Why Do You Usually Need a GC/TQ for Pesticide Residue Tests?

Application Note Abstract

Many pesticides are measured using an LC/TQ system, with electrospray ionization (ESI). However, several pesticides are not detected in ESI, and it was proposed to use negative atmospheric pressure chemical ionization (Ni-APCI) for their detection. Using Ni-APCI the analysis of PCNB has been shown in the literature with a precursor ion of m/z 275.5 and a ionization mechanism as the loss of HCl followed by formation of an ammonium ion adduct ion.

There are two intrinsic problems with this description:

1. The empirical formula for PCNB is $C_6Cl_5NO_2$, thus there is no hydrogen atom to lose as H-Cl
2. The formation of positively charged ammonium ions in negative ionization mode is highly unlikely.

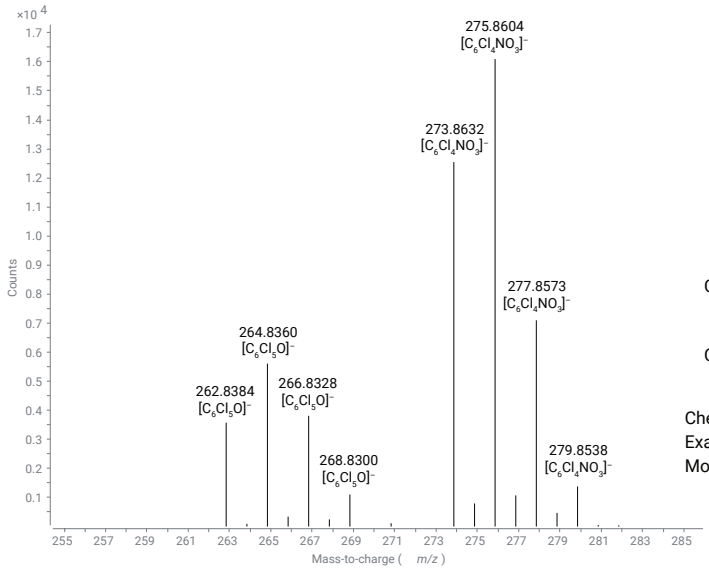
This application note demonstrates the correct ionization mechanism for PCNB using Ni-APCI LC time-of-flight mass spectrometry and evaluates the appropriateness of LC/TQ Ni-APC technique for detection of the analytes not responding in ESI.

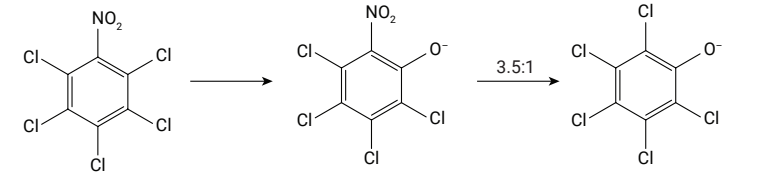
The analysis of PCNB and several other polychlorinated pesticides using LC/TQ with Ni-APCI results in nonselective precursor/product ion pairs. Furthermore, the nonlinear response and poor coefficients of determination (R^2) shown for these compounds in Ni-APCI LC/TQ disqualifies this analytical methodology for these analyses in certain regions, such as California and Canada. Learn more in the application note below.

Detailed application note

Why LC/MS/MS and GC/MS/MS Are Required for the Analysis of Certain Pesticides

Spectrum and Reaction Scheme for PCNB in Ni-APCI LC/Q-TOF Analysis





Chemical formula: $C_6Cl_5NO_2$
Exact mass: 292.8372
Molecular weight: 295.3210

Chemical formula: $C_6Cl_4NO_3^-$
Exact mass: 273.8638
Molecular weight: 275.8705

Chemical formula: $C_6Cl_5O^-$
Exact mass: 262.8397
Molecular weight: 265.3155

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DE.8174537037

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Published in the USA, June 1, 2020
5994-2127EN

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