Speciation of Rainwater and Aerosol during Rain Events in León, Spain, using High Resolution Mass Spectrometry

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A wide range of atmospheric compounds which are present in rainwater are often also present in aerosol. They can be taken up during cloud droplet formation (in-cloud scavenging) or washed out during precipitation (below-cloud scavenging). Such compounds including aromatic hydrocarbons and organic nitrogen containing compounds are hazardous to health.

In this study, the organic chemical composition of rainwater and aerosol from rain events in León, Spain, is being analysed using high resolution mass spectrometry. Collected rainwater along with high volume and low volume filters from rain events which occurred during spring, summer and winter of 2016 have been selected for analysis. Rainwater samples were prepared using Polymeric Reversed Phase Solid Phase Extraction (SPE) and filters have been extracted in water with and without SPE. Three different SPE polymer based sorbents were tested; one for extracting neutral compounds and two which are more suitable for extracting organic compounds containing sulphate and other polar functional groups. The sorbent for extracting neutral compounds was found to yield a higher number of compounds from the sample extraction than the other two varieties.

Kendrick masses, Van Krevelen plots and carbon oxidation states have been investigated to identify compounds and patterns. Preliminary results show a predominance in peaks with O/C ratios between 0.2 and 0.7 and H/C ratios between 1 and 2 in both rain and aerosol samples which indicates substituted aromatic compounds. Cellulose material and fatty acids may also be present. The rain samples also have a significant number of peaks with O/C ratios of 0.0 and H/C ratios between 0.5 and 1 which appear to be absent from the aerosol. These may be due to condensed aromatic rings and considering local meteorological factors will aid interpretation. More preliminary results show that on average 70% of assigned compounds in the rainwater contain nitrogen and 28% contain sulphur. In the aerosol, 54% of compounds contain nitrogen and 41% contain sulphur. Further analysis is also predicted to reveal significant seasonal trends between rainwater and aerosol samples."