Multimodal Ionization Strategies for Broad-Spectrum Threat Detection with a Miniature Field Mass Spectrometer

Dr. Nathan Grimes - United States - BaySpec

Abstract

Field teams need one instrument that can ionize everything from high-proton-affinity nerve-agent simulants to low-affinity petrochemicals. We have pursued two complementary strategies on the 22 kg Continuity portable linear ion-trap: (1) an atmospheric multimodal source that merges dielectric-barrier discharge ionization (DBDI), atmospheric-pressure chemical ionization (APCI), and atmospheric-pressure photoionization (APPI); and (2) a new configuration that retains DBDI and APCI in air while relocating the deuterium lamp behind the inlet orifice to enable vacuum ultraviolet photoionization (PI) inside the first vacuum stage.

For the atmospheric design, a patented coaxial manifold couples the DBDI plasma with an APCI corona needle and directs a 10.78 eV D_2 lamp into the same reaction volume. Bench testing with permeation-tube vapors showed mode-specific advantages: 2-butanone responded best in pure APCI, toluene radical cations dominated in APPI and DBDI, and dimethyl methylphosphonate gained an additional threefold in signal intensity when all three modes were active. Operating APPI and APCI concurrently raised total ion current for every analyte studied, confirming the predicted proton-transfer and photoionization synergy.

The vacuum PI variant addresses species whose proton affinities lie below that of water yet whose ionization energies fall under 10.78 eV, for example benzene and chlorinated benzenes. A 25 mm chamber extension positions the lamp at 7 torr, upstream of the ion funnel. Three low-profile DC lenses steer ions through the new region without additional RF, an arrangement validated in SIMION and confirmed experimentally.

We are actively comparing the atmospheric multimodal source with the vacuum-PI version to determine which excels at different target classes. By combining the DBDI, APCI, and photon-based ionization in a single adaptable front end, this approach expands chemical coverage and accelerates field detection capabilities without compromising portability.

Biography - Nathan Grimes

Nathan Grimes, Ph.D. is an Instrumentation and Application Scientist specializing in miniature linear ion trap mass spectrometry. He earned his Ph.D. in Analytical Chemistry with a focus on portable MS systems, instrumentation/ionization development, and differential ion mobility. His work spans electrical, mechanical, and software integration for field-deployable systems, as well as method development for detecting trace vapors, aerosols, and complex biological or environmental samples. Dr. Grimes has authored technical reports and proposals for defense and environmental applications, and has field experience in government and military collaborative projects.

Keywords

Portability, Photoionization, Multimodal, Corona