Referee comment on « Technical note: Determining chemical composition of atmospheric single particles by a standard-free mass calibration algorithm » by Shao Shi et al.

This study describe a standard-free mass calibration algorithm used for the detailed chemical caracterization of individual particles by single particle mass spectrometers. Their algorithm allows to improve mass accuracy by a factor of 20. In addition, it makes it possible to differentiate adjacent ions with similar m/z (difference of 0.05 Th) and to identify trace ions that were poorly studied in the litterature. Overall, the results of this article may help to improve our knowledge of atmospheric chemistry. However, some of the passages are difficult to read and the English should be revised. Some of the comments and suggested English corrections are listed below.

Abstract

1. Instead of using the terms "tentatively calibrated", I would recommend saying "pre-calibrated" or "initially calibrated" to better emphasise the provisional aspect. The same applies to the rest of the paper

2. L23 – 24 : Change

   « With maximum conformity, the optimal calibrated spectrum was obtained. »

   With

   « The optimum calibrated spectrum was obtained with maximum conformity. ».

Introduction

1. L42 – 43 : « The transformation could be described using mathematical functions (Kozhinov et al., 2013; Kolarova et al., 2017; Lou et al., 2010). ». This is not essential to understand, considering the following sentence.

2. L65 – 76 : Too much information for the introduction. Try to be concise and just present the study's plan.

3. L75 – 76 : « The improved understanding of particle composition was also proved by increased spectra entropy from an information theory perspective. ». This sentence comes out of nowhere.

Methodology

1. L150 – 151 : Change

   « encompassing a large amount of the chemical species and distribution patterns of high occurrence in ambient aerosols »

   with

« and includes a large number of chemical species and distribution patterns commonly found in ambient aerosols. »

2. L163 – 164 : Change

   « is suitable for the implementation of the algorithm, because of the absence of interference when calibrating different mass spectra spontaneously. »

   With

   « is suitable for implementing the algorithm because there is no interference in the spontaneous calibration of different mass spectra. »

3. L165 : Change

   « only ~12 hours was consumed. »

   With

   « only ~12 hours consumed. »

Results and dicussions

1. L177 : Replace « correctness » with « accuracy »

2. L206 – 207 : Change

   « with an accuracy of ~500 ppm (Fig. 4), whereas their presence is difficult to determine in the raw spectra, and thus these species were poorly studied before. »

   With

   « with a precision of ~500 ppm (Fig. 4), although their presence is difficult to detect in the raw spectra and has therefore been little studied in the literature. »

3. L 254 – 255 : Change

   « Principally, mass spectra are comprised of peak information. With our algorithm, calibration of adjacent m/z is achieved, thereby preserving crucial peak information. »

   With

   « Principally, mass spectra are made up of peak information. Our algorithm achieves calibration of adjacent m/z, thereby preserving critical peak information. »

4. Part 3.3 should be better explained as the Shannon entropy comes out of nowhere and is not explained.

Conclusions and implications

1. L275 : add « ppm » at « ~1000 »