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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 third 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. Unfortunately I failed to find any recommendations on not considering phosphorous

for molecular formulae assignment in Wozniak et al paper. The authors did consider this element and eliminated all molecular formulas containing phosphorous from the final list of formulae as they found them insignificant in their environment (and those environments considered by Wozniak et al references). As emphasised in my previous comment, this may not be the case for Yangtze river environment.

Reply: The referee is right in saying that Wozniak et al. not recommend to not consider phosphorous. Nevertheless, these authors clearly state that this element is insignificant and that a large majority of compounds can be assigned using only C, H, O, N and S elements. The statement that phosphorous is typically not a quantitatively significant component of atmospheric materials is supported by the literature (Chen et al., 2002; Grimshaw and Dolske, 2002; Baker et al., 2006). In addition, our sampling locations are away from the river and atmospheric aerosol samples are unlikely to be significantly impacted by the river spray, if there was any. Therefore, we choose to process our data similarly to recent studies dealing with environmental aerosol samples from various environments (rural, suburban, urban, Los Angeles, Shanghai, Pearl River Delta Region in China, East Asia) that is to say only involving C, H, O, N and S elements for molecular mass assignment (Fuller et al., 2012; Lin et al., 2012a; Lin et al., 2012b; Tao et al., 2014). In any case, if we do agree that the fact to take or not take into account phosphorous for molecular formula assignment in the case of environmental aerosol samples can be under debate, we think that it cannot be a reasonable reason to reject the present manuscript, given the recent literature on the subject.

2. Moreover, neither Fuller et al nor Wozniak et al (referenced paper in this section) provide any recommendation for not considering isotopic patterns. For molecular formulae assignment procedure, I strongly recommend considering isotopic pattern/ratio section of the highly cited work by Kind and Fiehn (2007) and references therein, which strongly emphasise the importance of this step for accurate molecular formulae assignment.

Reply: Similarly, the referee is right in saying that neither Fuller et al. nor Wozniak et al.

recommend to not consider isotopic pattern. Nevertheless, neither studies effectively used isotopic pattern for molecular formula assignment. In these studies, if a given m/z refers to a C13-containing compound (Fuller et al., 2012) or is 1.003 mass units greater than another detected peak (Wozniak et al, 2008), the peak is not further considered. Lin et al. (2012a) used C13 isotopic peaks only to determine the charge status of the ions. Tao et al. (2014) did not mention isotopic pattern at all. Only Lin et al. (2012b) mentioned isotopic pattern to support the assignment of S-containing formulae. But it is clearly stated that this is done only for intensive ions. In our study, in most cases, the isotopic peak is not detected due to the relatively low intensity of the quasi-molecular ion. One can thus consider that our assignments were done using the standard rules currently available in the literature of our field.

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