

Interactive comment on “Molecular Characterization of Alkyl Nitrates in Atmospheric Aerosols by Ion Mobility Mass Spectrometry” by Xuan Zhang et al.

Anonymous Referee #2

Received and published: 15 August 2019

The manuscript presents an application of Ion mobility mass spectrometry to alkyl nitrate characterization. The application is new for atmospheric chemistry experiments. The experiments are sound and well carried out. The results are well presented and discussed and I recommend publication of the manuscript after the following issues have been addressed.

Major issues:

The main issue is novelty and a very biased representation of the literature. In fact, the alkyl nitrates the authors target are explosives and their analysis by Ion mobility spectrometry has been studied by the security community for over a decade! So ig-

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noring this work is not appropriate! It is critical to actually include this and discuss what is novel here? What insights that are not already published have been gained and mostly how does this work relate in terms of selectivity and sensitivity to the existing literature. Even high resolution ESI-HRIMS work has been published nearly 10 years ago on RDX and similar compounds. It is amazing that this work (Hilton et al., 2010) is not referenced and discussed here. Also many other open literature papers are out there on “nitro explosive” detection which is the same as the alkylnitrates mentioned here.

A second, partially related issue that is critical to address is a lack of figures of merit in the abstract and very little to no discussions of figures of merit in the text. For an analytical paper it would be customary to have quantitative information in the abstract (e.g. LOD) and discussed in the text.

Relevant papers

Hilton C.K., Krueger C.A., Midey A.J., Osgood M., Wu J., Wu C. Improved analysis of explosives samples with electrospray ionization-high resolution ion mobility spectrometry (ESI-HRIMS) *Int. J. Mass. Spectrom.* 298, 64–71, 2010.

Kozole, J. et al., Gas phase ion chemistry of an ion mobility spectrometry based explosive trace detector elucidated by tandem mass spectrometry, *Talanta*, 140, 10-19, 2015.

But also:

Sivakumar N. et al., Development of an ion mobility spectrometer for detection of explosives. *Instrum. Sci. Technol.* 41:96–108, 2013.

And quite a few others... just replace alkyl nitrate with nitro explosives (same compounds!)...

Details:

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Please provide source information consistently for all your chemicals (target compounds).

Please provide quantitative information in the abstract (LODs) and also provide a comparison to the existing explosive literature.

Figure 2: Collision cross section typically has a unit (\AA^2).

Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2019-184, 2019.

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