



Supplement of

Chemical characterization of organic compounds involved in iodine-initiated new particle formation from coastal macroalgal emission

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S1. Integrated OH exposure measurement

SO₂ decay experiment was conducted to estimate integrated OH exposure in the experimental apparatus, following Lambe et al. 2015. We replaced the macroalgal emission flow by a humidified air flow containing 200 ppbv SO₂ from standard gas cylinder. SO₂ was consumed by the reaction with OH while flowing through 254 nm UV light and the bag reactor. SO₂ mixing ratio at the outlet of the bag reactor was measured with and without UV lamp on, using a Model 43i-TLE SO₂ analyzer (Thermo Scientific Inc.). OH exposure was calculated from the equation

$$OH_{exp} = ln(SO_{2 \text{ lamp off}}/SO_{2 \text{ lamp on}})/k_{OH+SO2}$$

where k_{OH+SO2} is 9.49×10^{-13} cm³ molecule⁻¹s⁻¹ (Burkholder et al. 2015).

SO_{2 lamp off} and SO_{2 lamp on} were measured to be 18 and 13 ppbv, respectively. OH_{exp} was then calculated to be to be 3.2×10^{11} molecules cm⁻³ s. This is equivalent to 2.4 days assuming 1.5×10^6 molecules cm⁻³ ambient average OH.

Reference

Burkholder, J. B., Sander, S. P., Abbatt, J., Barker, J. R., Huie, R. E., Kolb, C. E., Kurylo, M. J., Orkin, V. L., Wilmouth, D. M. and Wine P. H. "Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation No. 18," JPL Publication 15-10, Jet Propulsion Laboratory, Pasadena, 2015.

Lambe, A. T., Chhabra, P. S., Onasch, T. B., Brune, W. H., Hunter, J. F., Kroll, J. H., Cummings, M. J., Brogan, J. F., Parmar, Y., Worsnop, D. R., Kolb, C. E., and Davidovits, P.: Effect of oxidant concentration, exposure time, and seed particles on secondary organic aerosol chemical composition and yield, Atmos. Chem. Phys., 15, 3063-3075, 10.5194/acp-15-3063-2015, 2015.

S2. The measurement details of GC-MS and FIGAERO-iodide-CIMS

GC-MS

300 milliliters of air sample from the canister was pulled through a cryogenic trap in the quadrupole GC-MS system (model TH-300B) and cooled to -160 °C for preconcentration. After being trapped, the concentrated VOCs were flash desorbed by heating to 100 °C and transferred to a DB-624 column (60 m×0.25 mm×1.4 μ m). CO₂ and moisture are removed before injection. The initial temperature for the chromatographic column was 41 °C, maintained for 6 min, and then raised to 180 °C at a rate of 6 °C min⁻¹. Qualitative identification of VOCs was performed using a full MS scan from 50 to 500 Th. The most probable identity of an analyte was obtained based on the first ranked matching by comparing with the reference mass spectra in the NIST library.

FIGAERO-iodide-CIMS

A sample flow was directly drawn into a turbulent flow ion-molecule reactor (IMR). Gaseous products were ionized as their corresponding adduct ions with I⁻. Particulate products collected on the PTFE membrane filter were desorbed by a flow of heated UHP N₂. The temperature of the N₂ increased from 20 to 200 °C in 50 min. The desorbed molecules entered the IMR and were charged by the same ionization mechanism. Background HNO₃ was inevitable in the experimental apparatus containing macroalgae and natural seawater. So the cluster ions containing NO₃⁻ or HNO₃ were observed occasionally. ToF-MS was configured to measure singly charged molecular ions of 7-720 Th with a MS resolution of ~4500. Mass calibration was conducted using the ions of NO₃⁻, CF₃O⁻, C₂F₃O₂⁻, C₃F₅O₂⁻, I₃⁻ for gaseous products and NO₃⁻, I⁻, IHNO₃⁻, IC₂F₃HO₂⁻, I₃⁻ for particulate products. Reliable formula identification of ion peaks was corroborated by high accuracy of fits (<20 ppm) and isotope patterns. Background signal in the gas phase was determined by measuring a UHP N₂ flow. The signal during the last 3 minutes of the soak period of PTFE membrane filter was regarded as background signal in the particle phase. Background

signals were then subtracted from the intensities of compound formulas.



Figure S1. Particle number size distributions with and without room light and ozone.



Figure S2. Oxygen and carbon atom number distributions of particulate products measured by iodide-CIMS and ESI-orbitrap MS in a typical ozonolysis experiment (dynamic mode). Hatched bars indicate the fractions of formulas observed by both mass spectrometers.