Monitoring and Quantifying Toxic Industrial Compounds (TICs) with Proton-Transfer-Reaction Mass Spectrometry (PTR-MS)

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Abstract

Proton-transfer-reaction mass spectrometry (PTR-MS) is a powerful technology because of its wide spectrum of advantages, e.g. high sensitivity, low detection limit and fast response time. Therefore this technology is already well established in the fields of food and flavor science [1], environmental and biological research [2], medicine and biotechnology, etc. In contrast to chemical warfare agents (CWAs) which are very hard to get hold of by terrorists, toxic industrial compounds (TICs) are part of our everyday lives. Thousands of tons of TICs are used in chemical industry worldwide and can endanger human life either when accidentally released from factories or when misused as a weapon in terrorist attacks. Thus there is a need for a fast, sensitive and reliable method for the real-time detection and quantification of these compounds. Here we present (unpublished) results on our latest PTR-MS studies on different TICs. This study complements our previous work on the detection of explosives [3], CWAs [4] and illicit and prescribed drugs [5] and introduces PTR-MS as a universal detector for an ample number of potentially dangerous substances.

PTR-MS technology

In a hollow cathode ion source hydronium ions \( \text{H}_3\text{O}^+ \) are produced from water vapor at purity levels of >99%. Without the need of a mass filter the \( \text{H}_3\text{O}^+ \) ions are introduced into the adjacent drift tube where the proton transfer to all molecules that possess a lower proton affinity than water takes place. This ionization process is very soft (low fragmentation) and efficient, thus permitting real-time quantification and extremely low detection limits. Depending on the envisaged field of application the PTR part can be coupled either to a time-of-flight (TOF) or to a quadrupole mass spectrometer (QMS). The PTR-TOF 8000 instrument allows for the separation of many isobaric compounds because of the high mass resolution (e.g. up to 8 000 m/z for a PTR-TOF 8000 [6]), whereas the PTR-QMS is ideal for monitoring specific substances down to very low concentrations (below pptv level [7]) while keeping the overall dimensions of the instrument very compact.

Results

Chloroacetonitrile is a toxic substance which was commonly used as an eye irritant in the past. In the presented measurement the headspace of pure chloroacetonitrile was injected into a polypropylene (Teflon®) bag filled with nitrogen. We used a Teflon® bag since these sampling bags are widely used in analytical sciences. It can be seen that although the background signal (originating from the bag) at the nominal mass of chloroacetonitrile is rather high, the PTR-TOF 8000 instrument used for this study is still able to identify the chloroacetonitrile (m/z 93.010). Furthermore, due to the high mass resolution we could identify the background contamination peak at m/z 95.049 m/z as protonated phenol. Although the concentration of phenol is nearly as high as for the chloroacetonitrile and the mass difference is only 0.044 amu, both compounds can be monitored (and quantified) simultaneously. With a QMS based PTR-MS instrument the identification could be performed via the characteristic isotopic ratio for chlorine containing compounds (which is the case for many TICs).

References


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