Proton-Transfer-Reaction Mass Spectrometry: Improved Selectivity in Explosives and Designer Drugs Detection

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Abstract

A relatively new area of application for Proton-Transfer-Reaction Mass Spectrometry (PTR-MS) is in the field of safety and security, i.e. the detection of chemical warfare agents, toxic industrial compounds, explosives, illicit and prescribed drugs. The main reasons for the outstanding applicability of PTR-MS in this field are high sensitivity (down to the pptv level) and selectivity; simple sample handling (no preparation necessary) and short response time (down to 100 ms). Details about the performance data of the latest PTR-MS instrument generation are provided here. Furthermore we present details on recent studies that introduce a new dimension of selectivity to threat agent detection with PTR-MS, namely bias dependence in the detection sensitivity on the reduced electric field strength E/N. Following on from our explosive research programme, we present E/N studies on novel designer drugs. This current work emphasizes the use of PTR-MS as a broad-based and highly selective analytical technology for the detection of a large range of threat agents [1-6].

Experimental Setup

A typical PTR-TOFMS instrument consists of an ion source, where water vapor is converted into H3O+ in a hollow cathode discharge and an adjacent drift tube, where the actual proton transfer to the trace gas compounds takes place. The protonated product ions are finally analyzed and detected in a TOF mass spectrometer. We consecutively improved and optimized all of these parts, which in sum contributes to an increase in instrumental performance of over one order of magnitude (compared to the first generation of PTR-TOFMS instruments in 2009) without any decrease in mass resolution. On the left the schematic for a high mass-resolution (m/Δm up to 8000) "PTR-TOF 8000" is displayed. Below a picture of a test body for the explosives measurements is shown. These test bodies consist of aluminum foam containing a defined amount (< 1 mg) of the respective explosive and are used for evaluation of detection limits. PTR-TOFMS, combined with drift tube mass spectrometry, forms an excellent instrument platform that allows the measurement of relatively complex samples. This is the case with explosives, in which a large number of analogs can be found.

Performance Data

Measurement data obtained from a sample containing methylethylketone and butane to illustrate the importance of high resolution for isobaric separation.

Results of the LoD determination utilizing a gas standard. The LoDs were calculated using the common 3σ (standard derivation) method: limit of detection is about 200 pptv.

Results of the sensitivity determination utilizing a gas standard. Values are stated in cps/ppbv: maximum sensitivity is about 500 cps/ppbv.

Increased Selectivity

Above, E/N analyses of two test bodies containing PETN and TNT, respectively, are presented. The two explosives show completely opposite E/N behavior; i.e. the substance concentration and the amphetamine derivative 4-fluoroamphetamine) also possess characteristic E/N dependent branching ratios.

Novel Designer Drugs

Two very recent designer drugs (synthacaine, which should imitate the effects of cocaine and is sold without any information about its composition and ethylphenidate, which is an analogue to the controlled methenamine (aka Ritalin)) were legally bought from vendors in the internet. In contrast to ethylamine (right), which shows a surprisingly high purity of the active ingredient, synthacaine (left) turns out being a mixture of various chemicals, with methenamine (MPA; structural analog of methamphetamine) being the main active ingredient and benzocaine (local anesthetic) presumably being added for the cocaine-like feeling of numbness in the nose after snorting.

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References