

EGU21-14313

<https://doi.org/10.5194/egusphere-egu21-14313>

EGU General Assembly 2021

© Author(s) 2021. This work is distributed under the Creative Commons Attribution 4.0 License.



New halogenated trace gases discovered by non-target screening of the atmosphere at the Jungfrauoch high alpine station (Switzerland)

Myriam Guillevic¹, Martin K. Vollmer¹, Matthias Hill¹, Paul Schlauri¹, Aurore Guillevic², Lukas Emmenegger¹, and Stefan Reimann¹

¹Empa, Swiss Federal Laboratories for Materials Science and Technology, Air Pollution / Environmental Technology, Dübendorf, Switzerland (myriam.guillevic@empa.ch)

²Université de Lorraine, CNRS, Inria, LORIA, Nancy, France

Non-target screening consists in searching for all present substances in a sample, suspected or unknown, with very little prior knowledge about the sample. This approach has been introduced more than a decade ago in the field of water analysis or forensics, but is still very scarce in the field of indoor and atmospheric trace gas measurements, despite the urgent need for a better understanding of the composition of the atmosphere.

Recently, we have installed a novel analytical system at the Jungfrauoch high alpine station (3500 m.a.s.l., Switzerland), allowing us to conduct non-target screening of the atmosphere. The system is composed of a preconcentration unit followed by gas chromatography (GC), electron ionisation (EI), and time-of-flight high-resolution mass spectrometry (HRMS). This allows screening the air for all mass fragments from approx. 25 m/z up to 300 m/z, produced by compounds with boiling points from -128 °C (NF₃, CF₄) to +140 °C (e.g., CHBr₃, chlorobenzene, parachlorobenzotrifluoride PCBTF).

Here, we present a new and innovative method to detect and identify unknown organic substances in ambient air using GC-EI-HRMS. We developed an algorithm combining the identification of atom assemblage for the detected fragments and the reconstruction of a pseudo-fragmentation tree, linking fragments belonging to the same substance. This supports in particular the identification of substances for which no mass spectrum is registered in databases. Moreover, we developed a quality control strategy to ensure that the compounds have been correctly identified and are separated from potential coelutants.

Finally, we present a selection of halogenated compounds newly detected in air, measured for the first time at the Jungfrauoch station.