

Interactive comment on “Technical Note: Relating functional group measurements to carbon types for improved model-measurement comparisons of organic aerosol composition” by Satoshi Takahama and Giulia Ruggeri

Anonymous Referee #2

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The present paper is a technical note to already-published model-measurement comparison SOA studies (Ruggeri et al., ACP 2016). The general scientific objectives are already explained in the previous publications. Specifically, the Authors aim to exploit organic functional group distributions to constrain explicit-chemistry models of secondary organic aerosol (SOA) formation. The idea, although not new, is sound, because functional groups provide direct information about organic reactivity (like in the Carbon Bond Mechanism developed long ago for gas-phase reactions) and keep track of the chemical mechanisms that govern the enrichment of SVOC in the particulate phase. This technical note, in particular, focuses on the derivation of carbon-based

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metrics (such as oxidation state, and O/C ratios) from measurable functional groups distributions, with the aim to support and inform the comparison between FG-based techniques (such as FTIR) and more established mass spectrometric methods (AMS). The methodology is discussed in detail, and for the first time O/C ratios from FTIR measurements are reported taking into account the possible biases due to the selectivity of FTIR spectroscopy for specific FGs. I have only specific comments:

1. Simple examples, like the one shown in Figure 1, are essential for a chemist who is not familiar with linear algebra. I invite the Authors to comment such examples in the text, or in the Supplementary Information. For instance, it is not straightforward why negative values for phi can be obtained. This is important also to understand why values for lambda lower than 1/3 (the theoretical value for a tri-substituted carbon atom) are found in Table 2.
2. The three methods for carbon abundance estimation discussed in Section 2.4 are compared for the examples of SOA formation considered in this study (Table 2, Figures 8, 9), but it is difficult to derive general conclusions on their applicability. How much details on the qualitative composition (in “carbon types”) must be known *a priori*? It would be important to expand the paragraph about the type and nature of the datasets which the three methods rely on.
3. The paper makes use of the notion of “carbon types”. These are exemplified for simple molecules in Figure 1, and are otherwise listed as numbers in the other Tables and Figures. I suggest to explicit the full list in the Supplementary Information. It will be important to understand how many carbon types contain heteroatoms in functional groups (alcohols, carboxylic acids, nitro groups etc.), which seems to be the focus of the paper, instead of being included in the skeleton of the molecules (ethers, esters, etc.).