High Resolution Chemical Ionization Mass Spectrometry (ToF-CIMS): Application to Study SOA Composition and Processing

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Supplementary Material

Table S1: Voltages (V) applied on the HR-CIMS elements in positive mode for water and negative mode for acetate and iodide reagent ions. These elements are listed from left to right according their order in the mass spectrometer downstream from the sample inlet. A detailed description of the CI-ToFMS can be found in (Bertram et al., 2011)

Reagent ion	IMR	Nozzle	Q1 entrance plate	Q1 front	Q1 back	Lens skimmer	Skimmer	Q2 front	Q2 back
$(H_2O)_nH^+$	0	-3.3	0	-9.9	-2.1	0	0	-7.6	-9.5
$CH_3C(O)O^-$	0	3.3	6.6	17.9	-8.1	-7.2	-1.4	8.3	7.2
$I(H_2O)_n^-$	0	3.3	6.6	17.9	2.1	2.2	5.2	6.6	7.2

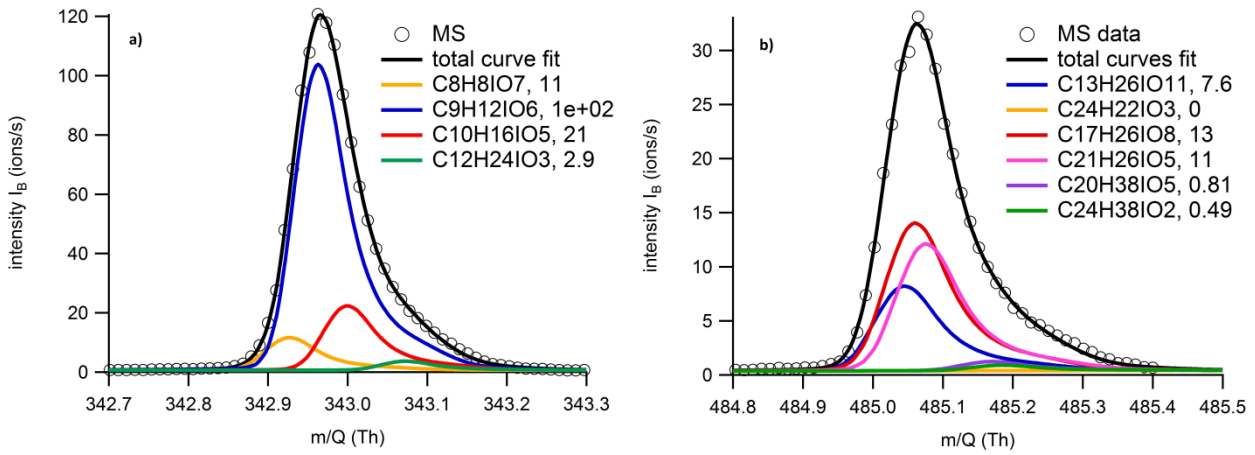

Figure S1: Mass spectral signal at m/z 343 and 485 for the WSOC before the oxidation using iodide reagent ion. The total fit trace is a linear combination of the fits of individual ions. The measured MS data are shown in black circles. Individual ion fits are shown in colours and the corresponding chemical formula are listed in the legend with the area covered by each ion listed next to the chemical formula in the legend.

Figure S1 (a) illustrates the fitting of peak at m/z 343, where four ions have been assigned to give the total curve fit area, and no other chemical formulas could be fitted under the peak to make the total curve fit closer to the MS data. On the other hand, the peak at m/z 485 is wider (a property of ToF mass analyzers that the peak width increases at higher m/z) as shown in Figure S1 (b) and more chemical formulas can be potentially used to fit the peak. For instance, $C_{17}H_{26}IO_8$, $C_{13}H_{26}IO_{11}$ and $C_{21}H_{26}IO_5$ can be used to fit the left half of the peak but it is hard to identify the contribution of those peaks to the measured mass spectral signal. The similar issue exist to the right half of the peak. The data presented here illustrates the ambiguous ion assignment of peaks appearing at the high m/z region.