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A vacuum ultraviolet ion source (VUV-IS) for iodide–chemical ionization mass spectrometry: a substitute for radioactive ion sources

Yi Ji et al.

Correspondence to: L. Gregory Huey (greg.huey@eas.gatech.edu)

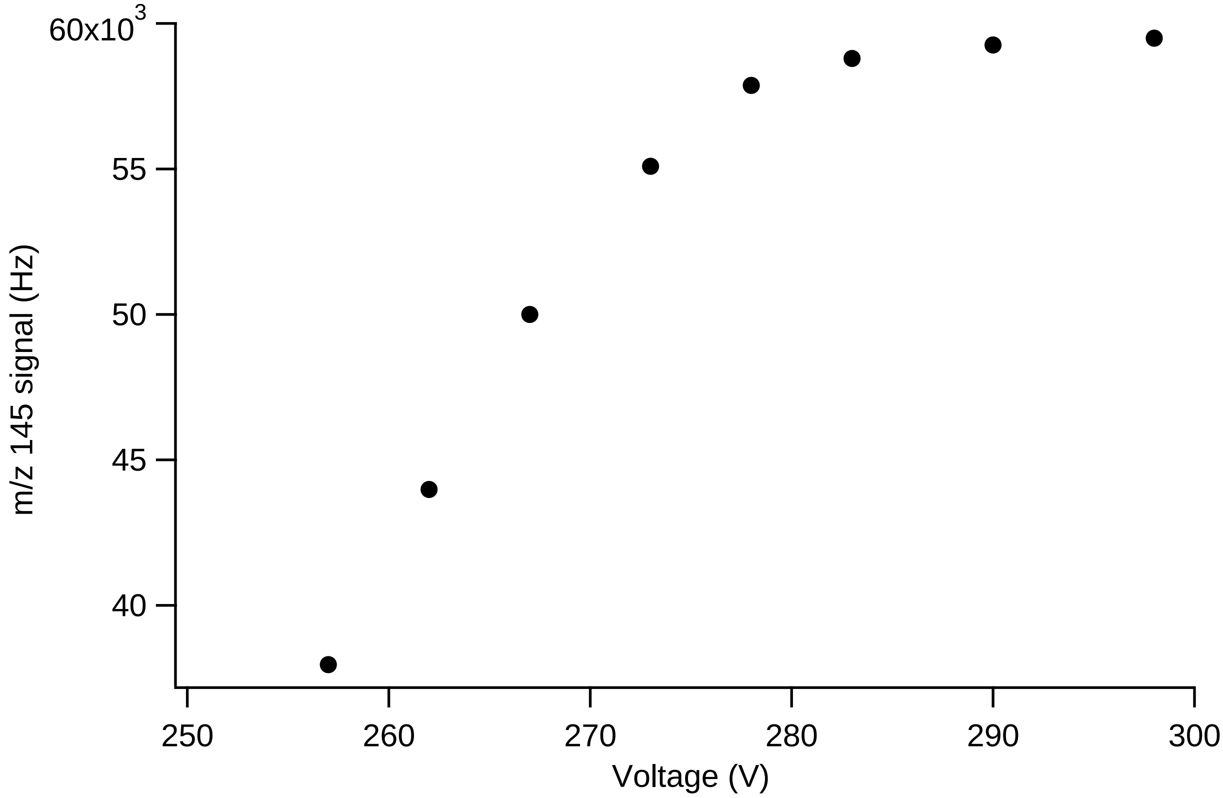

Figure S1. CIMS ion current at m/z 145 ($I^- \cdot H_2O$) as a function of voltage across the krypton. Note that the lamp ignites at voltage of ~280 V.

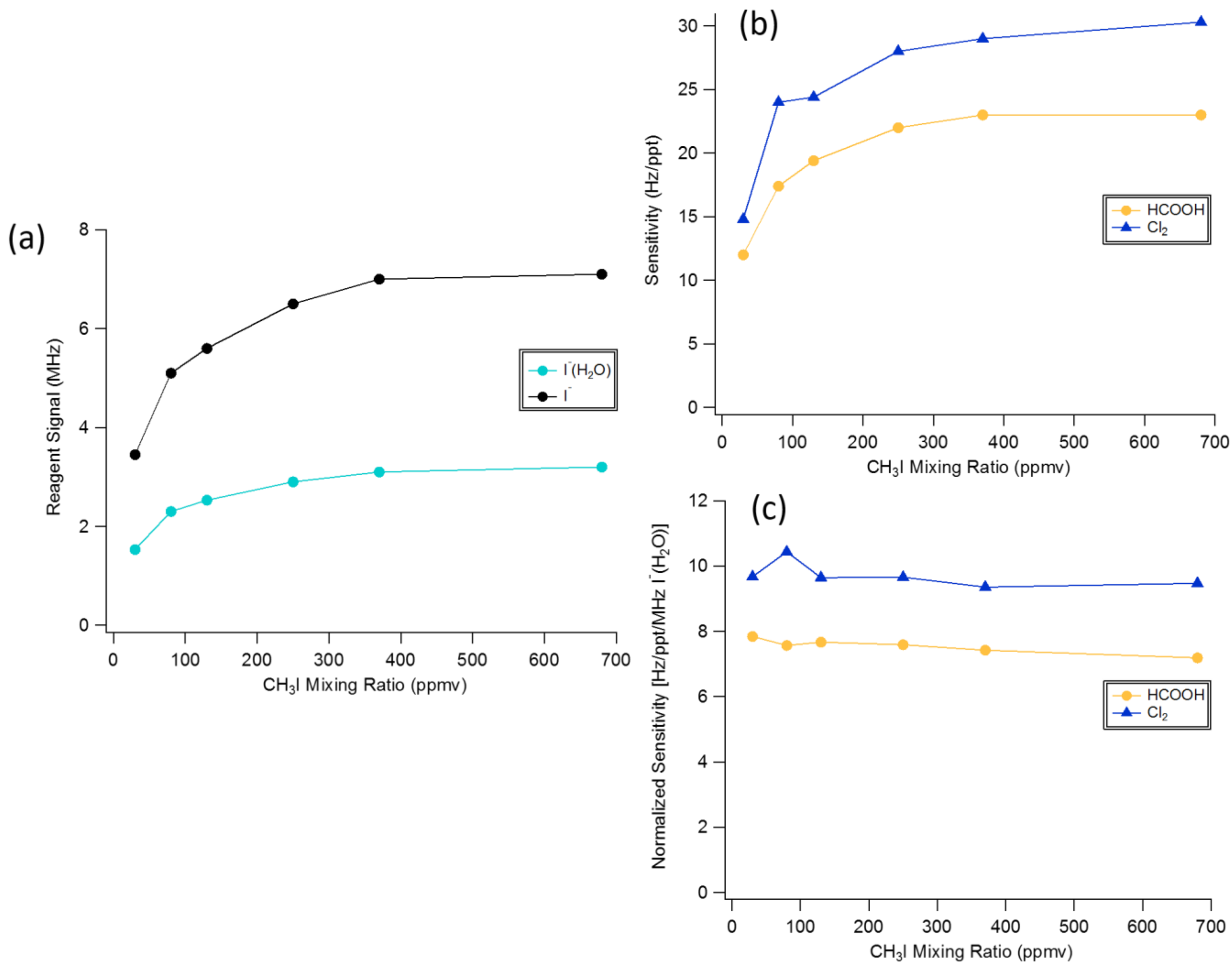

Figure S2. TOF-CIMS (a) reagent signal levels (b) sensitivity (c) normalized sensitivity as a function of CH_3I at 30 torr.

Peroxyacetyl nitrate (PAN) measurements using I^- -Q-CIMS

$$CH_3C(O)O_2NO_2 \xrightarrow{\Delta} CH_3C(O)O_2 + NO_2 \quad \text{(RS1)}$$

$$CH_3C(O)O_2 + I^- \cdot (H_2O)_n \rightarrow CH_3C(O)O^- \cdot (H_2O)_n + IO \quad \text{(RS2)}$$

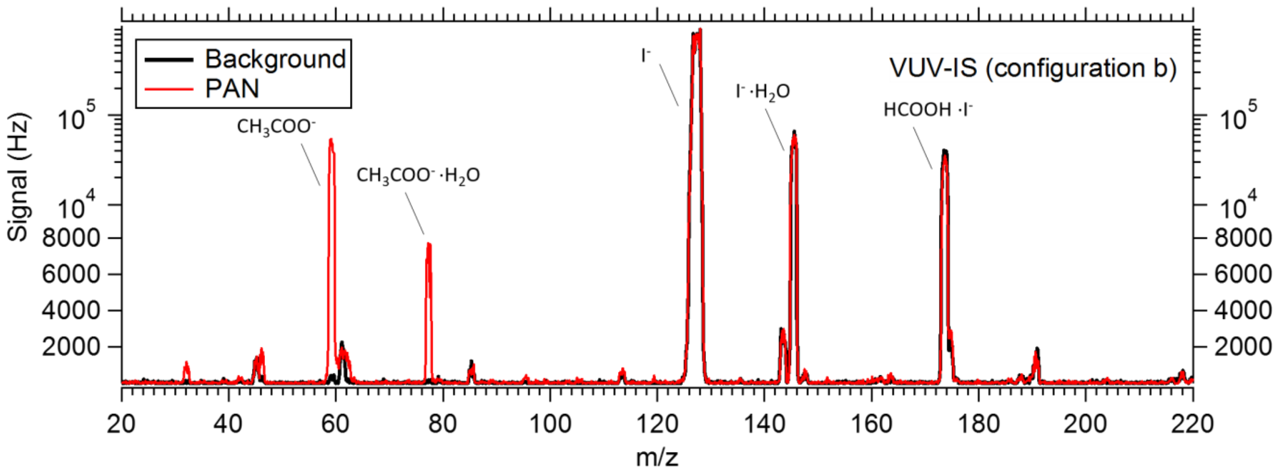

Figure S3. Mass spectra of zeroed ambient air with and without PAN calibration standard.

Organic acids measurements using SF_6^- -Q-CIMS

Detection of formic and acetic acid by the following reactions with SF_6^- (Nah et al., 2018).

$$SF_6^- + HC(O)OH \rightarrow HC(O)O^- \cdot HF + SF_5 \quad \text{(RS3)}$$

$$SF_6^- + CH_3C(O)OH \rightarrow CH_3C(O)O^- \cdot HF + SF_5 \quad \text{(RS4)}$$

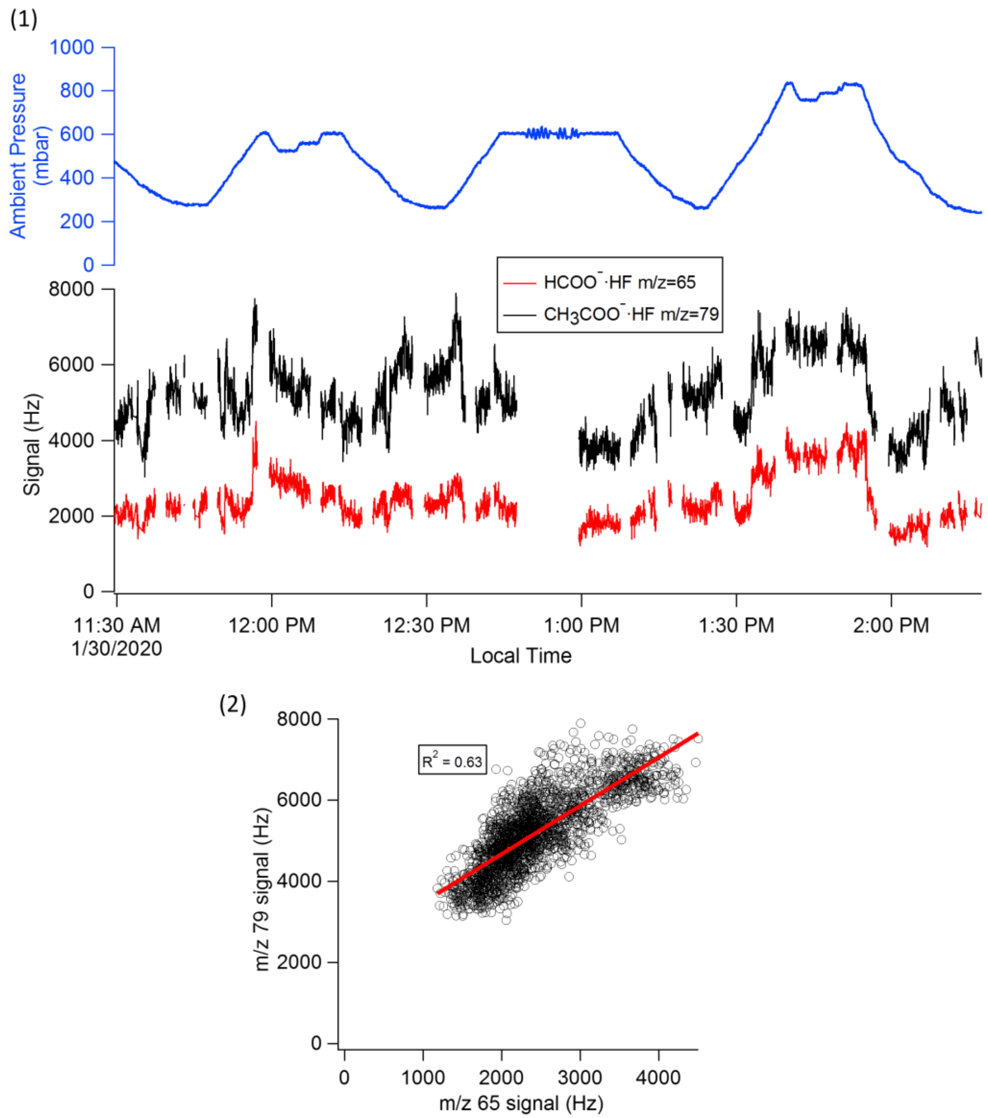

Figure S4. (1) Time series of formic acid signal ($HCOO^- \cdot HF$, m/z 65, red line), acetic acid signal ($CH_3COO^- \cdot HF$, m/z 79, black line), and ambient pressure (blue line). (2) A correlation plot of the $CH_3COO^- \cdot HF$ signal (m/z 79) versus $HCOO^- \cdot HF$ signal (m/z 65). Data was taken from the NCAR GV during a test flight based out of Broomfield, CO using a VUV-IS.

Sample Calculation of Absorption of VUV light by CH_3I

To calculate how much of the VUV light is absorbed, the Beer-Lambert Law is applied,

$$\frac{I(\lambda)}{I_0(\lambda)} = \exp(-\sigma(\lambda)nL)$$

where $I(\lambda)$ is the intensity of light at wavelength λ after absorption, $I_0(\lambda)$ is the original light intensity at wavelength λ, $\sigma(\lambda)$ is the absorption cross section of the absorber molecule at wavelength λ, n is number concentration of the absorber molecule, and L is the path length over which the light can be absorbed.

Sample calculation:

For 86.5 ppmv of CH_3I at a pressure of 20 torr

$n = 5.70\times10^{13}$ molecule cm^{-3}

$\sigma(\lambda) = 7\times10^{-17}$ cm^2 $molecule^{-1}$ (Olney et al., 1998)

$L = 21$ cm

$\frac{I(\lambda)}{I_0(\lambda)} = \exp(-\sigma(\lambda)nL) = 0.92$

Therefore, in this example ~8% of the light emitted from the VUV lamp is absorbed by the methyl iodide.