

Influence of Fast Temperature Program Rate and Fast Linear Velocity on GC-MS Analysis of Chemical Warfare Agent Degradation Products

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The chemical warfare agent O-ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate (VX) and numerous VX degradation products containing the diisopropylaminoethyl functional group are known to produce poorly-diagnostic mass spectra by gas chromatography-mass spectrometry (GC-MS) when typical 70 eV electron ionization (EI) is used with a quadrupole mass filter detector. To address this issue three detection methods were evaluated; lab based chemical ionization (CI) GC-MS, field portable ion trap GC-MS and vehicle based EI GC-MS. Chemical ionization reliably produced $M+H^+$ ions useful in the laboratory to definitively identify these analytes, but this method is less amenable for field deployment. Degraded VX was analyzed using a field-portable GC-MS system employing a cylindrical ion trap mass spectrometric detector, and ion/molecule reactions leading to formation of protonated species ($M+H^+$) were noted for all analytes studied. However, as the injected mass of analyte was increased the effects on resulting mass spectra observed included mass axis shifts due to space charge effects and pronounced signal for the dimer ($2M+H^+$) of the degradation product diethyl methanephosphonate. Additional samples were analyzed using a vehicle based GC-MS system equipped with a low thermal mass resistively heated GC column capable of completing rapid analyses. While the quadrupole mass filter used with this instrument and 70 eV EI predictably produced mass spectra for VX-related compounds with no discernible ion/molecule interactions, the lack of diagnostic mass spectra was problematic. This can be compensated through the use of GC retention index (RI) data.