EXTERNAL ELECTRON IONIZATION 7 T FOURIER TRANSFORM ION CYCLOTRON RESONANCE MASS SPECTROMETER FOR RESOLUTION AND IDENTIFICATION OF VOLATILE COMPLEX MIXTURES

Jinmei Fu (NHMFL Tallahassee), Jeremiah M. Purcell (FSU Chemistry & Biochemistry), John P. Quinn (NHMFL Tallahassee), Tanner M. Schaub (NHMFL Tallahassee), Christopher L. Hendrickson (NHMFL Tallahassee; FSU Chemistry & Biochemistry) Ryan P. Rodgers (NHMFL Tallahassee; FSU Chemistry & Biochemistry), and Alan G. Marshall (NHMFL Tallahassee; FSU Chemistry & Biochemistry)

Results and Discussion

An external electron ionization (EI) source has been interfaced to a 7 T Fourier transform ion cyclotron resonance mass spectrometer and tested for volatile complex mixture analysis. A new Sulfinert® deactivated inlet system provides continuous stable sample flow to the EI source, leading to stable ion signal (± 10% deviation) for 2 h from a 200 nL mixture of 15 n-alkylbenzenes. Ultrahigh mass resolving power, $m/\Delta m_{50\%} \approx 735,000$, was obtained for 1-bromo-2-chlorobenzene with accurate isotopic ratio measurement. Baseline resolution was observed (see Figure) for two of the closest commonly encountered mass doublets, $C_3/SH_4$ ($m_2 - m_1 = 3.4$ mDa at m/z 190) and $SH_3/C_4$ ($m_2 - m_1 = 1.1$ mDa at m/z 190), at mass resolving power, $m/\Delta m_{50\%} \approx 400,000$, by low-energy (18 eV) electron ionization of unprocessed diesel fuel from a 200 nL septum injection. Although hydrocarbons dominate the positive-ion 18 eV EI mass spectrum from diesel fuel, many sulfur-, nitrogen-, and oxygen-containing compounds were readily observed without prior fractionation. By comparing 18 eV EI FT-ICR mass spectra of unprocessed and processed diesel fuels, we were able to identify which heteroatom-containing species were removed by processing.

Acknowledgements

The authors thank Daniel McIntosh, Greg T. Blakney and Andy Powell for technical support. This work was supported by the NSF National High-Field FT-ICR Mass Spectrometry Facility (DMR 00-84173), Florida State U., and NHMFL.

References