GC/MS with a DART™ Ion Source

Introduction

The output of a gas chromatograph was connected to an AccuTOF-DART™ to provide a simple GC/MS interface.

GC/MS analysis can be carried out by connecting the GC output to the DARTTM ion source with a simple interface. Because the GC column is not introduced into vacuum, there are no restrictions on gas flow rates. No fragile electron filament is used. Conditions can be adjusted to produce chemical ionization (CI) mass spectra or mass spectra resembling electron ionization (EI) mass spectra.

Experimental Conditions

A JEOL AccuTOF-DART mass spectrometer was used as the detector. The GC/MS interface consisted of short piece of 1/8 inch OD copper tubing wrapped with heat tape. A thermocouple was used to check the interface temperature. The GC column extended about 1 cm from the tubing into the heated gas stream of the DART ion source and positioned directly in front of the sampling orifice for the mass spectrometer atmospheric pressure interface. The DART source was operated with helium gas with the gas heater set to 300 degrees C. The GC was operated with the standard GC column (30 m ID x 0.32 mm film thickness DB-5 column) used for GC/MS measurements in our laboratory. GC conditions for the Grob mix were: split injection, oven temperature ramped from 40 to 200 degrees at 6 degrees per minute.

Results and Conclusions

CI mass spectra are observed when operating the DART ion source under normal conditions (DART source ~1 cm from the API orifice, DART exit grid set to 250 V). Analysis of a Grob mix shows protonated and/or ammoniated molecules for all of the Grob mix components except the alkanes, which are not detected.

Moving the DART ion source as close as possible to the mass spectrometer orifice and setting the DART grid potential to maximum (650 volts) produces mass spectra that resemble electron ionization mass spectra. Ionization occurs by a combination of Penning ionization and/or charge-exchange with oxygen (O2+.) ions.

All of the components of the Grob mix were detected (Figure 1.) Mass spectra resembled electron ionization mass spectra, with two major exceptions. Both molecular ions and protonated molecules can be observed, and the relative abundance of these molecular species is very high. Figure 2 shows the DART mass spectrum of component 13 (methyl dodecanoate). This method has been applied to more complex mixtures (such as diesel oil) with excellent success. It is a simple solution for providing GC/MS capabilities with a DART ion source. The absence of vacuum interface, electron filament, and CI reagent gases offers a robust interface.

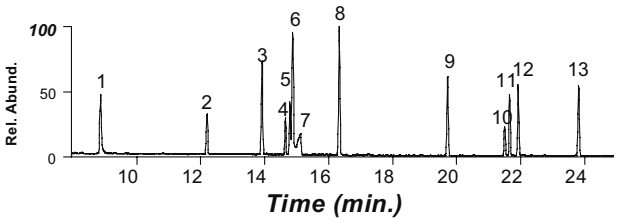

Figure 1. Grob mix analyzed by GC-DART. Peaks: 1 = 1,3-butanediol, 2 = decane, 3 =1-octanol, 4 = undecane, 5- nonanal, 6 - 2.6-dimenthylphenol, 7 = 2-ethylhexanoic acid, 8 = 2,6-dimethylaniline, 9 - methyl decanoate, 10 - surfynol, 11 = methyl undecenoate, 12 = dicyclohexylamine, 13 = methyl dodecanoate.

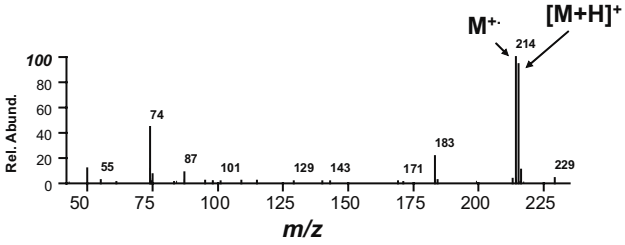

Figure 2. Mass spectrum of methyl dodecanoate.

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