MS and MS/MS Performance of a Field-Portable Ion Trap Mass Spectrometer for CWC Treaty Compounds

The pending ratification of the Chemical Weapons Convention (CWC) Treaty will trigger the on-site inspection of chemical production facilities all over the world. The treaty requires that inspections for scheduled compounds outlined in the treaty be made quickly and confidently, while maintaining the confidentiality of proprietary manufacturing processes and compounds. In addition, the analysis must be made in the presence of an expected excess chemical background. To meet this challenge, the Defense Nuclear Agency (DNA) has tasked the Chemical and Biological Defense Command (CBDCOM) of the US Army with the development of a field portable ion trap mass spectrometer (the Generic Detector) currently under development by Bruker-Franzen (Bremen, Germany). The instrument has full GC/MS/MS capabilities while possessing weight (<45 kg), size (< 0.12 cu. m) and power consumption (24 VDC, <500 W) figures of merit which are truly field-portable. In addition, the instrument uses no compressed gases for either the chromatography or the ion trap buffer gas, but rather uses air. This further reduces support requirements for field operation.

The design of field portable instruments often impose operational or performance restraints on the subsequent analysis. A recently completed study of the performance of the Generic Detector for the analysis of 24 chemical weapons related compounds (precursors, by-products or degradation products) demonstrates the capabilities of this instrument as a CWC treaty on-site inspection instrument. Chromatographic characteristics of these compounds when using air as the carrier gas on a short capillary column, vary widely and impact the subsequent detection limits. The detection limits for both MS and MS/MS modes of operation have been determined as well as calibration curves. The use of air as the ion trap buffer gas imposes some considerations for the resulting MS/MS spectra due to a larger mass targets as well as possible ion/molecule reactions with oxygen. As such, in addition to the analytical detection limits, MS/MS performance figures (isolation efficiency and MS/MS efficiency) have also been determined. The results from this unique instrument will be discussed in light of more conventional ion trap operational results when using helium as the buffer gas.

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