

Interactive comment on “Estimating mean molecular weight, carbon number, and OM/OC with mid-infrared spectroscopy in organic particulate matter samples from a monitoring network” by Amir Yazdani et al.

Anonymous Referee #2

Received and published: 19 June 2020

Yazdani et al. obtained important characteristics (mean molecular weight, carbon number and OM/OC) of ambient organic particles using the aliphatic C-H absorbance profile in mid-infrared spectrum. The method applied is solid and the analysis is comprehensive with the results clearly presented. The authors also did careful comparison with some previous studies using other techniques. As the molecular weight, carbon number and OM/OC can be used in recent models or parameterizations characterizing organic aerosol (OA) evolution or other physical properties, this study is timely and I recommend the publication after the following comments can be addressed.

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Major comments:

It is nice that in the introduction the authors have tried to compare the advantages and disadvantages of several techniques determining organic aerosol compositions, e.g., GC/MS, FT-IR and AMS. However, discussions on soft ionization methods are limited (Line 14-16). In recent years soft ionization methods have been frequently used characterizing elemental compositions of ambient organic aerosols (Mazzoleni et al., 2010; Romonosky et al., 2017) and the elemental composition information has been used predicting physicochemical properties of OA, e.g. volatility (Li et al., 2016; Lin et al., 2016; Xie et al., 2020) and phase state (DeRieux and Li et al., 2018; Li et al., 2020). Though the soft ionization methods have shortcomings such as ionization efficiency as the authors pointed, they give more detailed chemical composition information of OA, i.e., the number of C, H, O, N, S, comparing with the mid-infrared spectroscopy used in the study. I suggest more discussions about the advantages and disadvantages of soft ionization methods and the mid-infrared spectroscopy should be added (Nizkorodov et al., 2011; Laskin et al., 2016). I also suggest the authors could add more discussions about the future development of the mid-infrared spectroscopy, for example, how to characterize the characteristics of nitrogen- and sulfur- containing compounds? The compounds used in this study to produce laboratory standards (Table 1) contain only CH and CHO compounds. Does it mean the method developed in this study can only be applied to CH and CHO compounds? However, ambient OA contain heteroatoms.

Minor comments and technical corrections:

- (1) Figure 9: what is the criteria of the liquid and solid phase state? Did the authors measure the viscosity of these compounds or the phase state was estimated? How about the semi-solid phase state, e.g., oil or gel?
- (2) Caption of Table 2: better clarify the first 6 principal compounds were listed in Table 1.
- (3) Line 13, Page 14: the authors described “Many spectra, particularly urban ones,

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are clustered close to tetradecane for the first 4 PCs (Fig. 10)". However, it is difficult to differentiate which points indicate "urban particles" in Fig. 10.

(4) Line 4, Page 11: should be "into" not "in to".

(5) Figure 4 vertical axis: should be "percentage" not "precentage".

(6) Line 13, Page 15: should be "There" not "The is".

(7) Line 4, Page 17: there are two "of" before "the mixture".

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Interactive comment on *Atmos. Meas. Tech. Discuss.*, doi:10.5194/amt-2020-79, 2020.

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