Response to Delphine Farmer review of:
"Calibration of Hydroxyacetonitrile ($HOCH_2CN$) and Methyl isocyanate (CH_3NCO) Isomers using I^- Chemical Ionization Mass Spectrometry (CIMS)", Finewax, Chattopadhyay, Neuman, Roberts, and Burkholder
Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2024-94, 2024

The authors thank the reviewer for their careful reading and constructive comments regarding our manuscript.

Reviewer Comment:
The reviewers concerned with wording in the following abstract sentence "These results contradict several recent field studies that have reported the detection of MIC using I-CIMS instruments.", which was interpreted to imply a controversy.

Author Response:
It was not our intention to imply a controversy as the results from our study are definitive in that I-CIMS instruments are not sensitive to MIC and, therefore, previous studies have mis-attributed the observed C2H3NO I-CIMS signal to MIC.

Action to be taken:
Revise the abstract text "These results contradict several recent field studies that have reported the detection of MIC using I-CIMS instruments. This study demonstrates that HAN, rather than MIC, was most likely the C_2H_3NO isomer observed in those field studies, although the source chemistry for HAN remains uncharacterized."
as follows:
"~~These~~ The present results ~~contradict~~ show that several recent field studies ~~that have reported the detection of MIC~~ using I-CIMS instrument detection have misattributed the C_2H_3NO signal to MIC. This study ~~demonstrates~~ proposes that HAN, rather than MIC, was most likely the C_2H_3NO isomer observed in those field studies, although the source chemistry for HAN remains uncharacterized. This study demonstrates the importance of applying absolute calibration standards in the identification and quantification of isomeric compounds.".

Reviewer Comment:
I encourage the authors to consider this question - what makes I-CIMS so sensitive to hydroxyacetonitrile, and not to methyl isocyanate?

Author Response:
We did not provide an explanation for the difference in sensitivity between the MIC and HAN isomers in our original submission. Reviewer #2 has provided an explanation in their review, which we agree with. We will add text and citation to two references that addresses this point

Action to be taken:
We have added text and citation to two references in the conclusion section as follows: Iyer et al, (2016) and Hyttinen et al, (2018) provide an explanation for the significant difference in the I-CIMS sensitivity for MIC (CH_3NCO) and HAN ($HOCH_2CN$), due to the stability of I- cluster binding energies. That is, the H-bonding with the HO group in HAN leads to a stable I- cluster, while MIC would not form a stable I- cluster.

Hyttinen, N., Otkjaer, R. V., Iyer, S., Kjaergaard, H. G., Rissanen, M. P., Wennberg, P. O., and Kurten, T.: Computational comparison of different reagent ions in the chemical ionization of oxidized multifunctional compounds, J. Phys. Chem. A., 122, 269-279, https://doi.org/10.1021/acs.jpca.7b10015, 2018.

Iyer, S., Lopez-Hilfiker, F., Lee, B. H., Thornton, J. A., and Kurten, T.: Modeling the detection of organic and inorganic compounds using iodide-based chemical ionization, J. Phys. Chem. A, 120, 576-587, https://doi.org/10.1021/acs.jpca.5b09837, 2016.