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Molecular composition of atmospheric aerosols from Halley Bay, Antarctica, using ultra-high resolution mass spectrometry

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Antarctica is one of the few pristine places to study natural processes of atmospheric aerosols and anthropogenic impacts on the clean remote atmosphere. Although stratospheric aerosol in Antarctica has now been explored in some detail because of the ozone depletion phenomenon, tropospheric aerosol particles in Antarctica remain very little studied.

The main goal of this work is to identify in detail the organic chemical composition of aerosol from Halley Bay station, which is located on the Brunt Ice Shelf floating on the Weddell Sea in Antarctica. In this study we characterise the molecular composition of aerosols from three seasons (summer, autumn and winter in 2012) using ultra-high resolution mass spectrometry (UHRMS). The technique provides high accuracy and high mass resolving power that allows determining unambiguous number of organic compounds present in complex organic mixtures (Noziere et al., 2015). The molecular composition interpretation was facilitated using visualisation methods (e.g. double bond equivalent, Van Krevelen diagrams, Kendrick mass analysis, and carbon oxidation state), which allowed to identify patterns, such as differences between sampling times and atmospheric processes. The majority of the identified compounds were attributed to nitrogen and sulphur containing species which exhibited very strong seasonal trends. Relatively large fraction (up to 30% of the total number of molecules) of these species contained very low hydrogen to carbon ratios (below 1) indicating that the site is impacted by anthropogenic emissions. Influences of the meteorological parameters and air mass trajectories on the molecular composition are discussed.

Nozière et al., The Molecular Identification of Organic Compounds in the Atmosphere: State of the Art and Challenges, Chem. Rev., 115, 3920-3983, 2015.