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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Distinguishing molecular characteristics of aerosol water soluble organic matter from the 2011 trans-North Atlantic US GEOTRACES cruise" *by* A. S. Wozniak et al.

Anonymous Referee #1

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Overview: The presented publication reports molecular characteristics of aerosol water-soluble organic matter (WSOM) collected as part of the 2011 trans-North Atlantic US GEOTRACES cruise. Aboard the ship, a high volume filter sampler was used to collect 24 individual samples Nov 7, 2011 - Dec 9, 2011. The samples were analyzed using ultrahigh resolution FT-ICR MS. Using multivariate statistical analysis the identified molecular formulas were used to separate the 24 samples into 5 key groups associated with the air mass histories. For each of the groups, the molecular characteristics are described based on the unique molecular formulas identified using the PCA. Overall, this is an interesting piece of work with very high quality data. The molecular

insights to marine organic aerosol from this paper represent a substantial contribution of interest to the readers of ACP.

Specific Comments: Several specific comments are listed here in no particular order. 1) P6428, L26: The following includes a typo, "higher O/C ratios and lower O/C ratios". 2) P6432, L09: The PCA was done on selected assigned molecular formulas and not on the MS data. 3) P6434, L14: Please note the addition of HCl may catalyze many oligomerization reactions. Also, methanol has been shown by Bateman et al. ES&T 2008 to contribute to artifacts from acetal reactions. 4) P6435, L01 – L22: Molecular formula assignments appear to be limited only the elemental ratios, mass accuracy and the number of heteroatoms. Are there additional measures to ensure data quality? The method described by Kujawinski et al., 2009 is more extensive than just the number of heteroatoms. They also advocate using formula extensions because mass accuracy alone is insufficient with the high number of elemental combinations. Furthermore, the limit on the O/C is relatively low for atmospheric aerosol. 5) P6440, L03 – L18: Why are the compounds considered ubiquitous? Perhaps they are strongly associated with biogenic hydrocarbons? A similar statement about "terpene-like" molecular formulas that has been presented in Schmitt-Kopplin et al., 2010 and Mazzoleni et al., 2012. This underlines the significance of biogenic hydrocarbons as sources of atmospheric OA components. 6) P6443, L03 -06: How do you explain the amino functional groups in negative ion mode? Typically the H-affinity of amines is so high, that the multifunctional compounds (amino acids) will be zwitterions in the negative ion mode unless there are multiple deprotonations. However, most of the studied OM components have been singly charged. Several of the tentative structures drawn in Figure 7 do not seem likely to be observed in the negative ion mode as indicated on P6433. 7) P6449, L08 – 09: How was the WSOM defined as combustion-influenced? Or, how was the contribution of biogenic SOA removed from the complex mixture to better understand the composition of the combustion influence? How does the fossil fuel combustion composition differ from biomass burning? 8) P6451, L23 - 27: A lack of condensed aromatic compounds could be a result of other factors. For example, aerosol-aging processes

may promote transformation of the compounds over the longer distances. Have condensed aromatic compounds been observed in the remote atmospheres previously? 9) Figure 6: A few figure labels are missing or use different fonts. 10) Figure 1: Only 3 of the 5 groups are shown here. Why?

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