

Supplement of

Impact of temperature on the role of Criegee intermediates and peroxy radicals in dimers formation from β -pinene ozonolysis

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Table S1. Main updates to the formation of β -pinene-derived Criegee intermediates suggested for MCM v3.3.2.

No.	Modified reaction	Branching ratio in MCM	Updated branching ratio	Reference
1	BPINENE + O ₃ →NOPINONE + CH ₂ OOF	0.40	0.20	Ma and Marston, 2008; Nguyen et al., 2009; This work
2	BPINENE + O ₃ →NOPINOOA + HCHO	0.60	0.80	Ma and Marston, 2008; Nguyen et al., 2009; This work
3	CH ₂ OOF→CH ₂ O	0.37	0.50	Ahrens et al., 2014; Winterhalter et al., 2000; Zhang and Zhang, 2005
4	CH ₂ OOF→HO ₂ +CO+OH	0.13	0.30	Atkinson et al., 1992; Nguyen et al., 2009
5	CH ₂ OOF→CO	0.50	0.20	This work
6	NOPINOOA→NOPINOO	0.17	0.40	Ahrens et al., 2014; Winterhalter et al., 2000; Zhang and Zhang, 2005
7	NOPINOOA→NOPINDO ₂ + OH	0.50	0.30	Atkinson et al., 1992; Nguyen et al., 2009
8	NOPINOOA→C ₈ BC	0.33	0.30	This work

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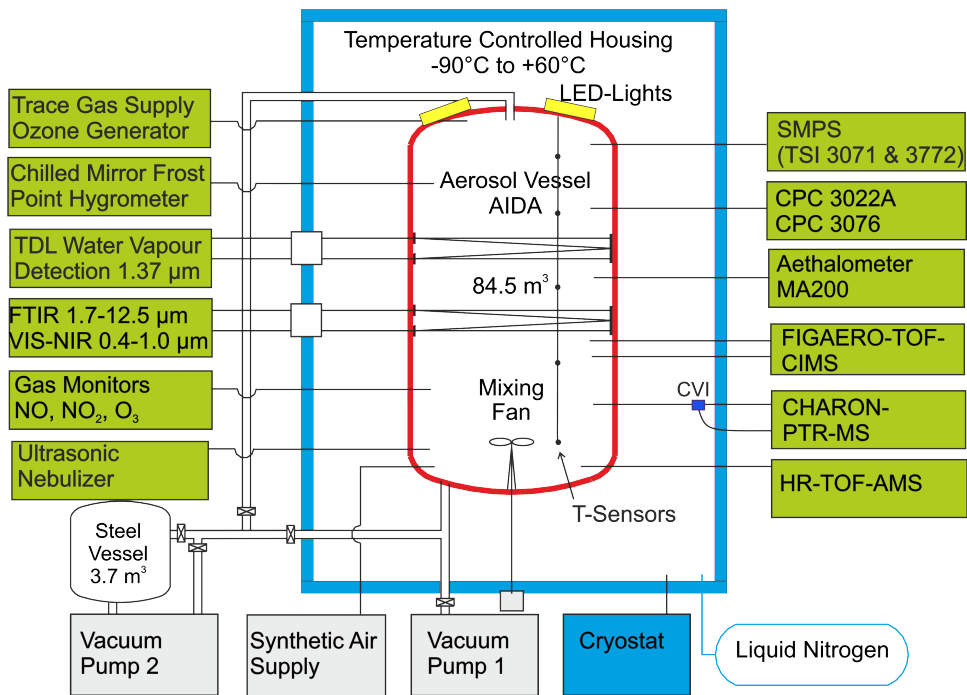


Figure S1. Schematic of the AIDA simulation chamber with the typical instrumentation.

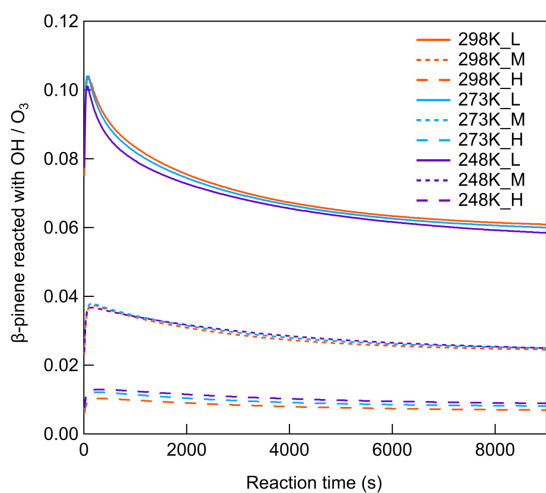


Figure S2. The ratio of the accumulated amount of β -pinene reacted with OH versus O_3 at different $[HO_2]/[RO_2]$ conditions and different temperatures (Exp. 298abc, 273abc, 248abc).

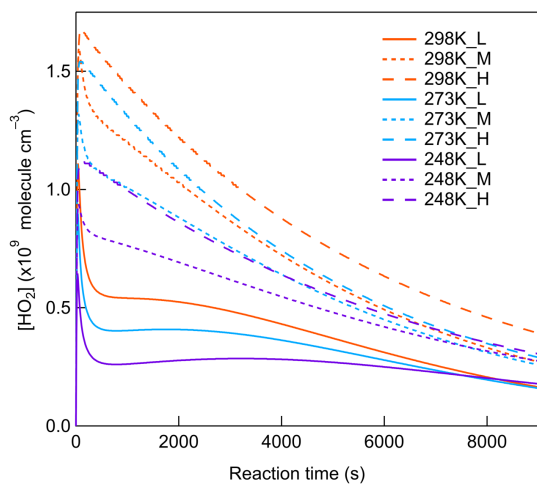


Figure S3. Simulated HO₂ concentration as a function of reaction time at different [HO₂]/[RO₂] conditions and different temperatures (Exp. 298abc, 273abc, 248abc).

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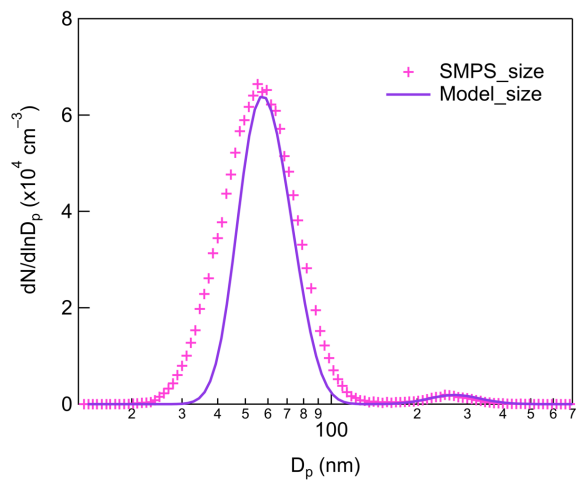


Figure S4. Particle size distribution from SMPS measurement and COSIMA model result at 7000 s of reaction (Exp. 298a).

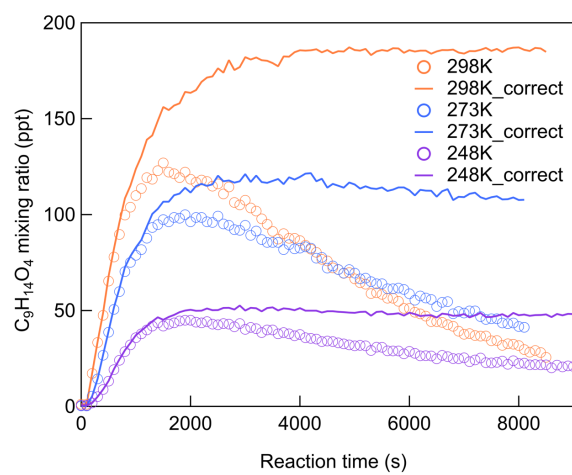


Figure S5. The mixing ratio of gas-phase $C_9H_{14}O_4$ before (measured) and after wall loss correction (modeled) at different temperatures (Exp. 298a, 273a, 248a).

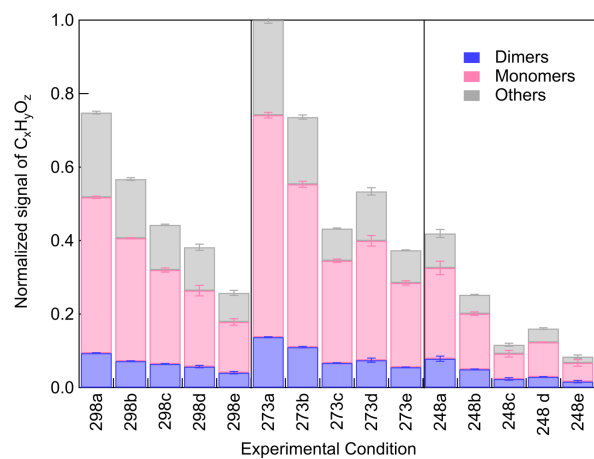
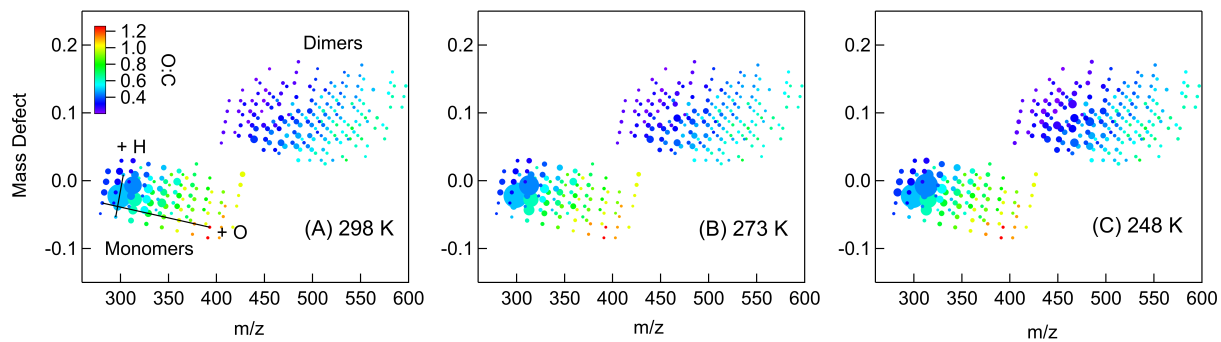


Figure S6. Normalized signals of all particle-phase $C_xH_yO_z$ compounds for different experimental conditions.



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Figure S7. Mass defect plots of particle-phase monomers and dimers (with Γ^-) at different temperatures (Exp. 298a, 273a, 248a). Markers are sized by the square root of their signals and colored by the O/C ratio.

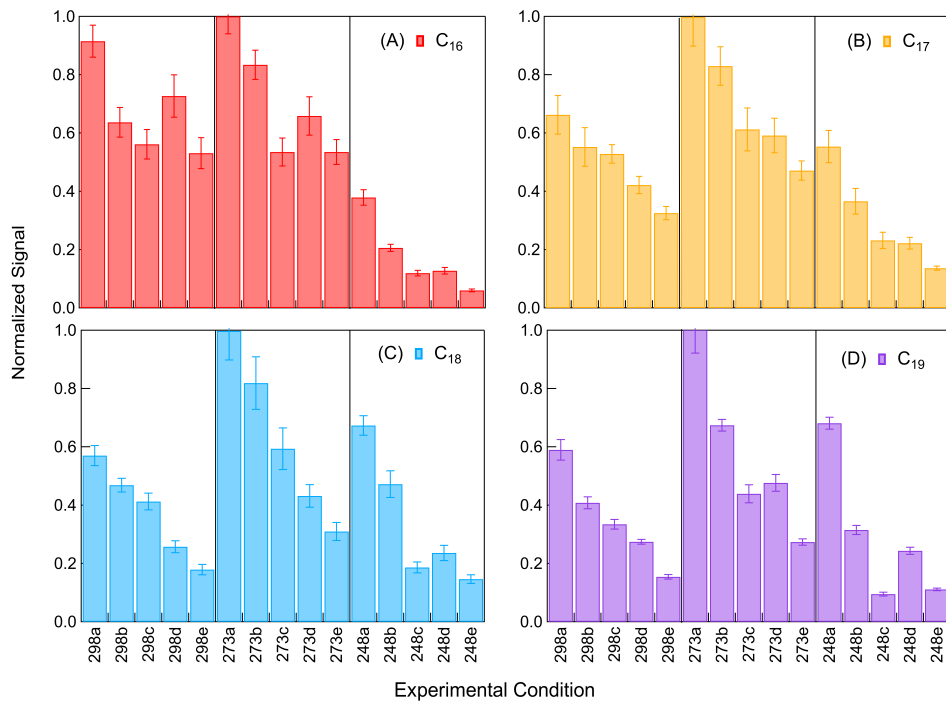


Figure S8. The particle-phase signals of (A) C_{16} (B) C_{17} (C) C_{18} (D) C_{19} dimers normalized to the peak intensity under different experimental conditions.

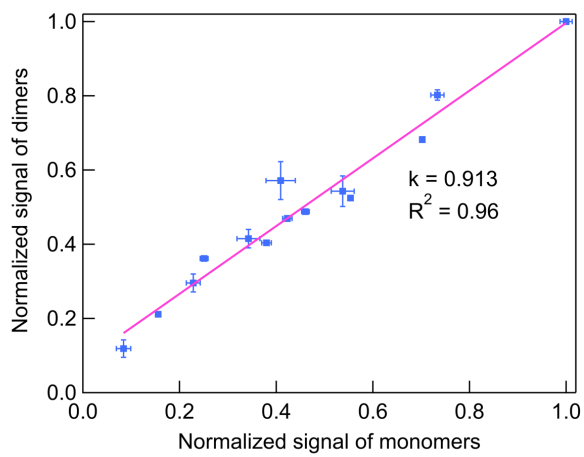
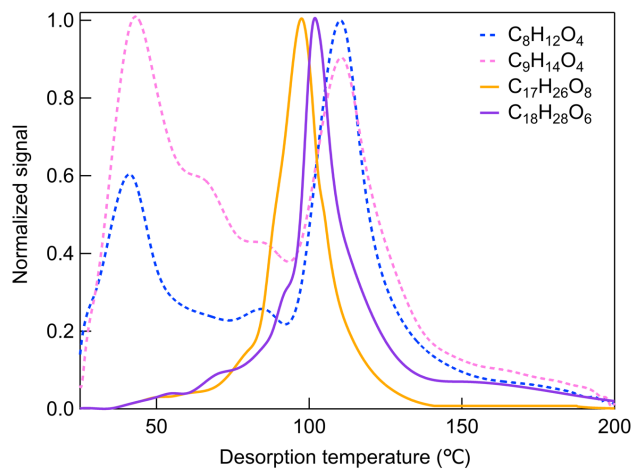
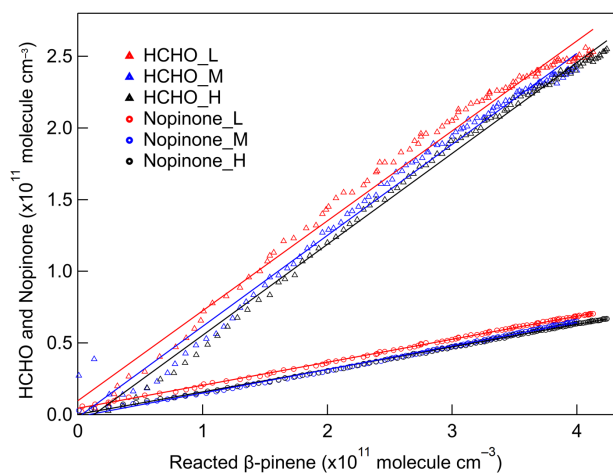


Figure S9. The correlation between particle-phase normalized signal of dimers with normalized signal of monomers. The solid line shows a linear fit.

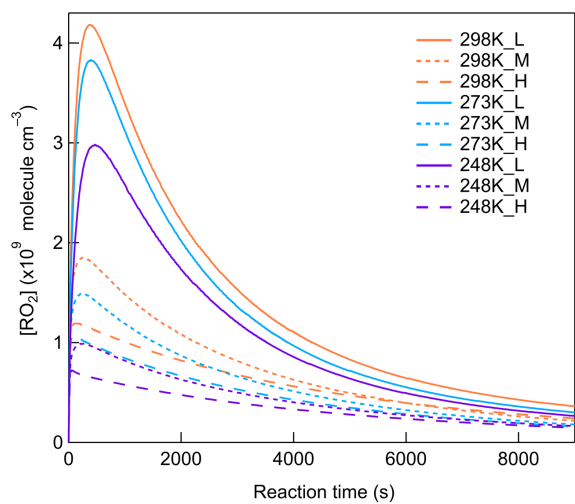
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65 **Figure S10. Thermograms of abundant monomers (C₈H₁₂O₄ and C₉H₁₄O₄) and dimers (C₁₇H₂₆O₈ and C₁₈H₂₈O₆), i.e., the normalized signals versus desorption temperature.**



70 **Figure S11.** The formation of formaldehyde (HCHO) and nopinone as a function of β -pinene reacted at 298 K for different $[\text{HO}_2]/[\text{RO}_2]$ (Exp. 298abc). The lines represent linear fits and R^2 values are larger than 0.95.



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Figure S12. Simulated RO₂ concentration as a function of reaction time at different [HO₂]/[RO₂] conditions and different temperatures (Exp. 298abc, 273abc, 248abc).

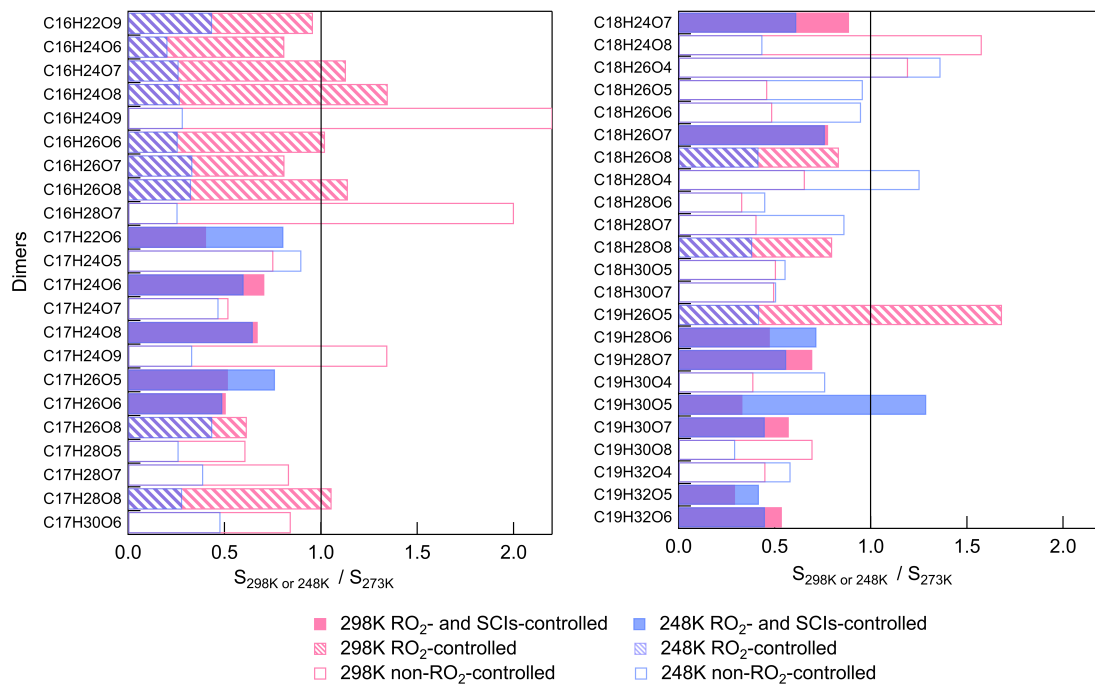


Figure S13. The relative changes of RO₂-controlled and non-RO₂-controlled abundant dimers at 298 K or 248 K versus 273 K (The relative standard deviations are within 25 %).

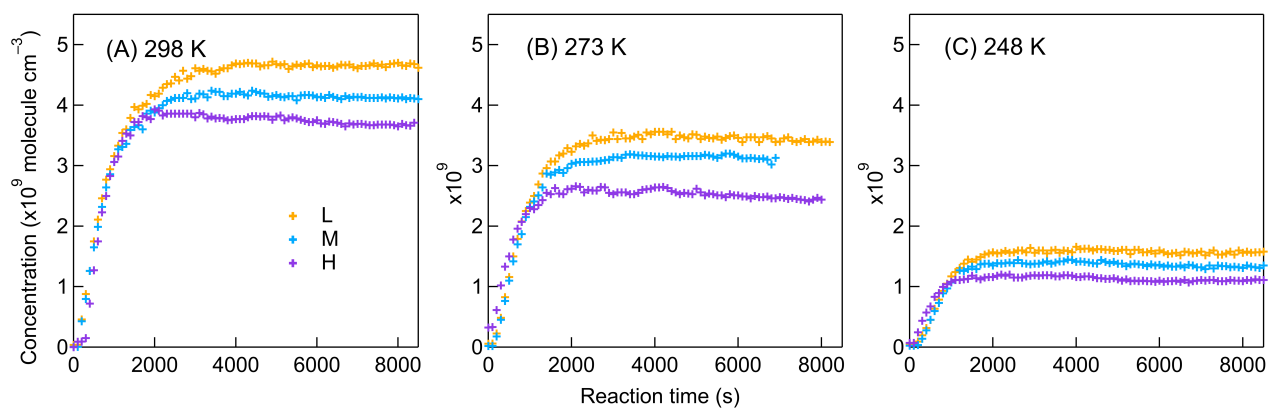


Figure S14. The impact of $[HO_2]/[RO_2]$ on the gas-phase concentrations of $C_9H_{14}O_4$ at (A) 298 K (B) 273 K (C) 248 K after wall loss correction (Exp. 298abc, 273abc, 248abc).