

Interactive comment on “Analysis of functional groups in atmospheric aerosols by infrared spectroscopy: method development for probabilistic modeling of organic carbon and organic matter concentrations” by Charlotte Bürki et al.

Anonymous Referee #1

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The manuscript describes a statistical model and a probabilistic framework to characterize combinations of organic matter, organic carbon and functional groups obtained from the Fourier transform infrared (FTIR) spectra of fine particulate matter (PM_{2.5}). The model was found to be consistent with field measurements of organic carbon (OC). The Development of these models and frameworks is important and timely as they can be used in developing machine learning algorithms.

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The manuscript is publishable after addressing the following minor comments:

The abstract is too long. Consider shortening.

The introduction is missing a discussion on the results obtained from NMR spectroscopy in the characterizing organic aerosols and using multivariate analysis to correlate functional groups with sources of aerosols. For example, see Chapter Two - NMR Studies of Organic Aerosols, Annual Reports on NMR Spectroscopy, Volume 92, 2017, Pages 83-135.

Figure 4: this figure has 12 sub figures; each is labeled with a 'cluster' number and contain a number of overlapping spectra as judged by the gradation in the line colors. The caption needs to be modified to refer the reader to appropriate table or graph containing the definition of each cluster.

Figure 7: The caption needs to be modified to refer the reader to appropriate table of graph containing the definition of parameters in the y- and x-axes.

Figure 8,9,10,11: the use of three-letter abbreviation for seasons that do not correspond to the actual name of the season is confusing: DJF = winter, MAM = spring, JJA = summer, and SON = fall. It is better to use WR = winter, SG = spring, SR = summer, and FL = fall.

Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2019-333, 2019.

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