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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.

Anonymous Referee #3

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General comments

This is the first study combining UPLC separation with UHRMS (Orbitrap) to characterize organosulfates (OSs) present in ambient samples. The UPLC separation allows detection of isomers, which offers another dimension of information in comparison with the previous fused-injection UHRMS studies of OSs. Such data is valuable in advancing our understanding of OSs, although the authors could have done a better job exploring information derived from this unique combination of information (see details in specific comments).

The uses of wording such as "seasonal" and "diurnal" are misleading as a very small number of samples (a total of 8 samples spread over three cities and two seasons) were characterized and it is over-stretched to argue these snapshots represent seasonal and diurnal variation for a location. The authors also noted that the NJ daytime sample was different from other (pp21425, lines 18-19), illustrating the danger of using one single sample to represent one type of atmospheric conditions). In related to this concern, the abstract needs re-phrasing to indicate sample-to-sample variation, instead of generalizing as seasonal or diurnal variation.

Specific comments

1. Abstract: "…detection of about two hudred particulate organosulfates (OSs), including dozens of nitroxy-organosulfates…". This statement appears to refer to the number of unique formulas, not counting isomers sharing the same formula. This needs to be clarified. It will also be good to indicate the number of OS chromatographic peaks detected (i.e, counting the isomers).

2. Abstract: winter versus summer comparison for WH and SH is better removed or rephrased as sample-to-sample variation instead of generalizing as seasonal variation considering the small number of samples at each location and in each season (as there is only one 24-h summer sample and one 24-h winter sample in WH, one day sample and one night sample in SH in each season).

3. Considering the ability of detecting isomers is a unique result with this work, Fig. S1 deserves to be shown in the main text. I also suggest that the authors include example chromatograms showing isomer presence for a few monoterpene-derived OSs that have been reported in the smog chamber experiments and other ambient studies. For example, [M-H]- at m/z =251.0595 (or neutral mass 252.0673) could be a limonene-derived OS. In current work, 5-7 of isomers at this neutral mass were detected, possibly indicating VOCs other than limonene could also be precursors. Such information is useful in guiding future LC/MS quantification of common OSs.

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4. For the abundant OS formulas shown in Fig. 2 (i.e., A, B, . . .,J.K), I suggest including a table to show the isomer ratios in the samples and possible VOC precursors for these abundant OS formulas. Also comment on the ratio variability among different samples. This information can be useful for LC/MS quantification studies of OSs with lower mass resolution instruments.

5. Figure 2 caption, line 4: a given species -> a given formula

6. Re-organize Tables S3-S10 to list the formulas from the three sites side by side. I suggest combining into one single table to facilitate cross-sample comparison. Also include the retention time data as this also offers information on the compound polarity. It will be also helpful to label the formulas that match those reported in the smog chambers of known precursors.

7. As sulfate is the common precursor for all the OSs, the level of sulfate in each sample could be useful to understand the sample-to-sample variation of OSs detected. I suggest including sulfate data in the manuscript.

8. Figs. 3 and 4: please add a brief note in the caption to indicate what the series (1,2,3,..) are.

9. Fig. 4 (f): series (3) appear twice but series (2) is missing.

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