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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Identification of particulate organosulfates in three megacities at the middle and lower reaches of the Yangtze River" *by* X. K. Wang et al.

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RE: A point-to-point response to referee #1's second comments

"Identification of Particulate Organosulfates in Three Megacities at the Middle and Lower Reaches of the Yangtze River" (acp-2015-393) by X. K. Wang , S. Rossignol , Y. Ma, L. Yao, M. Y. Wang, J. M. Chen , C. George, and L. Wang

We are grateful to referee #1 for his/her valuable comments. A point-to-point response to this reviewer's comments is given below.

1. I have a short remark to the authors comment on 'Bearing in mind the availibility of

instruments having resolutions better than 1 ppm, and the availablitly of the environmental samples as those considered here, we do believe having conducted our study according to the best available standards.' As mentioned in the main the text of the paper-the authors used a mass tolerance of 2 ppm and only C, H, O, N, and S elements for their formulae assignments. This would be valid if you have authentic standards or/and compared your chromatographic RTs as well as the MSn fragmentation patterns with the literature data for all of the suggested OSs. The riverine environments (including Yangtze River region) are not only rich in nitrogen but also phosphorous (e.g. Li et al., 2007, Duan et al., 2009, Hou et al., 2009). Therefore, not considering phosphorous and isotopic ratios for the most abundant elements (i.e. C, N, S and P) could lead to significant formulae misassignments, especially for the ions with m/z >300. The authors describe their formulae assignment procedure by referring to Wozniak et al. (2008). However, the work by Wozniak et al. (2008) does consider phosphorous and isotopic ratios in their molecular formulae assignment procedure. References: M. Li et al. Long-term variations in dissolved silicate, nitrogen, and phosphorus flux from the Yangtze River into the East China Sea and impacts on estuarine ecosystem, Estuar. Coast. Shelf Sci., 71 (2007), pp. 3–12; S.W. Duan, et al. Seasonal changes in nitrogen and phosphorus transport in the lower Changjiang River before the construction of the Three Gorges Dam, Estuar. Coast. Shelf Sci., 79 (2008), pp. 239–250 L.J. Hou, et al. Phosphorus speciation and availability in intertidal sediments of the Yangtze Estuary, China. Appl. Geochem., 24 (2009), pp. 120–128; A.S. Wozniak et al. Technical Note: Molecular characterization of aerosol-derived water soluble organic carbon using ultrahigh resolution electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry, Atmos. Chem. Phys., 8 (2008), pp. 5099-5111.

Reply: Thank you very much for your interest. It is perfectly correct that the work by Wozniak et al. (2008) does consider phosphorous and isotopic ratios in their molecular formulae assignment procedure. However they concluded (Page 5102, Section 3.1.1): "Phosphorous is typically not a quantitatively significant component of atmospheric materials (Chen et al., 2002; Grimshaw and Dolske, 2002; Baker et al., 2006); therefore

all molecular formulas containing phosphorous were eliminated for ease of processing". We therefore indeed just followed their recommendations.

Phosphorus should be considered when dealing with sediment and water samples (e.g. Li et al., 2007, Duan et al., 2009, Hou et al., 2009) because this element is rich in riverine environment. However, here we focus on analysis of organics organosulfates in atmospheric aerosol samples. We revised our title into “Molecular Characterization of Atmospheric Particulate Organosulfates in Three Megacities at the Middle and Lower Reaches of the Yangtze River” to avoid this misunderstanding.

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 21415, 2015.