

Detection of the Peroxide Explosives TATP and HMTD

Introduction

The explosive peroxide compounds triacetone triperoxide (TATP) and hexamethylenetriperoxide diamine (HMTD) are difficult to detect by conventional mass spectrometry methods. These compounds can be easily detected by the Direct Analysis in Real Time (DART™) ion source.

Experimental

Measurements were made with the AccuTOF-DART mass spectrometer operated in positive-ion mode under standard conditions. Little or no heat was required to observe these compounds. Dilute solutions of standard samples of TATP and HMTD were analyzed by dipping melting point tubes into the liquid and dangling the melting point tubes in the DART ion source. Dilute aqueous ammonium hydroxide on a cotton swab was held in the DART gas stream to enhance detection of TATP as the ammoniated molecule.

Results

TATP is readily detected as $[M+NH_4]^+$ at m/z 240.1447 (Figure 1). A trace fragment at m/z 91.0399 is assigned as the $C_3H_7O_3^+$ fragment. Exact mass measurements allow the assignment of the peak at m/z 223.0968 as $C_{12}H_{15}O_4^+$, which is assigned as monobutyl phthalate $[M+H]^+$. Exact mass measurements avoid a mistaken assignment of this peak as protonated TATP (m/z 223.1182), which is not observed.

HMTD is observed as the protonated molecule at m/z 209.0776. This is major species observed. A few small characteristic fragment ions may also be observed in the HMTD mass spectrum.

Conclusion

Peroxide explosives TATP and HMTD were easily detected by the AccuTOF-DART with no sample preparation. Both compounds were detected at trace levels on a variety of surfaces including fingertips, boarding passes, and cloth. Exact mass measurements confirmed the compositions and avoided mistaken assignment of a contaminant as a target analyte peak.

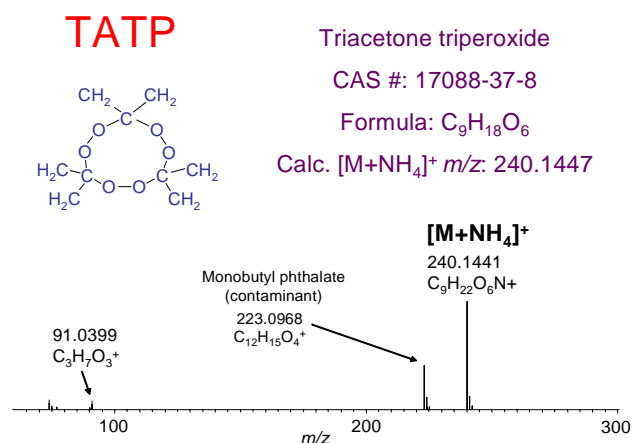


Figure 1. AccuTOF-DART mass spectrum of TATP

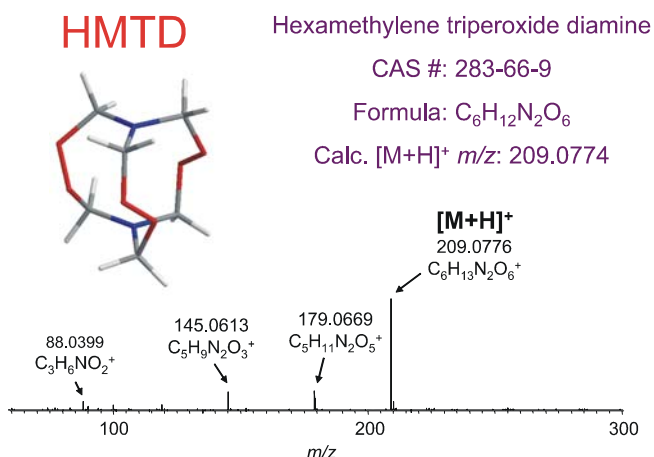


Figure 2. AccuTOF-DART mass spectrum of HMTD