Determination of PM-bound organosulfates in the atmosphere of Athens: Seasonal cycles and source apportionment

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Organosulfates (OS) are components of secondary organic aerosols, which contain sulfate ester functional group in their molecules. OS are assumed to form through various pathways in heterogenous particle phase reactions, which explains the diversity and ubiquity of OS. However, the lack of authentic standards complicates the quantitation of their abundances and contribution to PM mass. In this study, the molecular composition of PM-bound OS was examined. PM_{2.5} samples were collected from January to November 2015 and were analyzed with RPLC-qToF-MS. Eleven OS were identified and quantified using synthesized authentic compounds. More than 40 other OS have been identified using data for their exact masses from the literature and have been quantified using the response factors from the synthesized or other surrogate compounds.

The mean contribution of the total quantified OS to the total PM_{2.5} mass was $0.92\pm1.1\%$, reaching the maximum contribution during the summer period $(2.5\pm1.2\%)$. Different seasonal trends were observed, with the OS derived from isoprene and monoterpenes reactions presenting higher concentrations during the summer period. On the contrary, OS derived from anthropogenic compounds (PAHs, 1,3,5-TMB, decalin, cyclohexane, cyclodecane, etc) showed higher concentrations during autumn/winter. OS with multiple sources, such as, alkylOS, glycolic and lactic acids sulfates presented mixed seasonal trends. Isoprene-derived OS was the most abundant group with mean concentrations ranging from 12,9 (winter) to 271 (summer) ng m⁻³. Among the isoprene OS, the OS215, which is attributed to the sulfate ester of 2-methylerythritol, presented a noteworthy increase during the summer period which is approximately 54 times higher than that measured during winter. Nitrooxy-Organosulfates of biogenic compounds were also abundant, highlight an indirect impact of the increased ambient NO_x and SO₂ levels. References:

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