APPLICATION NOTE 5981-A

QUANTITATION OF CHLORINATED DIBENZOFURANS IN PCBs USING THE TAGA™ 6000 MS/MS SYSTEM

Current chemical methodology for the measurement of PCBs in environmental samples entails perchlorination and gas chromatographic quantitation of the resulting decachlorobiphenyl. Of even greater interest are the more toxic decomposition products of PCBs; chlorinated dibenzofurans. Chlorinated dibenzofurans, which are generally in much lower concentration than PCBs, are converted to the octachloro species when subjected to perchlorination. It is the decachlorobiphenyl (DCB), octachlorodibenzofuran (OCDF) mixture which results from the workup of environmental samples for PCB analysis. Quantitation of OCDF in the DCB matrix can be accomplished using the TAGA™ 6000 MS/MS more rapidly and with greater specificity than is afforded by GC or GC/MS.

The analysis was carried out by ionizing the sample at atmospheric pressure using hexafluorobenzene as a charge transfer agent. This reagent selectively ionizes only the OCDF and not the DCB. After passage into the vacuum only positive ions with m/z 440 (corresponding to the OCDF molecular ion with eight ^{35}Cl) were selected by the first quadrupole (Q1), and collided with the target gas in Q2. The daughter ion spectrum obtained by scanning Q3 is shown in Figure 1.

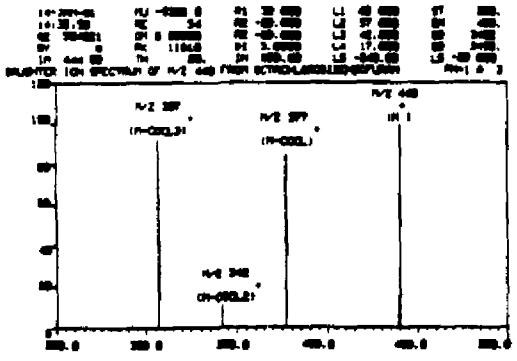

Figure 1. Daughter Ion Spectrum of m/z 440 From Octachlorodibenzofuran.

Quantitation was achieved by flash desorption from a direct insertion probe at atmospheric pressure, and multiple ion monitoring was used to examine the most intense parent m/z 444 (M^+), and two daughters, m/z 381 ($[M\text{-}CO^{35}Cl]^+$) and m/z 311 ($[M\text{-}CO^{35}Cl_3]^+$). The computer soft-

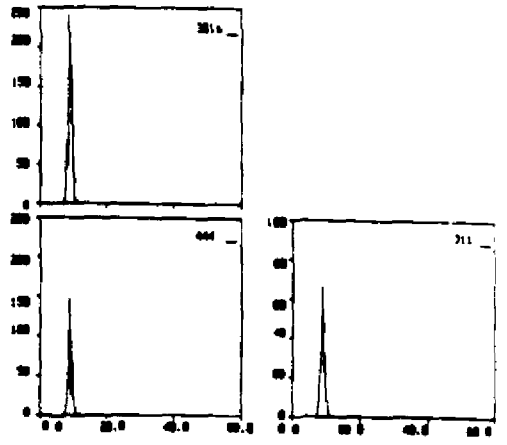

Figure 2. Multiple Ion Scan for the Flash Desorption of Octachlorodibenzofuran Standard Solution

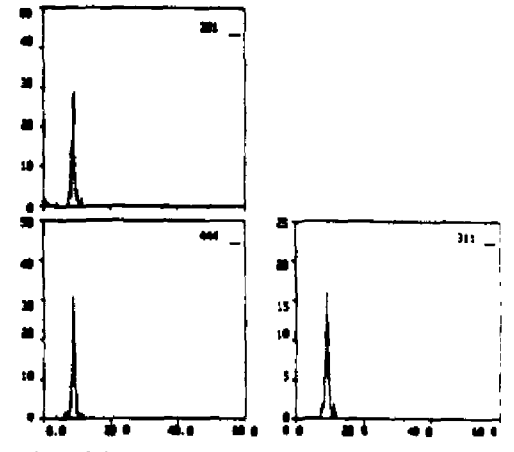

Figure 3. Multiple Ion Scan for the Flash Desorption of Octachlorodibenzofuran in Decachlorobiphenyl

SCIEX INC

MONS 214305

ware controls the flash evaporation and displays and integrates the desorption curve, as shown in Figure 2 for a standard OCDF solution. The branching ratios for fragmentation are very specific for each parent ion and these are used to confirm the presence of OCDF in environmental samples. In the case of OCDF in the DCB matrix (Figure 3) the branching ratios are within 4% of those determined from the standard solution of OCDF (Figure 2). While sensitivity to OCDF in the matrix is somewhat reduced when compared to the standard, the branching ratios remain constant (indicating no interferences from decachlorobiphenyl) and the detection limit (S/N = 3) is projected as less than 10ppm of OCDF in DCB.

If OCDF is the primary target for analysis this could be carried out in the extract without the perchlorination since no interferences have been observed for OCDF in Aroclor matrices.

In conclusion, the TAGA™ 6000 MS/MS has the demonstrated ability to measure OCDF in environmental samples without interference from other ubiquitous chemical pollutants.

Copyright © 1981 by SCIEX INC

55 Glencameron Road, #202
Thornhill, Ontario, Canada L3T 1P2

Telephone: (416) 881-4646 / (416) 223-9077 • Telex 06-964722

MONS 214306