# Determination of benzene, toluene and xylene concentration in humid air using differential ion mobility spectrometry and partial least squares regression

M. Maziejuk, A. Szczurek, M. Maciejewska, T. Pietrucha, M. Szyposzyńska


www.elsevier.com/locate/talanta

PII: S0039-9140(16)30064-9
DOI: http://dx.doi.org/10.1016/j.talanta.2016.01.064
Reference: TAL16316

To appear in: *Talanta*

Received date: 1 December 2015
Revised date: 22 January 2016
Accepted date: 30 January 2016

Cite this article as: M. Maziejuk, A. Szczurek, M. Maciejewska, T. Pietrucha and M. Szyposzyńska, Determination of benzene, toluene and xylen concentration in humid air using differential ion mobility spectrometry and partia least squares regression, *Talanta,* http://dx.doi.org/10.1016/j.talanta.2016.01.064

# Determination of benzene, toluene and xylene concentration in humid air using differential ion mobility spectrometry and partial least squares regression

M. Maziejuk[b)], A. Szczurek[a)], M. Maciejewska[a,*)], T. Pietrucha [a)], M. Szyposzyńska[b)]

[a)]Wroclaw University of Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

[b)]Military Institute of Chemistry and Radiometry, al. gen. A. Chruściela 105, 00-910 Warsaw, Poland

monika.maciejewska@pwr.edu.pl

**Abstract:** Benzene, toluene and xylene (BTX compounds) are chemicals of greatest concern due to their impact on humans and the environment. In many cases, quantitative information about each of these compounds is required. Continuous, fast-response analysis, performed on site would be desired for this purpose. Several methods have been developed to detect and quantify these compounds in this way. Methods vary considerably in sensitivity, accuracy, ease of use and cost-effectiveness. The aim of this work is to show that differential ion mobility spectrometry (DMS) may be applied for determining concentration of BTX compounds in humid air. We demonstrate, this goal is achievable by applying multivariate analysis of the measurement data using partial least squares (PLS) regression. The approach was tested at low concentrations of these compounds in the range of 5-20 ppm and for air humidity in a range 0-12 g/kg. These conditions correspond to the foreseeable application of the developed approach in occupational health and safety measurements. The average concentration assessment error was about 1 ppm for each benzene, toluene and xylene. We also successfully determined water vapor content in air. The error achieved was 0.2 g/kg. The obtained results are very promising regarding further development of DMS technique as well as its application.

**Keywords:** BTX, DMS, PLS, multivariate analysis



## 1. Introduction

Benzene, toluene and xylene (BTX compounds) are chemicals of greatest concern because of their widespread distribution and multiple impacts on the environment and human health. They may contribute to the formation of ground-level ozone and photochemical smog, which can cause damage to plants and materials. BTX compounds are considered harmful to aquatic organisms. The investigation of these substances, especially in drinking water at low levels, is critical to protect public health. Benzene, toluene, and xylene may be highly flammable. They have a characteristic sweet, aromatic and “solvent-like”, strong odor. Benzene, toluene, and xylene pose human health concerns. They are regulated toxic compounds. Exposure to BTX compounds occurs in occupational or environmental settings through inhalation or dermal contact. It can create a number of adverse health effects.

For the above mentioned reasons it is important to have access to the quantitative information about each of these compounds. In many applications, there is strong need for continuous, fast-response analysis of BTX compounds on site. Several methods have been developed to detect and quantify these compounds in this way. They vary considerably in