Poster Abstract

A Study of How Alternative Buffer Gases can Affect Energetic Material Detection in an Ion Trap Mass Spectrometer

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Due to their inherent nature, energetic materials are more reactive than the traditional hydrocarbons and are better able to undergo the substitution of one or more groups located in the alpha position to the electron withdrawing nitro group. The mass spectra of various high explosives were determined using electron ionization and an ion trap containing nitrogen gas. The spectra obtained displayed characteristic fragmentation in accordance with their respective structures. When the nitrogen gas was replaced with labile deuterium gas, the spectrum for certain compounds of interest showed an increase in the M+1 and M+2 peaks indicating whether the compound had been mono or di-substituted with deuterium. Due to the small potential well on the miniature ion traps and the ability to undergo many neutral collisions, it is an ideal environment to couple chemistry with ion fragmentation to reduce false positives in the spectrum. As hydrocarbons and even some energetic materials do not undergo these substitutions, one can rapidly test (1-2 minutes) for a specific group of high explosives by identifying the M+1 and M+2 peaks. The ideal high explosives are stable enough to undergo electron ionization and substitution without completely decomposing, yet not so stable that they do not substitute at all.