

Interactive comment on “Coupling a gas chromatograph simultaneously to a flame ionization detector and chemical ionization mass spectrometer for isomer-resolved measurements of particle-phase organic compounds” by Chenyang Bi et al.

Anonymous Referee #1

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Review of “Coupling a gas chromatograph simultaneously to a flame ionization detector and chemical ionization mass spectrometer for isomer-resolved measurements of particle-phase organic compounds” AMT 2020-264 Bi et al.

Summary: The authors describe a new instrument consisting of an aerosol impactor, thermal desorption unit, GC, and split column effluent to an FID detector and an iodide-adduct chemical ionization mass spectrometer. The separate components of this in-

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strument have been described previously; the combination of the simultaneous FID and CIMS measurement is novel. The goals of this instrument are to (1) isomerically resolve chemical compounds in an aerosol sample, and (2) determine the sensitivity of the CIMS detector to each chemical species. A second novel instrument technique is also described, in which a combination of air and iodide are used as reagent ions in the CIMS. The purpose of this is to ionize both high- and low-polarity compounds.

Major comments: The manuscript is generally well-written and well-organized. The use of chromatography to interpret CIMS spectra is not especially inventive, and because it is so complicated, this instrument will likely not see widespread use in its current form. However, this is a particularly useful instrument because it addresses two major problems with CIMS in atmospheric science: the spectra may be complicated to interpret, and the sensitivities to individual species are difficult to determine. Used under carefully-controlled conditions in a small number of laboratories, this instrument could provide important reference information to interpret iodide-CIMS measurements from field studies.

The analysis of the number of detected isomers was done very well and it is very useful to see the comparison to other studies.

The inclusion of the air/iodide mixed-reagent-ion technique is interesting, but does not seem to really belong here. It is not even indicated in the title of paper and does not address the motivations mentioned in the introduction. This is better suited to a separate manuscript. If this is retained, it needs to be better explained how the mixed-reagent-ion approach relates to the other capabilities of the instrument. An additional figure or other concrete example should be shown to demonstrate how chemical information can be derived from this technique.

Instead of the mixed-reagent ion description, it would be better to include an assessment of the FID-enabled determination of CIMS sensitivities. This is stated several times as the major benefit of the FID. However there are no data shown to demon-

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strate this utility. This is a significant weakness of the manuscript. The manuscript could be published with some minor revisions, but would have a much larger impact if the use of the FID to determine sensitivity is demonstrated.

Specific/minor comments: Section 2.3. It would be helpful to summarize the major technical challenges of CIMS/FID split flow at the top of this section.

Page 6 line 166- 170. I don't understand the purpose of the EI-MS experiment. Please explain.

Page 10 Line 235: Wouldn't decomposition during TD change the parent formula as well?

Page 11 Line 260: This statement should be qualified with the volatility- or carbon-number-range analyzed.

Page 11 lines 264-266: Could you not use the EI-MS and identify the isomers via matching to a NIST library?

Page 14 lines 330-358: Can you provide an example of how this can be used? This seems to subvert the main benefits of CIMS, which are a 1:1 correspondence between molecule and product ion, and the retention of the parent ion (low fragmentation). If the only benefit is that it allows detection of some other compounds with the CIMS, why not just use the FID, which detects everything and with roughly equal sensitivity? The spectra are probably too complicated to interpret without GC-preseparation. Maybe there is some information about the structure of the isomer, given the observed mixed I-/O₂- product ions. If so, can you provide some examples? Please comment on the use of this method to interpret the non-adduct ions typically observable in I- CIMS spectra. Can you state anything concrete about the identity of these ions, given the results of your experiments?

Technical corrections: Line 221: "magnitudes" -> "magnitude"

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