From source to the environment

Strategies for identification and determination of hydroxylated polycyclic aromatic hydrocarbons in complex particulate matrices

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Abstract

Adverse health effects have been linked to exposure to particulate matter, and wood combustion is considered as an important source of harmful particulate matter in the urban air and environment. Hydroxylated polycyclic aromatic hydrocarbons are a group of compounds with toxic, endocrine disrupting and carcinogenic properties. Sources of hydroxylated polycyclic aromatic hydrocarbons are different incomplete combustion processes, such as coal and wood combustion. They can also be formed by microbiological and/or photochemical degradation of polycyclic aromatic hydrocarbons in the environment.

This thesis describes analytical strategies and methods that have been developed and used for screening, tentative identification and determination of hydroxylated polycyclic aromatic hydrocarbons in wood combustion and urban air particles. Conventional targeted analytical methods have been developed for compounds with available reference standards, while suspect and non-target screening strategies have been used for the identification of suspects and unknown compounds lacking reference standards. Each step of the developed analytical methods is described and discussed: the choice of the analytical strategy, sampling of the matrices, extraction, clean-up, instrumental analysis, data processing and validation of the methods.

The influence of wood type (birch, spruce, pine and aspen) and burning conditions (nominal and high burn rate) on the hydroxylated polycyclic aromatic hydrocarbon emissions has been examined, showing that emissions from nominal burn rate combustion correspond on average to 14 % of the emissions from high burn rate combustion. It has been shown that spruce and pine have the highest emissions for nominal burn rate and high burn rate combustion, respectively.

The composition of wood combustion particles has been examined and 32 suspect hydroxylated polycyclic aromatic hydrocarbons have been tentatively identified together with 20 other oxygen-containing small molecular weight compounds. Furthermore, the presence of hydroxylated polycyclic aromatic hydrocarbons in airborne particles from an urban background and a car tunnel has been investigated, and nine target and 11 suspect hydroxylated polycyclic aromatic hydrocarbons have been determined and tentatively identified, respectively.

In summary, this thesis has shown that wood combustion is an important emission source of hydroxylated aromatic hydrocarbons and that the chemical composition of the emitted particles strongly depends on both burning conditions and wood type. Furthermore, the findings suggest that there might be other sources of these compounds in the urban environment than wood burning, such as the traffic. Thus, further investigations are required to fully understand the formation, sources and presence of hydroxylated polycyclic aromatic hydrocarbons in the atmosphere. The suitability of different analytical strategies and methods for identification and determination of hydroxylated polycyclic aromatic hydrocarbons is also discussed.

Keywords: OH-PAHs, hydroxy-PAHs, particulate matter, PM, airborne particles, combustion particles, wood combustion, suspect screening, non-target screening, high resolution mass spectrometry, HRMS, atmospheric pressure photoionization, APPI.

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