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# Analysis of triacetone triperoxide complexes with alkali metal ions by electrospray and extractive electrospray ionisation combined with ion mobility spectrometry and mass spectrometry

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**The complexation of triacetone triperoxide (TATP) with a range of alkali metals has been studied by electrospray ionisation mass spectrometry to yield $[M + Cat]^+$ ions for all of the alkali metals. The formation of $[2TATP + Li + LiX]^+$ (X = Br, Cl) sandwich complexes was also observed. Collision cross-sections for the lithium-containing complexes of TATP were measured by travelling wave ion mobility spectrometry mass spectrometry and compared well with computationally determined structures. Extractive electrospray ionisation (EESI) using a lithium-doped electrospray is demonstrated for the detection of TATP vapours desorbed from a metal surface. The limit of detection for EESI was shown to be 20 ng using the $[TATP + Li]^+$ ion.**

*Keywords*: triacetone triperoxide, ion mobility mass spectrometry, collision cross-section, extractive electrospray ionisation

## Introduction

The peroxide-based explosive triacetone triperoxide (TATP) has gained notoriety through its use by terrorist organisations. Its straightforward synthesis, availability of the starting products and an explosive power comparable to that of TNT have led to its involvement in a number of incidents,[1,2] including the London bombings of 2005.[3]

Many chemical-based explosive detection systems rely upon the presence of a nitro group or a metallic element within the explosive; the lack of these in TATP makes detection difficult using these approaches.[4,5] Mass spectrometric analysis of TATP allows the identification of the explosive through accurate mass measurement and tandem mass spectrometry. However, the protonated TATP molecule generated in atmospheric pressure ionisation ion sources fragments readily, making detection of the intact $[M + H]^+$ ion by electrospray and atmospheric pressure chemical ionisation problematic.[6–8] Complexation of the peroxide with either ammonium or alkali metal ions has been shown to improve the stability of TATP and facilitate mass spectrometric detection of intact TATP complexes.[8–10] Oligomeric peroxides of TATP have also been observed by electrospray ionisation mass spectrometry (ESI-MS) through the formation of sodium adducts.[11–13] TATP has been extracted from a range of surfaces by desorption electrospray ionisation (DESI) using an electrospray doped with ammonium or alkali metal ion and with low limits (nanograms) of detection.[6,14] Ion mobility measurements have shown the potential to detect TATP from hair samples with the use of an ammonium ion dopant.[15] Hyphenated gas chromatography

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