Interactive comment on “An automated gas chromatography time-of-flight mass spectrometry instrument for the quantitative analysis of halocarbons in air” by F. Obersteiner et al.

Anonymous Referee #2

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This study reports on a GC-TOF instrument and its performance in measuring halocarbons in air. The TOF studied was an instrument from TOFWERK. They investigated several aspects of the TOF including the sensitivity, linearity etc. and factors that influence these. The authors put a good deal of work into this paper and the technique shows lots of promise. The paper definitely addresses relevant scientific questions and novel concepts and tools are presented. The experimental work appears sound but needs some tightening up in places. I recommend publication after some minor considerations. Some specific comments follow.

Abstract: The abstract is concise and well written.
Introduction: The introduction is concise and clear.

Technical description: Looks fine except the authors should include a little more discussion on what is used for calibrating the instrument – it is briefly mentioned that the calibration is performed by comparing to a calibrated air sample. Please explain how the air sample was calibrated or from whom the calibrated air sample was obtained with specified certification, etc.

Better define chromatographic mass traces.

Better define the concept of nominal masses and how in practice these are extracted from the data.

Better development of the discussion around Figure 8 is needed.

9459 – line 11: Change to Magnesium perchlorate

9459 line 17: cryofocusation – new word - would not recommend. Use cryofocusing instead

9465 line 9 – Awkward sentence – rewrite – not clear what achievable calibration quality if referring to. Also data “were” analyzed.

9466 line 27: not clear what is meant by “lower arrival time distribution”.

9468 line 2: Table 1 shows found fragmentation... awkward

Suggest to define spectral skew – not all readers will be familiar with this: e.g., relative intensity of mass spectral peaks due to the changes in concentration of the analyte in the ion source as the mass spectrum is scanned.

9469 line 16: The key parameter ... I would say A key parameter or one of the two key parameters...

9470 line 22: the calculation gives a LOD of 0.016 – you sure about this?

9473 line 9 – change to these findings imply...
9475 line 15: a large substance portfolio? (not sure the meaning of this – reword. Reword sentence – also because it is not necessary to say “with the instrument ion discussion”

9478 lines 25-28: Rewrite these sentences for clarity.