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Supplement of

SIM-HOM (version 1.0): a mechanistic module for the formation of highly oxygenated organic molecules from isoprene, monoterpene and sesquiterpene evaluated with ADCHAM (version 1.0)

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S1. Species naming convention

In Caltech isoprene mechanism, names of most species generally follow the stable precursor names (e.g., ISOP for isoprene, MVK for methyl vinyl ketone, MACR for methacrolein). Functional groups are added to the precursor name based on their position, with the carbon number of the attached functional group preceding it in ascending order (i.e. groups on C1 are listed before those on C2). Carbon numbers are those assigned to the parent compound (isoprene, MVK, or MACR). For stereoisomers, the designation "E", "Z", "c" (cis) or "t" (trans) is appended to the end of the name. Stabilized Criegee Intermediate (SCI) are marked with "ci" before the precursor name and "OO" following. Hot radicals are denoted by a lowercase "x" at the end of the name, while alkyl radicals are denoted by an "R" at the radical position. And MCM naming convention primarily composed of the total number of carbon atoms in the carbon backbone, unique numbers and specific functional groups attached to the backbone. The following summarizes the different names for the two mechanisms and elemental composition of substances in the isoprene oxidation system:

Table S1. Correspondence and elemental composition of species in Caltech and MCM

NrC	NrH	NrN	NrO	Caltech name	MCM name
1	2	0	2	HCOOH	HCOOH
1	2	0	2	ciCH2OO	CH2OOE
1	3	0	2	CH3OO	CH3O2
2	2	0	2	GLYX	GLYOX
2	4	0	2	GLYC	HOCH2CHO
5	8	0	0	ISOP	C5H8
4	6	0	1	MACR	MACR
4	6	0	1	MVK	MVK
3	4	0	2	MGLY	MGLYOX
3	5	0	2	CH3COOCH2	CH3C2H2O2
2	2	0	3	FAH	CHOOCHO
3	6	0	2	HAC	ACETOL
2	3	0	3	CH3CO3	CH3CO3
2	4	0	3	HPETHNL	HCOCH2OOH
5	6	0	1	M3F	M3F
5	9	0	1	ISOP1OHc	CISOPA
5	9	0	1	ISOP4OHc	CISOPC
5	9	0	1	ISOP1OHt	TISOPA
5	9	0	1	ISOP4OHt	TISOPC
4	6	0	2	ciMVKOO	MVKOOA
4	6	0	2	ciMACROO	MACROOA
4	6	0	2	MACROO	MACROO
4	6	0	2	MVKOO	MVKOO
4	6	0	2	MACR1OH	MACO2H
4	6	0	2	MVKENOL	HVMK
4	6	0	2	MACRENOL	HMAC
4	6	0	2	HMACR	HMACR

3	4	0	3	PYRAC	CH3COCO2H
3	6	0	3	HPAC	HYPERACET
2	3	0	4	HPA	HOCH2CO3
2	4	0	4	HPMF	CHOOCH2OOH
5	6	0	2	ISOP1CO4CO	C4MDIAL
4	4	0	3	MVK3CO4CO	CO23C3CHO
5	8	0	2	ISOP1OH4CO	HC4ACHO
5	8	0	2	ISOP3CO4OH	HCOC5
5	8	0	2	ISOP1CO4OH	HC4CCHO
4	5	0	3	MACR2O3CO	C3MDIALO
4	5	0	3	MVK3O4CO	C4CO2O
4	5	0	3	MVK3CO4O	BIACETO
4	5	0	3	MACR1OO	MACO3
5	9	0	2	ISOP1OH2O	ISOPBO
5	9	0	2	ISOP1OH4Oc	CISOPAO
5	9	0	2	ISOP3O4OH	ISOPDO
5	9	0	2	ISOP1O4OH	CISOPCO
5	9	0	2	ISOP1OH4Ot	ISOPAO
4	6	0	3	HMML	HMML
4	6	0	3	MVK3OH4CO	CO2H3CHO
4	6	0	3	MACR1OOH	MACO3H
4	6	0	3	MVK3CO4OH	BIACETOH
4	6	0	3	MACR2OH3CO	C3MDIALOH
5	10	0	2	ISOP1OH2OH	ISOPBOH
5	10	0	2	ISOP1OH4OH	ISOPAOH
5	10	0	2	ISOP3OH4OH	ISOPDOH
4	7	0	3	MVK3OH4O	HMVKAO
4	7	0	3	MACR2O3OH	MACRO
4	7	0	3	MACR2OH3O	MACROHO
4	7	0	3	MVK3O4OH	HMVKBO
4	8	0	3	MACR2OH3OH	MACROH
4	8	0	3	MVK3OH4OH	HO12CO3C4
5	5	0	3	ISOP1CO4O4CO	C3MCODBCO2
5	5	0	3	ISOP1CO1O4CO	MC3CODBCO2
5	6	0	3	ISOP1CO1OH4CO	MC3ODBCO2H
5	8	0	3	ISOP1CO23O4OH	IEB1CHO
5	8	0	3	ISOP1OH3CO4OH	C524CO
5	8	0	3	ISOP12O3OH4CO	IECCHO
5	8	0	3	ISOP1OH23O4CO	IEB4CHO
5	8	0	3	ISOP1CO1OH4OH	HC4CCO2H
5	8	0	3	ISOP1OOH4COc	C5HPALD2
5	8	0	3	ISOP1CO4OOHc	C5HPALD1
5	8	0	3	ISOP1OH4CO4OH	HC4ACO2H

5	8	0	3	ISOP1CO2OH34O	IEACHO
4	5	0	4	MVK3CO4OO	BIACETO2
4	5	0	4	MACR2OO3CO	C3MDIALO2
5	9	0	3	ISOP1OH3O4OH	C524O
5	9	0	3	ISOP1OH2OO	ISOPBO2
5	9	0	3	ISOP1OH4OOc	CISOPAO2
5	9	0	3	ISOP3OO4OH	ISOPDO2
5	9	0	3	ISOP1OO4OHc	CISOPCO2
5	9	0	3	ISOP1OH4OOt	ISOPAO2
5	9	0	3	ISOP1OO4OHt	ISOPCO2
4	6	0	4	MVK3CO4OOH	BIACETOOH
4	6	0	4	MACR2OOH3CO	C3MDIALOOH
4	6	0	4	MVK3OOH4CO	C4CO2OOH
5	10	0	3	ISOP1OH2OOH	ISOPBOOH
5	10	0	3	ISOP1OH4OOHt/c	ISOPAOOH
5	10	0	3	ISOP3OOH4OH	ISOPDOOH
5	10	0	3	ISOP1OOH4OHt/c	ISOPCOOH
5	10	0	3	ISOP12O3OH4OH	IEPOXC
5	10	0	3	ISOP1OH2OH34O	IEPOXA
5	10	0	3	ISOP1OH3OH4OH	C524OH
5	10	0	3	ISOP1OH23O4OHc(t)	IEPOXB
4	7	0	4	MACR2OO3OH	MACRO2
4	7	0	4	MACR2OH3OO	MACROHO2
4	7	0	4	MVK3OH4OO	HMVKAO2
4	7	0	4	MVK3OO4OH	HMVKBO2
4	8	0	4	MACR2OOH3OH	MACROOH
4	8	0	4	MACR2OH3OOH	MACROHOOH
4	8	0	4	MVK3OH4OOH	HMVKAOOH
4	8	0	4	MVK3OOH4OH	HMVKBOOH
5	5	0	4	ISOP1CO4OO4CO	C3MCODBCO3
5	5	0	4	ISOP1CO1OO4CO	MC3CODBCO3
5	6	0	4	ISOP1CO4CO4OOH	C5PACALD2
5	6	0	4	ISOP1CO1OOH4CO	C5PACALD1
5	7	0	4	ISOP1CO1OO4OH	HC4CCO3
5	7	0	4	ISOP1OH4CO4OO	HC4ACO3
5	7	0	4	ISOP1CO2O3OH4CO	C4M2ALOHO
5	8	0	4	ISOP1CO2OH3OH4CO	C4M2AL2OH
5	8	0	4	ISOP1CO1OOH4OH	HC4CCO3H
5	8	0	4	ISOP1OH4CO4OOH	HC4ACO3H
4	5	0	5	MACR2OH3CO3OO	CHOMOHCO3
4	5	0	5	MVK3OH4CO4OO	CO2H3CO3
5	9	0	4	ISOP1CO2OH3O4OH	C57AO
5	9	0	4	ISOP1OH2O3CO4OH	C59O

5	9	0	4	ISOP1CO2O3OH4OH	C57O
5	9	0	4	ISOP1OH2O3OH4CO	C58O
5	9	0	4	ISOP1OH2OH3O4CO	C58AO
5	9	0	4	ISOP1OH3OO4OH	C524O2
4	6	0	5	MVK3OH4CO4OOH	CO2H3CO3H
4	6	0	5	MACR2OH3CO3OOH	CHOMOHCO3H
5	10	0	4	ISOP1OH3OOH4OH	C524OOH
4	8	0	5	MVK3OOH4OOH	DHPMEK
4	8	0	5	MACR2OOH3OOH	DHPMPAL
5	7	0	5	ISOP12O3OH4CO4OO	IECCO3
5	7	0	5	ISOP1CO1OO2OH34O	IEACO3
5	7	0	5	ISOP1CO2OO3OH4CO	C4M2ALOHO2
5	8	0	5	ISOP1CO1OOH2OH34O	IEACO3H
5	8	0	5	ISOP12O3OH4CO4OOH	IECCO3H
5	8	0	5	ISOP1CO2OOH3CO4OH	IEC2OOH
5	8	0	5	ISOP1CO2OOH3OH4CO	C4MALOHOOH
5	9	0	5	ISOP1CO2O3OOH4OH	C526O
5	9	0	5	ISOP1OH2OO3CO4OH	C59O2
5	9	0	5	ISOP1OH2O2COH3CO4OH	C525O
5	9	0	5	ISOP1OH2OOH3O4CO	C527O
5	9	0	5	ISOP1OOH2O3OH4CO	HPC52O
5	10	0	5	ISOP1OH2OOH3OH4CO	C58OOH
5	10	0	5	ISOP1OH2OOH3CO4OH	C59OOH
5	7	0	6	ISOP1CO2O3OH4CO4OOH	C535O
5	7	0	6	ISOP1CO1OOH2O3OH4CO	C534O
5	9	0	6	ISOP1CO2O3OOH4OOH	C536O
5	9	0	6	ISOP1OOH2OOH3O4CO	C537O
5	9	0	6	ISOP1CO2OO3OOH4OH	C526O2
5	9	0	6	ISOP1OH2OOH3OO4CO	C527O2
5	9	0	6	ISOP1OH2OO2COH3CO4OH	C525O2
5	9	0	6	ISOP1OOH2OO3OH4CO	HPC52O2
5	10	0	6	ISOP1OH2OOH2COH3CO4OH	C525OOH
5	10	0	6	ISOP1OH2OOH3OOH4CO	C527OOH
5	10	0	6	ISOP1OOH2OOH3OH4CO	HPC52OOH
5	10	0	6	ISOP1CO2OOH3OOH4OH	C526OOH
5	7	0	7	ISOP1CO2OO3OH4CO4OOH	C535O2
5	7	0	7	ISOP1CO1OOH2OO3OH4CO	C534O2
5	8	0	7	ISOP1CO2OOH3OH4CO4OOH	C535OOH
5	8	0	7	ISOP1CO1OOH2OOH3OH4CO	C534OOH
5	9	0	7	ISOP1OOH2OOH3OO4CO	C537O2
5	9	0	7	ISOP1CO2OO3OOH4OOH	C536O2
5	10	0	7	ISOP1CO2OOH3OOH4OOH	C536OOH
5	10	0	7	ISOP1OOH2OOH3OOH4CO	C537OOH

5	9	0	8	ISOP1OOH2OOH3OH4CO4OO	HPC52CO3
5	10	0	8	ISOP1OOH2OOH3OH4CO4OOH	HPC52CO3H

S2. Chamber runs

The model simulations were constrained by the CLOUD chamber conditions. Specifically, the initial mixing ratios of VOCs and O_3, together with the chamber irradiation settings, were prescribed according to the experimental setup (see Table 1). These inputs provide the precursors and oxidants required for HOM formation.

The simulations were performed with the Aerosol Dynamics gas- and particle-phase chemistry model for laboratory CHAMber studies (ADCHAM)(Roldin et al., 2014). In this framework, the default chemical module was replaced by a detailed gas-phase kinetic mechanism generated by the Kinetic PreProcessor (KPP)(Damian et al., 2002). This mechanism, referred to as SIM-HOM (Sesquiterpene, Isoprene and Monoterpene-derived HOM mechanism), integrates the peroxy radical autoxidation mechanism (PRAM)(Roldin et al., 2019), the Master Chemical Mechanism version 3.3.1 (MCMv3.3.1), the Caltech isoprene mechanism(Wennberg et al., 2018), and additional reactions relevant for HOM formation. SIM-HOM explicitly represents peroxy radical (RO_2) chemistry and the production of highly oxygenated molecules (HOMs). A complete list of reactions is provided in the Code and data Availability section.

The removal of HOM was mainly through wall loss, which were parameterized by assuming irreversible uptake due to the extremely low vapor pressures of HOMs. Diffusion coefficients (D_i) were estimated as:

$$D_i(cm^{-3}s^{-1}) = 0.31 \cdot {M_i}^{-1/3} \quad (1)$$

where M_i (g mol^{-1}) is the mass of the molecule. The wall loss rate inside the chamber at each temperature is determined from the following expression:

$$k_{wall}(T) = C_{wall}(T) \cdot \sqrt{D_i} \quad (2)$$

where C_{wall} is an empirical parameter and set to 0.0075 cm^{-1} s$^{-0.5}$ at 5 °C in this study.

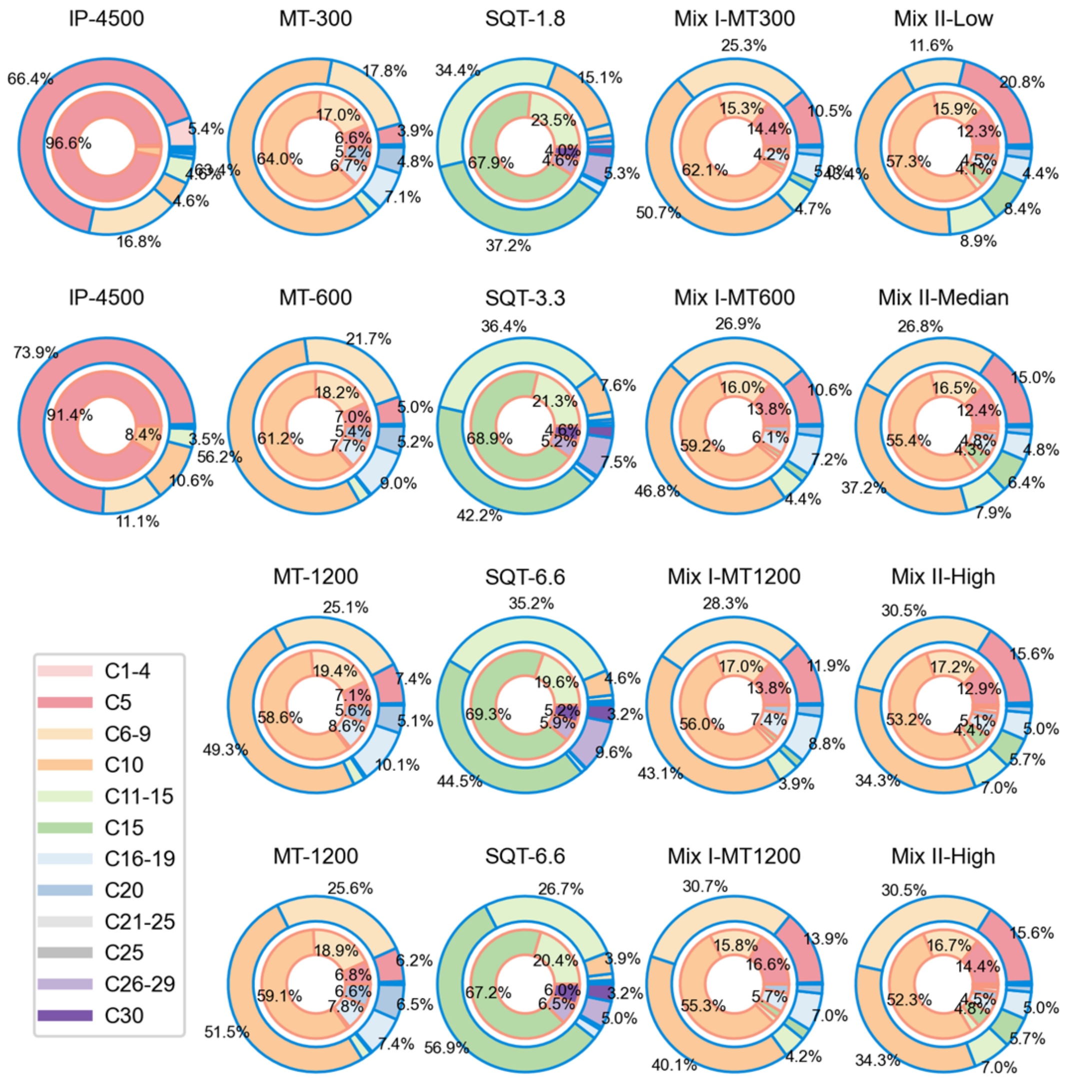

Figure S1. Carbon distributions in each system under all different experimental conditions. Blue and outer circles indicate observed values, pink and inner circles indicate simulated values. From left to right, they represent pure isoprene, monoterpene, and sesquiterpene systems, the mixed system of isoprene, monoterpene, and the mixed system of the three VOCs. The specific experimental conditions are shown in Table 1.

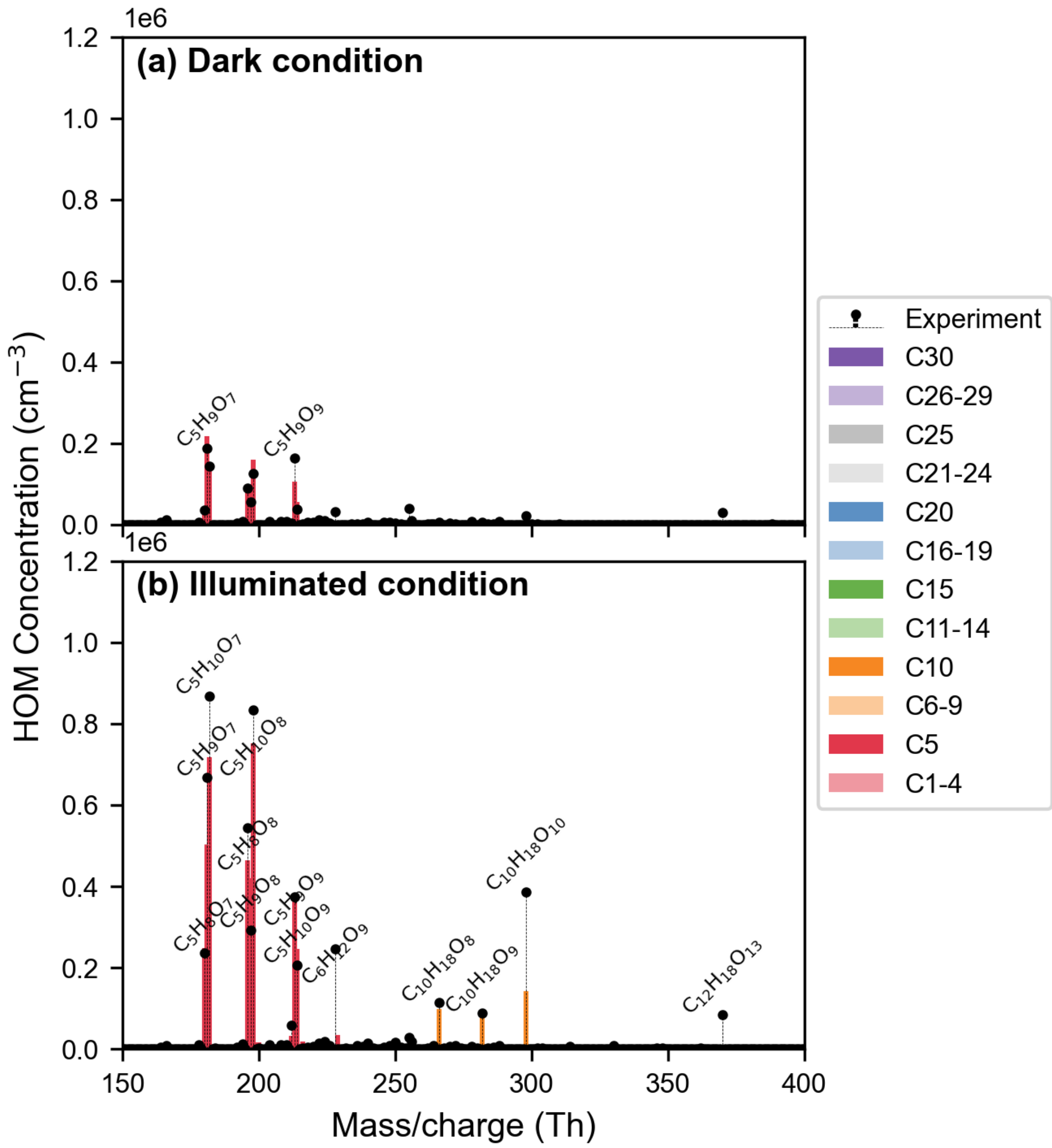

Figure S2. Comparisons between modeled and observed spectrum in isoprene oxidation experiment with around 4.5 ppb isoprene in (a) dark condition and (d) UV excimer laser (UVX) on. Mass/charge ratio is plotted in units of thomsons (Th) and it should be noted that the nitrate reagent ions has been removed from mass.

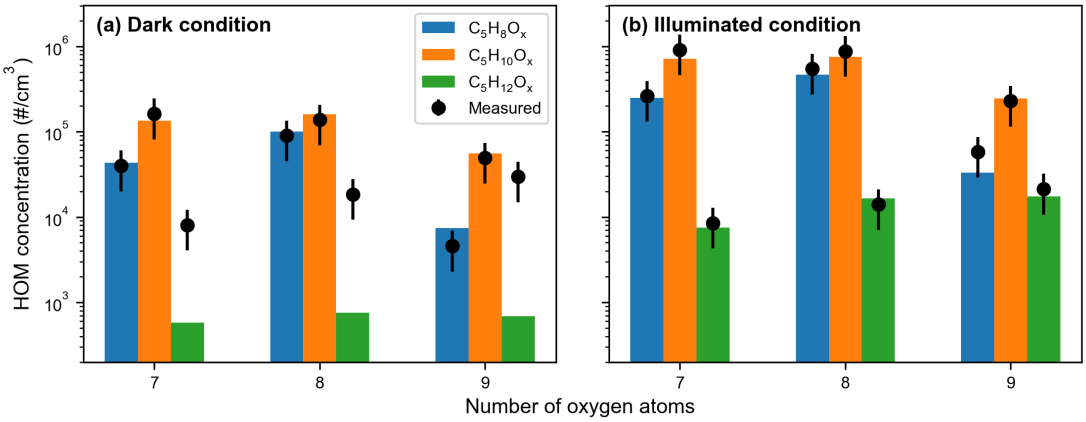

Figure S3. Comparison of simulated and observed representative oxidation products with 5 carbons for isoprene oxidation experiments. Blue, orange, and green colors indicate oxidation products with molecular formula $C_5H_8O_x$, $C_5H_{10}O_x$ and $C_5H_{12}O_x$, respectively. The measurement error of the HOM concentration varies within 50 % in experiments.

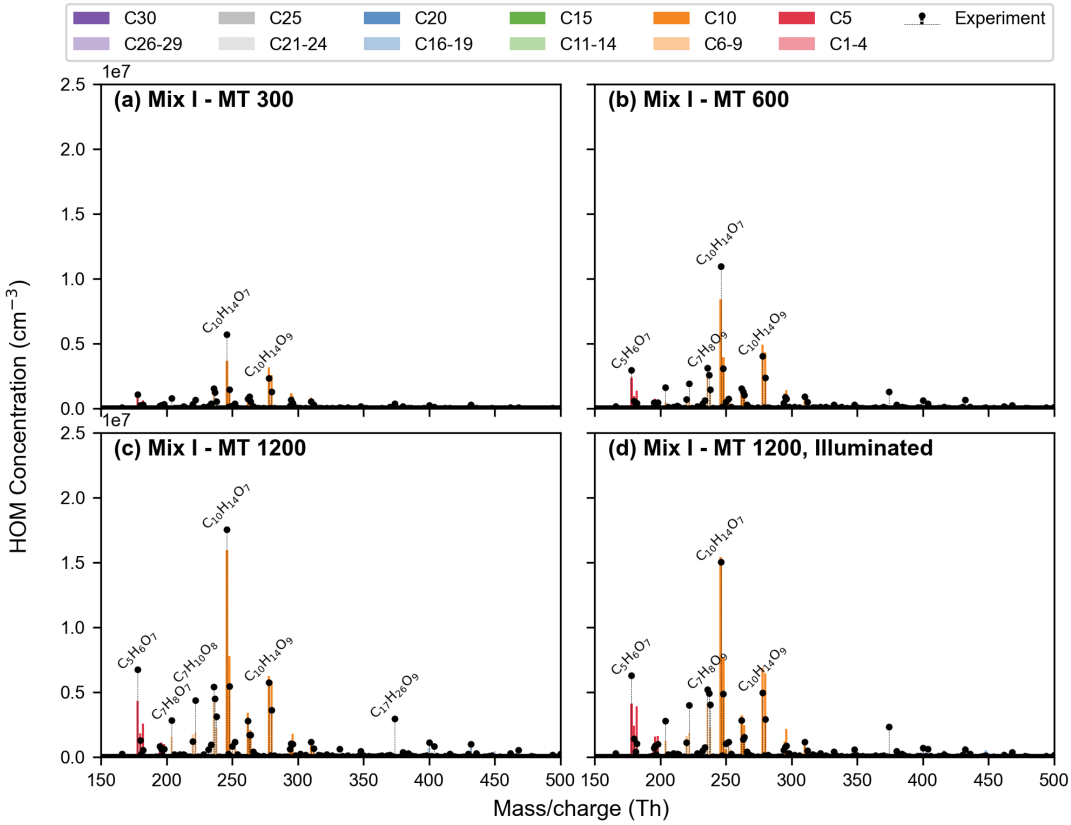

Figure S4. Comparisons between modeled and observed spectrum in mix system I of isoprene and monoterpene. These experiments are conducted under (a) 3962 ppt isoprene and 317 ppt monoterpene, (b) 3780 ppt isoprene and 618 ppt monoterpene, (c) 3588 ppt isoprene and 1116 ppt monoterpene and (d) 3396 ppt isoprene and 1096 ppt monoterpene in (a-c) dark condition and (d) Hamamatsu UV lamps (UVH) and UV excimer lasers (UVX) on. Mass/charge ratio is plotted in units of thomsons (Th) and it should be noted that the nitrate reagent ions has been removed from mass.

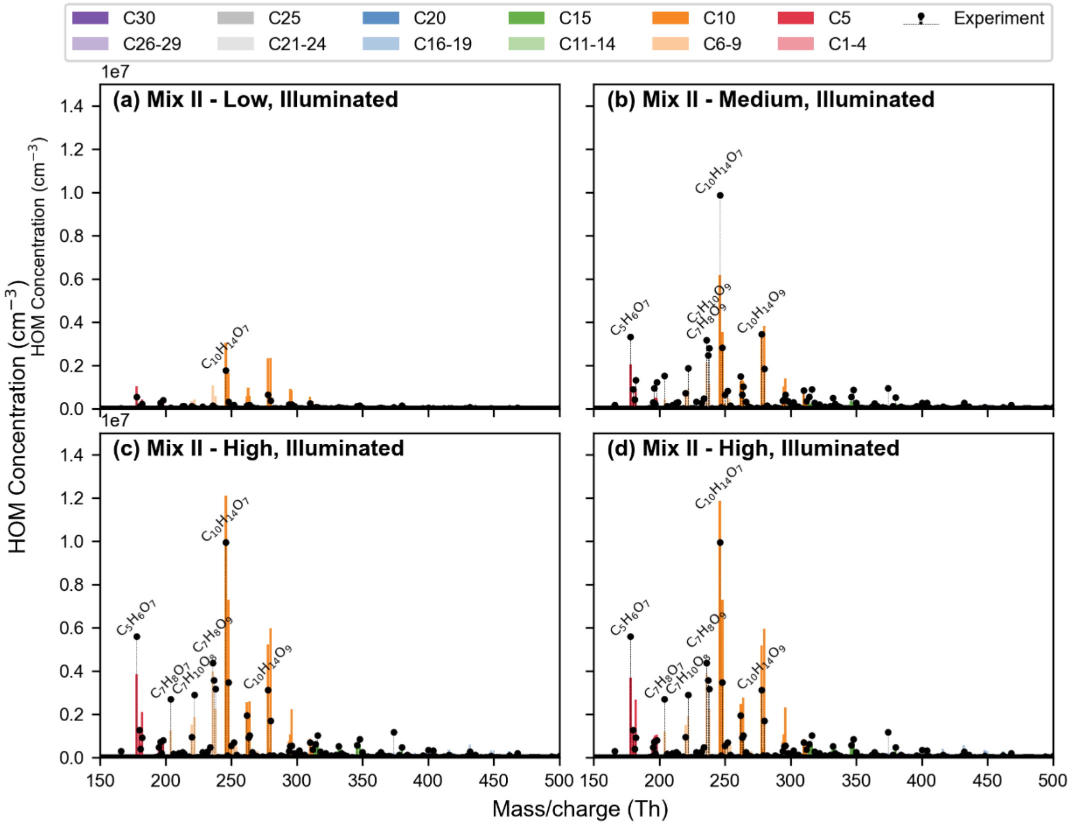

Figure S5. Comparisons between modeled and observed spectrum in mix system II of isoprene, monoterpene and sesquiterpene. These experiments are conducted under (a) 1471 ppt isoprene, 303 ppt monoterpene and 3 ppt sesquiterpene, (b) 2695 ppt isoprene, 578 ppt monoterpene and 7.1 ppt sesquiterpene, (c) 5749 ppt isoprene, 1168 ppt monoterpene and 15.8 ppt sesquiterpene and (d) 4578 ppt isoprene, 974 ppt monoterpene and 15.8 ppt sesquiterpene in (a-d) UVH on and (d) UVX on. Mass/charge ratio is plotted in units of thomsons (Th) and it should be noted that the nitrate reagent ions has been removed from mass.

Reference

Damian, V., Sandu, A., Damian, M., Potra, F., and Carmichael, G. R.: The kinetic preprocessor KPP - a software environment for solving chemical kinetics, Comput. Chem. Eng., 26, 1567-1579, 10.1016/s0098-1354(02)00128-x, 2002.

Roldin, P., Eriksson, A. C., Nordin, E. Z., Hermansson, E., Mogensen, D., Rusanen, A., Boy, M., Swietlicki, E., Svenningsson, B., Zelenyuk, A., and Pagels, J.: Modelling non-equilibrium secondary organic aerosol formation and evaporation with the aerosol dynamics, gas- and particle-phase chemistry kinetic multilayer model ADCHAM, Atmospheric Chemistry and Physics, 14, 7953-7993, 10.5194/acp-14-7953-2014, 2014.

Roldin, P., Ehn, M., Kurtén, T., Olenius, T., Rissanen, M. P., Sarnela, N., Elm, J., Rantala, P., Hao, L., Hyttinen, N., Heikkinen, L., Worsnop, D. R., Pichelstorfer, L., Xavier, C., Clusius, P., Öström, E., Petäjä, T., Kulmala, M., Vehkamäki, H., Virtanen, A., Riipinen, I., and Boy, M.: The role of highly oxygenated organic molecules in the Boreal aerosol-cloud-climate system, Nat. Commun., 10, 4370, 10.1038/s41467-019-12338-8, 2019.

Wennberg, P. O., Bates, K. H., Crounse, J. D., Dodson, L. G., McVay, R. C., Mertens, L. A., Nguyen, T. B., Praske, E., Schwantes, R. H., Smarte, M. D., St Clair, J. M., Teng, A. P., Zhang, X., and Seinfeld, J. H.: Gas-Phase Reactions of Isoprene and Its Major Oxidation Products, Chem. Rev., 118, 3337-3390, 10.1021/acs.chemrev.7b00439, 2018.