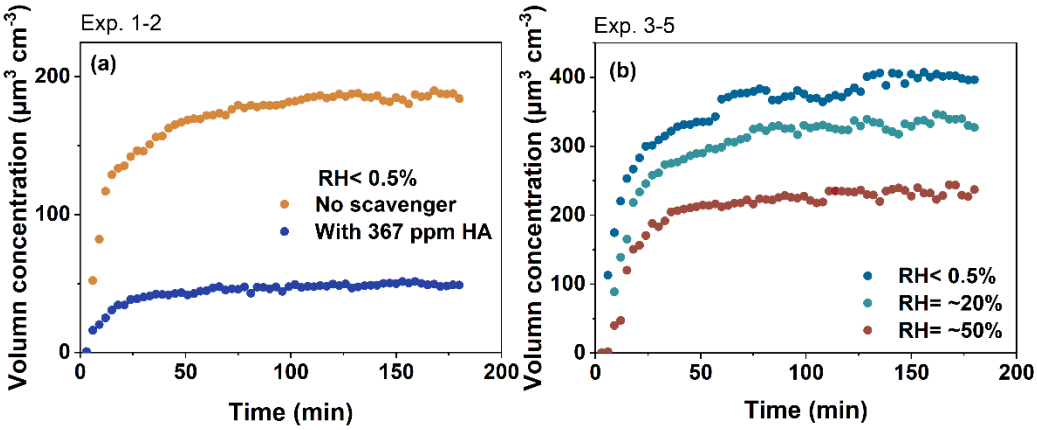


Figure S2 Time series of particle volume concentration in myrcene ozonolysis under different condition. (a) depict particle formation processes in Exp. 1-2 from Table 2, while (b) illustrate particle formation processes in Exp. 3-5 of Table 2.

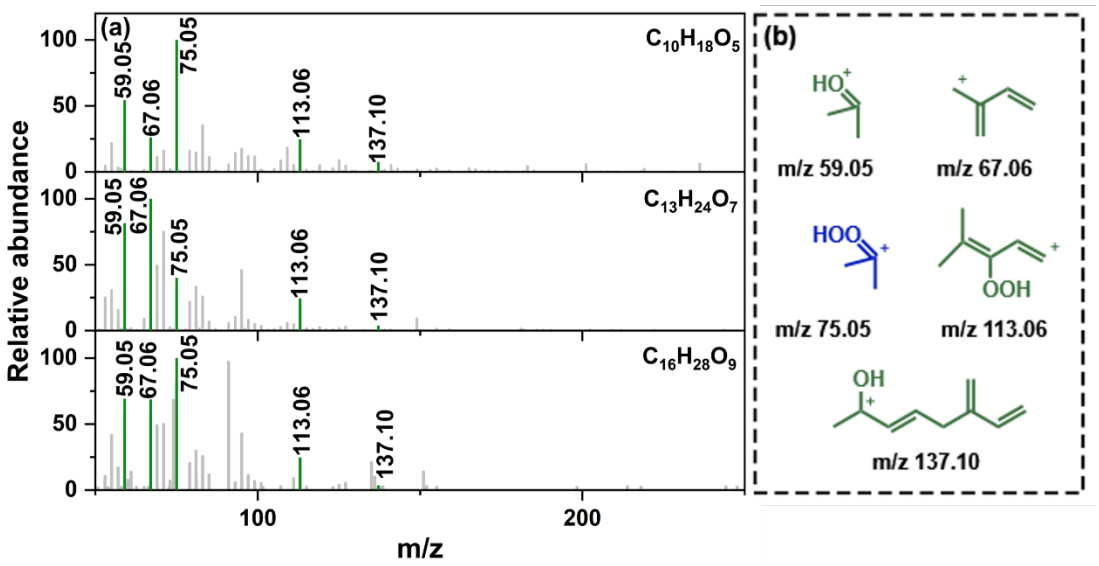
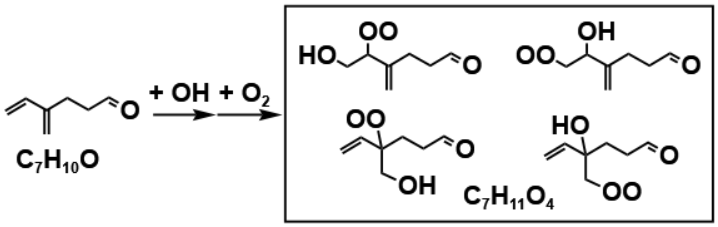


Figure S3 The MS/MS of $C_{10}H_{17}O_5$ + n-C3-SCIs + HO_2 sequence (a) and chemical structures of ions corresponding to major fragment peaks in MS/MS spectra (b).



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