Supporting Information (SI) for

Real-time Characterization of Negative Air Ions-Induced Decomposition of Indoor Organic Contaminants by Mass Spectrometry

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Supporting Information includes experimental section (reagents, apparatus, probe preparation); MS characterization of untreated laboratory air (Figure S1); measurement of tungsten-tip voltage (Figure S2); MS spectrum of NAIs (Figure S3); and optimization of flow rates of IOCs (Figure S4).

Experimental Section

Reagents

Synthetic air (21 % O_2 + 79 % N_2 Hai Pu Co., Ltd., China), formaldehyde solution (Xilong Chemical Co., Ltd., China), benzaldehyde (Bodi Chemical Co., Ltd., China), salicylaldehyde, di-(2-ethylhexyl) phthalate (Sinopharm Chemical Reagent Co., Ltd., China), methylbenzene (North Fine Chemicals Co., Ltd., China), paraxylene (Coupling Reagent Co., Ltd., China), ethylbenzene (Adamas Reagent Co., Ltd., China), propylbenzene, phenylacetaldehyde, and phenylpropionaldehyde (Aladdin reagent Co., Ltd. Shanghai, China), ethyl acetate (Three Chemical Reagent Factory, China), demethyl phthalate (Beijing Chemical Reagent Company, China), and dibutyl phthalate (Fuchen Chemical Reagent Factory, China) were used as obtained. Freshly deionized water from an ultraviolet ultrapure water system (18.3 MΩ cm, Millipore purification system, USA) was used throughout the experiments.

Apparatus

A laboratory-made high-voltage power supply (0−30 kV) was used for electrospray ionization. The syringe pump (Harvard Apparatus, USA) was used for controlled the flow rate of IOCs solution. The temperature of DL in mass spectrometry (Shimadzu, LCMS-8030, Japan) was set as 250 ℃ while heat block was 400 ℃. The intermediates generated during the interaction between NAIs and IOCs spray were detected in real-time by MS under the negative mode. The obtained MS data were analyzed using the software package provided by Shimadzu (Japan).

Probe Preparation

The probe tungsten probe was designed with a point radius of 10.0μm, shaft diameter of 0.5 mm and length of 38mm. The probe was connected to NAIs generator (Sunyou Electric, China) for electrospray ionization based on corona discharge. The tungsten-made probes (99.9% tungsten, ST20-2, purchased from GGB Industries Inc.) were initially washed with methanol/water (1:1) to clean its surface and then soaked in 5%

HNO_3 for 5 min. Afterward, the probes were washed with ultrapure water, methanol/water (1:1), and ethanol. Regeneration of the probes was quite simple. The used probes were washed with methanol/water (1:1), ultrapure water, and ethanol. To avoid contact with outside air, the tungsten probe was sealed inside a laboratory-made T-shaped silicate tube (10 cm long horizontal channel and 5 cm long vertical channel). Afterward, the probes could be used again. By applying a high voltage, an electrospray cone could be formed from the liquid droplet on the probe tip.

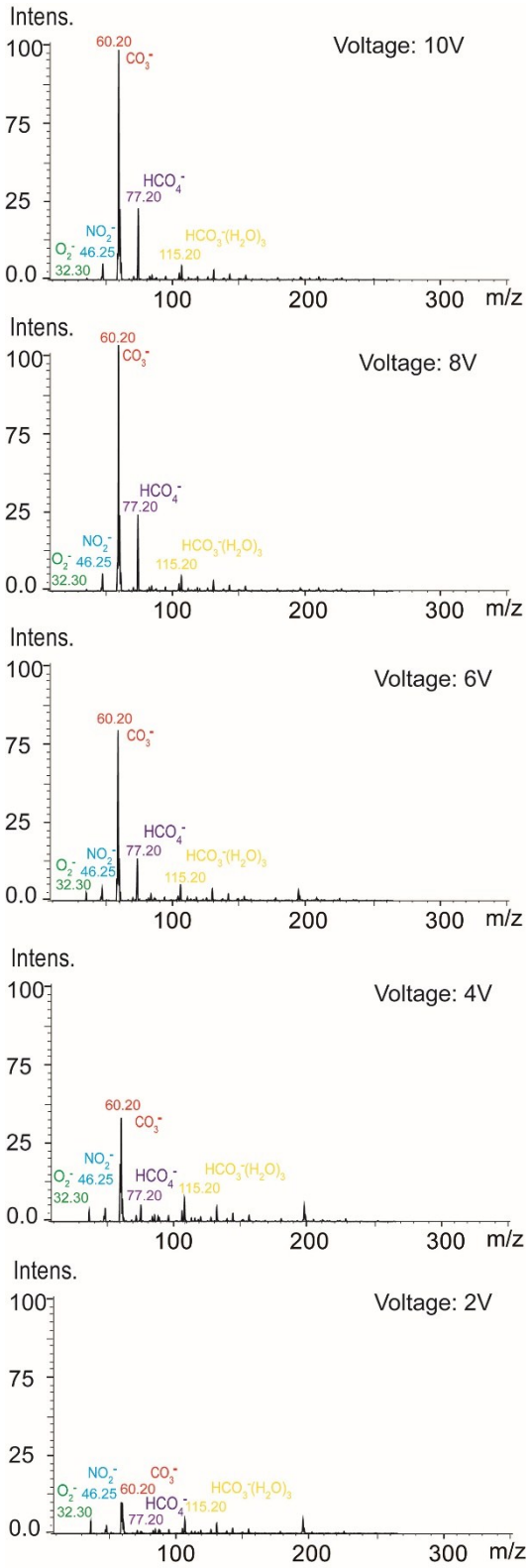

Figure S1 MS characterization of untreated laboratory air. Output voltage of 12 V, L of 3 mm, and D of 8 mm.

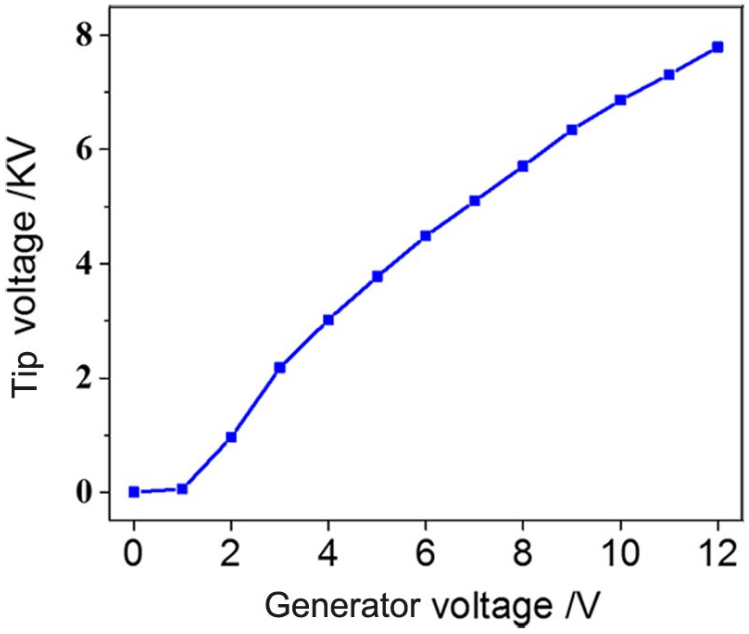

Figure S2 Characterization of the tungsten-tip voltage (absolute voltage) versus the output voltage from NAIs generator.

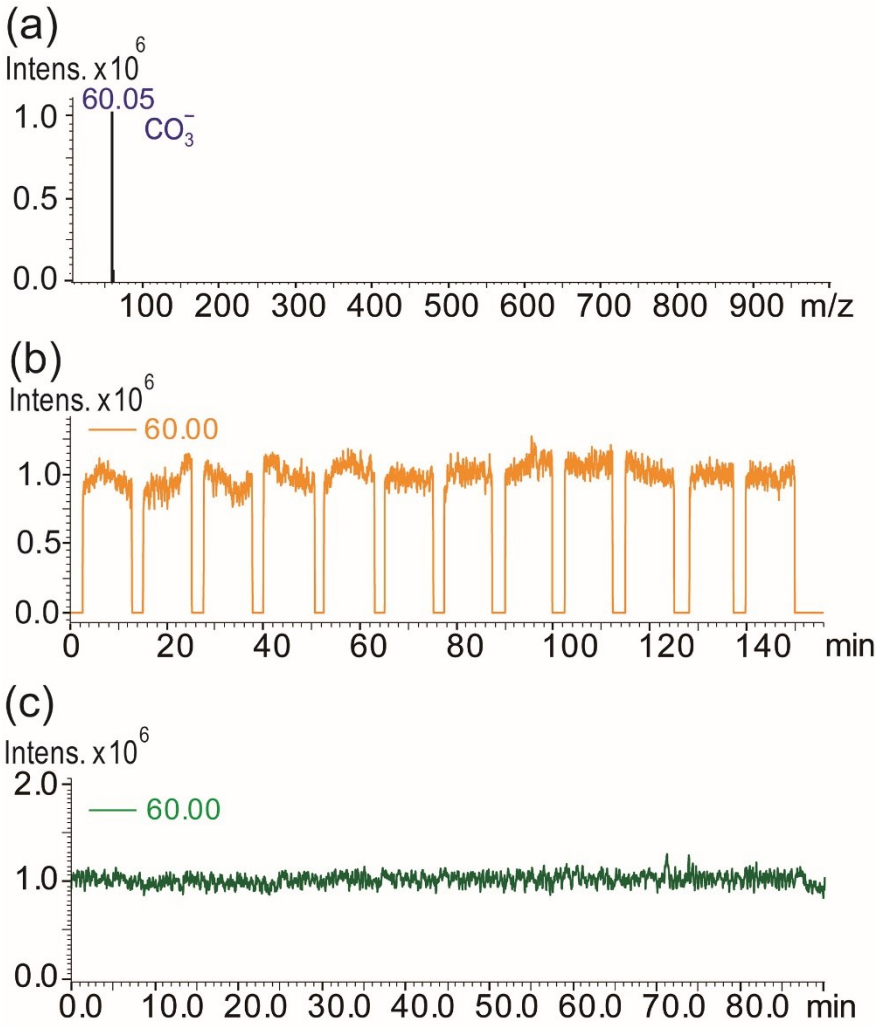

Figure S3 (a) MS spectrum in the range of 10 to 1000 (m/z ratio) to characterize NAIs under the optimized parameters. (b) Reproducibility and (b) Long-time stability of NAIs. Output voltage of 5 V, synthetic air flow rate of 5 L/min, L of 3 mm, and D of 8 mm.

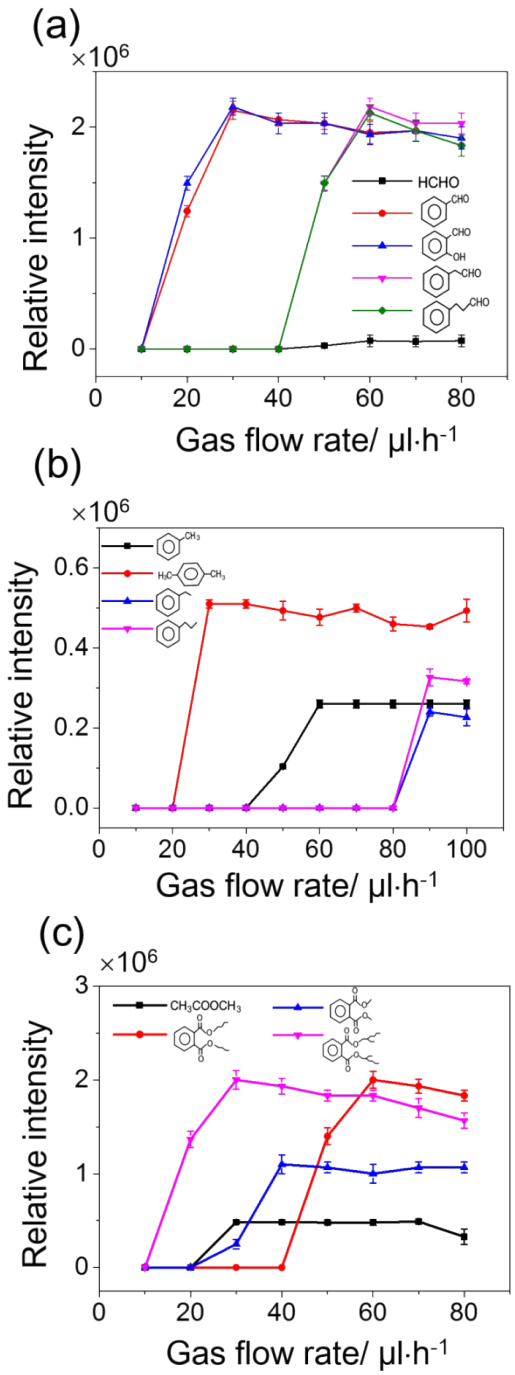

Figure S4 Optimization of flow rates of IOCs. (a) The optimal flow rates of formaldehyde, benzaldehyde, salicylaldehyde, phenylacetaldehyde, and phenylpropionaldehyde are 60, 30, 30, 60, and 60 μL/h, respectively. (b) The optimal flow rates of methylbenzene, paraxylene, ethylbenzene, and phenylpropane are 60, 30, 90, and 60 μL/h, respectively. (c) The optimal flow rates of ethyl acetate, demethyl phthalate, dibutyl phthalate, and Bis-(2-ethyl-hexyl) phthalate are 30, 60, 30, and 20 μL/h, respectively.