



Review

Ion chromatography-mass spectrometry: A review of recent technologies and applications in forensic and environmental explosives analysis



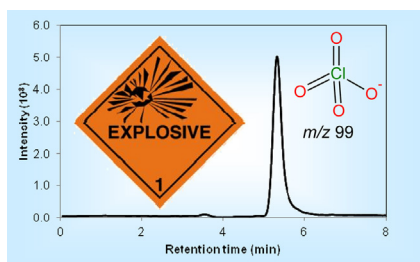
Leon Barron*, Elizabeth Gilchrist

Analytical & Environmental Sciences Division, Dept. Forensic & Analytical Science, School of Biomedical Sciences, King's College London, 150 Stamford Street, London SE1 9NH, United Kingdom

HIGHLIGHTS

- A critical review of the evolution of IC-MS and its application to low-order explosives detection.
- Comprehensive comparison of reported method performances at the fg–μg level.
- A review of auxiliary on-line approaches to maximise MS detector sensitivity.
- A comparison of IC-MS to other confirmatory analytical technologies.
- Emerging future areas for IC-MS in forensic and environmental explosives analysis.

GRAPHICAL ABSTRACT



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ABSTRACT

The development and application of ion chromatography (IC) coupled to mass spectrometry (MS) is discussed herein for the quantitative determination of low-order explosives-related ionic species in environmental and forensic sample types. Issues relating to environmental explosives contamination and the need for more confirmatory IC-MS based applications in forensic science are examined. In particular, the compatibility of a range of IC separation modes with MS detection is summarised along with the analytical challenges that have been overcome to facilitate determinations at the ng–μg L⁻¹ level. Observed trends in coupling IC to inductively coupled plasma and electrospray ionisation mass spectrometry form a particular focus. This review also includes a discussion of the relative performance of reported IC-MS methods in comparison to orthogonal ion separation-based, spectrometric and spectroscopic approaches to confirmatory detection of low-order explosives. Finally, some promising areas for future research are highlighted and discussed with respect to potential IC-MS applications.

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* Corresponding author. Tel.: +44 20 7848 3842; fax: +44 20 7848 4980.
 E-mail address: leon.barron@kcl.ac.uk (L. Barron).

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Leon Barron received his Ph.D. in 2005 from Dublin City University focussing on ion chromatography-mass spectrometry (IC-MS) of disinfectant by-products. He then spent 4 years as a research fellow at the Irish Separation Science Cluster. In 2009, he took up a Lectureship at King's College London where he established his own research group. His interests incorporate all fundamental and applied aspects of separation science, particularly the development of on/off-line sample pre-treatment technologies, portable/miniatuised analytical systems, novel monolithic materials for capillary-scale separations, advancing the fundamental understand-

ing of a range of separation modes, and development of high resolution analytical methods for multi-analyte screening in complex matrices (e.g. illicit drugs/metabolites in wastewater and biota; and explosive residues in human fingermarks). His research is applied across the forensic and environmental science sectors. He is the Editor-in-Chief of *Science & Justice*, Journal of the Forensic Science Society (Elsevier). This review is dedicated to his son, Luc, who was born during its compilation.



Elizabeth Gilchrist is a Ph.D. candidate within the Analytical & Environmental Sciences Division at King's College London. She received her B.Sc. in chemistry at the University of Liverpool in 2009 followed by an M.Sc. in forensic science from King's College London in 2010. Her Ph.D. research lies in the development of capillary ion chromatography and ion chromatography-high resolution mass spectrometry (IC-HRMS) technologies for trace analysis of low-order energetic material residues at the fg–pg level. She has published several papers on the characterisation of gunshot residue and black powder substitutes specifically regarding the determination

of low molecular weight inorganic and organic ion species in latent and chemically enhanced fingermarks. Her M.Sc. and Ph.D. research have been performed in collaboration with the Metropolitan Police Service (UK). In 2012, she was employed as an analyst at the Anti-Doping Science Centre for the 30th Olympic Games in London.

1. Introduction

With the apparent increased use of explosives in recent years [1], the ability to quickly, sensitively and reliably identify and determine a wide range of chemical components is essential both in forensic and environmental investigations. Some of the recent high-profile terrorist attacks using improvised explosive devices (IEDs) include those used in London (1999, 2005), Norway (2011) and Boston (2013) amongst several others. The devices used in these events highlighted the array of possible chemicals that may exist and, in some cases, the relative ease in obtaining them. Therefore, the significant challenges placed on analytical scientists to prepare for and hopefully prevent such events, despite their complexity, is unfortunately an ongoing problem.

Explosives can be sub-divided by compound sensitivity into primary, secondary and tertiary explosives as shown in Fig. 1. Primary explosives are highly sensitive, unstable materials and can ignite by shock, friction, heat or impact. Triacetone triperoxide (TATP) is an example of a primary explosive and one which can be analytically challenging to determine due to this instability [2–4]. Secondary organic explosives typically contain a nitro

group such as 2,4,6-trinitrotoluene (TNT) or nitroglycerin (NG). These are comparatively more stable [5] and are frequently used with a small amount of primary explosive to initiate a detonation. They are regularly mixed with gels, sensitisers or stabilisers depending on the application requirement. Primary and secondary explosives are generally termed “high-order explosives” as they detonate upon discharge. The majority of inorganic compounds, containing salts of chlorate, perchlorate or nitrate ions for example, are considered “low-order explosives”. These materials generally deflagrate and are often used in pyrotechnics and propellants. However, some inorganic compounds, such as ammonium nitrate, are still classed as high-order explosive materials and are known as tertiary explosives. These are very insensitive to shock and require an explosive booster of secondary explosive. Any of the above explosive types can be used in IEDs, and the identification of the components present can be used to determine the source and possibly provide a link to a suspect [6]. The term “pre-blast” describes a point in time before an explosion has occurred. Conversely, “post-blast” pertains to a time-point after discharge of an explosive. Pre-blast detection of explosives can either involve bulk (mg to kg) analysis of the charge itself, or trace analysis (fg to mg) of the

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