Chapter 4

Application of the Dual-Cell Fourier Transform Mass Spectrometer

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The differentially-pumped, dual cell geometry has improved the performance of Fourier transform mass spectrometry (FTMS) for a variety of analyses, including combined gas chromatography/mass spectrometry, laser desorption mass spectrometry, and MS/MS. The ability to accommodate higher source pressures has also permitted the coupling of supercritical fluid chromatography with FTMS. The dual cell geometry has demonstrated improved resolution and accurate mass measurements under analytical conditions; added benefit results from isolating sample ions from reactive neutrals.

The potential benefits of Fourier transform mass spectrometry have been evident ever since the introduction of the technique by Comisarow and Marshall in 1974 [1], but it is only in recent years that major developments in the technology have caused an increased acceptance of FTMS into the mainstream of analytical mass spectrometry. In particular, the development of differentially-pumped systems including the tandem quadrupole-FTMS [2], the dual-cell geometry [3,4], and external sources [5], have overcome the difficulties associated with the requirement that FTMS analysis be accomplished at low pressures (e.g., less than 10^{-7} torr) for best results. Efforts to develop FTMS for high mass detection [6,7], in particular, the work by Shabanowitz, et al. [8] with the detection of insulin and cytochrome C, have demonstrated that large ions can be formed with sufficiently long lifetimes to be detectable on the FTMS timescale, proving that FTMS is a viable technique for the analysis of molecules in the "middle-mass" range (e.g., 1,000-15,000 amu). The tailored-excitation method developed by Marshall [9,10] provides a means to overcome several limitations of current ion excitation methods, and promises to bring about significant improvements in the overall performance of FTMS, particularly FTMS/MS [11].

In this article, we describe some of the recent developments and applications of the dual-cell Fourier transform mass

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spectrometer to a variety of chemical problems and mass spectrometric techniques.

Experimental

All experiments were performed using a Nicolet Analytical Instruments FTMS-2000 dual-cell Fourier transform mass spectrometer with optional GC and laser desorption interfaces. The FTMS-2000 dual cell is specially constructed of stainless steel with low magnetic susceptibility. This permits very efficient ion transfer between the source and analyzer cells, if the cells are properly aligned in the magnetic field.

The superconducting magnet was operated at a field strength of 3 Tesla. This instrument has been described in previous publications [4] to which the reader is referred for a more detailed description. Specific details of the various experiments described in this report will be included in the individual sections pertaining to those experiments.

Results and Discussion

Gas Chromatography/FTMS. The differentially pumped, dual-cell geometry has permitted the practical realization of combined gas chromatography/Fourier transform mass spectrometry (GC/FTMS) by providing a means to deal with the higher pressures associated with the GC carrier gas [12]. Using the dual-cell instrument, we have shown that it is possible to obtain high resolution mass spectra, even for small sample quantities. For example, we were able to detect ions from a 125 pg splitless injection of naphthalene at a resolution of 15,000 over the mass range 120 to 130 amu with a signal-to-noise ratio of 10:1[4].

Figure 1. resolution

Once the carrier gas pressure has been eliminated as a factor, the major factor affecting the resolution obtainable for GC/FTMS spectra is the trade-off between the mass spectral data acquisition time (observation time and number of signal-averaged transients) and the data acquisition rate required for high resolution capillary gas chromatography. In order to maximize mass spectral resolution, it is desirable to observe the transient signal for as long a time as possible. However, the width of chromatographic peaks places a limit on how long an observation time may be employed without affecting chromatographic resolution. Typically, peaks in capillary gas chromatography are about 3 seconds wide, which means that, ideally, mass spectra should be acquired about once per second.

In order to demonstrate that it is possible to obtain very high mass resolution without sacrificing chromatographic resolution, we made a splitless injection of an activity mix (SGE Activity Mix A) containing approximately 50 ng each of naphthalene, 2,6-dimethylphenol, and 2,4-dimethylaniline. The mass spectrometer was set up to operate in heterodyne (high resolution) mode [13] to monitor masses within the range 119-129 amu. Two transients were collected and signal-averaged per spectrum, with 64K data points acquired per data set.

Figure 1 shows the molecular ion of naphthalene, detected at a resolution of 340,000. The total acquisition time per transient

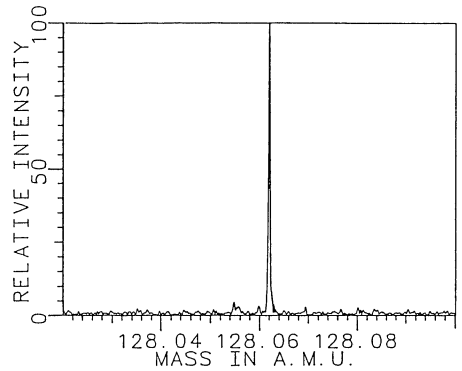

Figure 1. GC/FTMS: Naphthalene molecular ion detected at a resolution of 342,000.

was 1.2 seconds. By observing the transients, it could be seen that only one of the two averaged transients contributed signal. This suggests that the optimum conditions would be to collect only one transient per spectrum, which would reduce the total acquisition time to 1.2 seconds per spectrum. This data shows that it is possible to obtain ultra-high mass resolution (greater than 100,000) on a time scale that is consistent with high chromatographic resolution.

The major application of high resolution mass spectrometry is for obtaining accurate mass measurements in order to determine elemental compositions. The present FTMS calibration equation, derived by Ledford, et al. [14] shows that the mass-to-charge ratio m/z of a given ion is related to the magnetic field, B, the electric field, E, and the measured frequency, F, by a relation having the form:

$$m/z = k_1 + B/f + k_2 E/f^2$$

where k_1 and k_2 are constants, and the electric field term is related to the trap voltage and the number of ions in the cell. Wilkins, et al. have demonstrated accurate mass measurements in the low part-per-million range for GC/FTMS, using a calibration performed just prior to the sample analysis [15]. The success of this method is based upon the fact that the calibration is performed under conditions which are virtually identical to those employed for the sample measurement, and hence the total number of ions is approximately the same for both measurements.

It is also possible to improve the accuracy of the mass calibration by making use of a peak of known composition to correct the electric field term for changes in the number of ions [16]. In other words, if the identity of some component of the mixture is known by its retention time and/or mass spectrum, a peak of known mass in the mass spectrum may be used to apply a correction factor, x, to the electric field term in the calibration equation, which may be rewritten as:

$$m/z = k_1 B/f + k_2 (E+x)/f^2$$

where m/z is chosen to be the mass of the known peak, and f is the measured frequency of that peak. Subsequent mass measurements using the corrected calibration equation will have a higher mass measurement accuracy than those using the uncorrected equation.

This is illustrated for the activity mix in Table 1. Masses for ions within the 119-129 amu mass range were measured for the three compounds, using a calibration taken prior to the measurement. The average deviation for six ions is found to be 6.9 ppm. If we were certain of the identity of the molecular ion from naphthalene (e.g., if naphthalene had been deliberately added to the mixture), we could use the molecular ion as an "internal standard" to determine the appropriate correction to the electric field term in the calibration. From Table 1, we see that the result of this "one point" correction is a significant improvement in the mass measurement accuracy, with the average deviation in the measurements of the remaining five ions being only 0.8 ppm

This sort of correction should be helpful for improving specific mass measurements for GC/FTMS analyses where it is possible to add a calibrant compound to the mixture, or where some component is known to be present. Unlike the method where a static

Table I.
Mass Measurement Accuracy
from High Resolution GC-FTMS Run

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Mass Measurement Accuracy
from High Resolution GC-FTMS Run

COMPOUND	PRIOR CALIBRATION		ONE POINT CALIBRATION	
	Mass (amu)	Deviation (ppm)	Mass (amu)	Deviation (ppm)
2,6-Dimethylphenol	122.072316	7.0	122.072674	-0.5
2,4-Dimethylaniline	120.080473	7.1	120.080819	-0.4
	121.088187	8.0	121.088539	0.5
Naphthalene	126.046190	6.0	126.046572	-1.4
	127.053994	6.1	127.054382	-1.2
	128.061660	7.3	128.062054	-0.01
	AVERAGE	6.9		0.7

calibration compound is present, the "internal calibrant" here is separated by the gas chromatograph from the sample compounds, and does not interfere with the mass spectra of the remaining compounds. It should be noted that the best results are achieved when the ion chosen to determine the correction is close in mass to the ions to be measured.

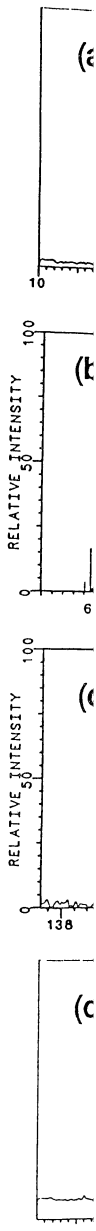
The additional information available from high resolution GC-MS may be illustrated by examining a portion of the data from a peppermint oil analysis. Figure 2a shows the total ion chromatogram for a sample of a peppermint flavor extract. Some of the components are clearly unresolved with these chromatographic conditions. If we look at the mass spectrum of the component eluting at 15 minutes (Figure 2b), we can see a resolved doublet at m/z 139. The doublet is shown in an enlarged view of the region of the mass spectrum around m/z 139 (Figure 2c).

If we were to look at a single-mass chromatogram for mass 139 (+/- 0.5 amu), we would see only two clearly-defined chromatographic peaks (Figure 2d). But if we choose a more selective mass range to take advantage of the high resolution information, we can clearly identify several other components. In fact, three isobaric ions may be identified, two of which are associated with the sample, and one which is present in the background. The high-resolution single-ion reconstructions (Figure 3) clearly show which ion is associated with which eluting components.

The background ion is only identifiable from its suppression when components are eluting. This sort of phenomenon is known to occur in conventional GC/MS analyses; in our case the phenomenon may be associated with dynamic range considerations [17]. From analysis of this same mixture by MS/MS, [18], we have identified the $C_9H_{15}O^+$ peaks as fragments from menthol and menthone. The $C_{10}H_{19}^+$ peaks are assigned as fragments from menthyl acetate, menthyl valerate, and cadinene.

The use of the dual-cell FTMS to perform a typical target compound analysis may be illustrated by the identification of cocaine in a human urine extract. To determine the retention time of cocaine, a drug standard containing 10 ng of cocaine was injected using splitless injection onto a 20 meter BP-1 column with a 200 micron ID. The column was heated from 90 to 250 degrees at 10 degrees per minute. Under these conditions, the component eluting at 15.8 minutes (Figure 4a) was identified as cocaine. The mass spectrum corresponding to this peak (Figure 6a), shows the molecular ion at m/z 303, as well as characteristic fragment ions. The total ion chromatogram (Figure 4b) from the urine extract is quite complex and does not have a strong peak at 15.8 minutes. However, by plotting mass chromatograms (Figure 5) of the base peak in the mass spectrum of cocaine (m/z 82) for both the standard and the urine extract, one can see a large peak at an elution time of 15.8 minutes.

The mass spectrum corresponding to this peak (Figure 6b) matches well with the spectrum obtained from the drug standard, and also with the (Wiley NBS) library spectrum. Using the accurate mass measurements obtained on the FTMS data, comparisons can be made between the standard and the unknown. Based on twelve



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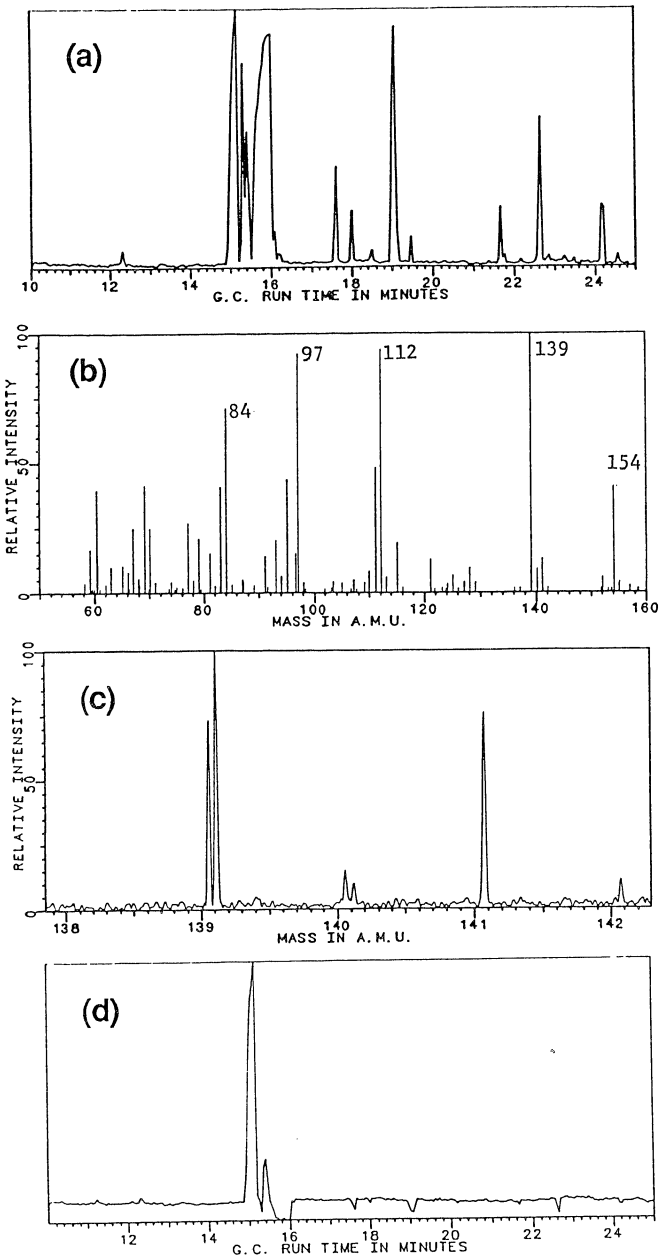


Figure 2. Peppermint oil analyzed by GC/FTMS: (a) total ion chromatogram; (b) mass spectrum of component eluting at 15 minutes; (c) enlargement of region around m/z 139 from (b); (d) mass chromatogram for m/z 139 +/- 0.5 amu.

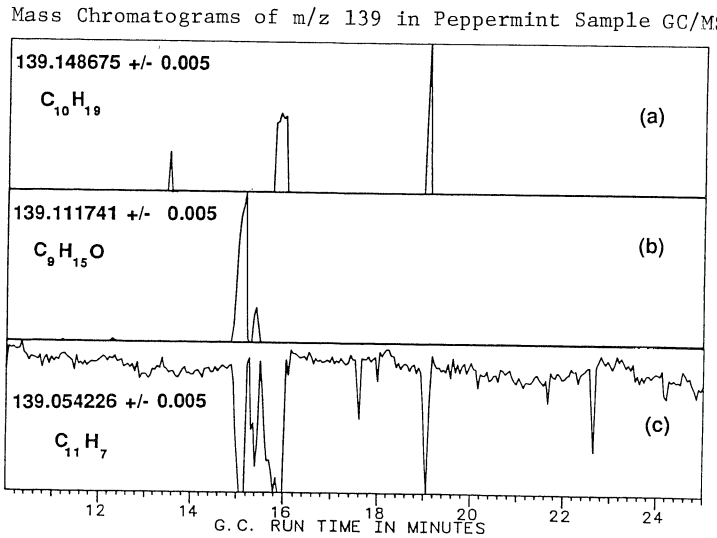


Figure 3. High resolution mass chromatograms for m/z 139: (a) mass chromatogram for $C_{10}H_{19}^+$; (b) mass chromatogram for $C_9H_{15}O^+$; (c) mass chromatogram for $C_{11}H_{17}^+$ (background peak).

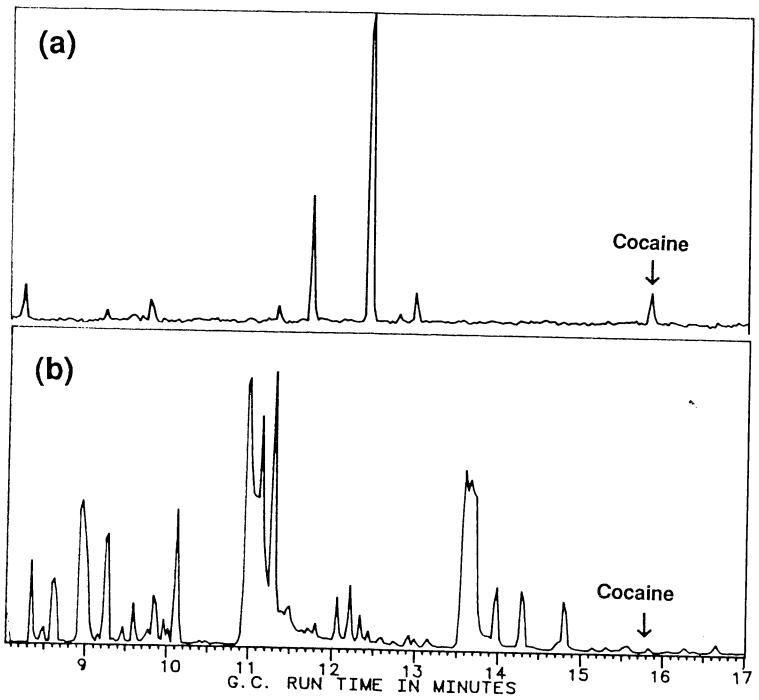
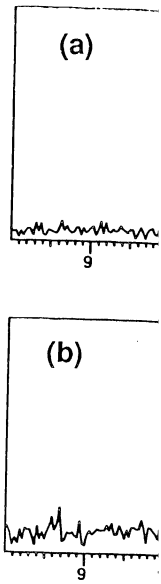


Figure 4. (a) chromatogram for drug standards including cocaine; (b) Chromatogram for urine extract.



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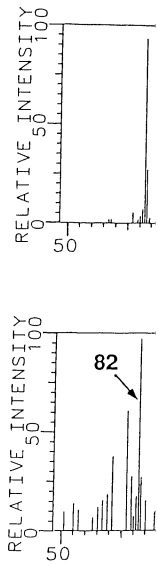

Figure 6. (a)
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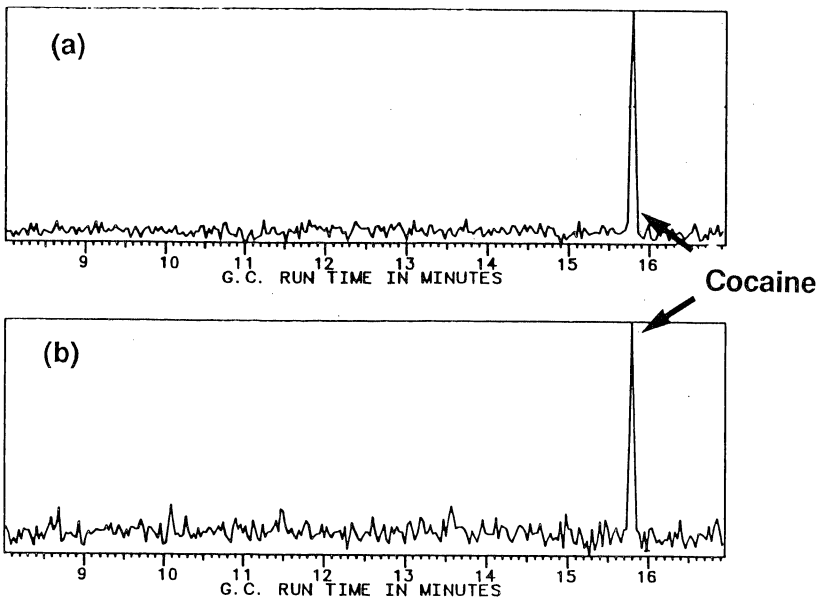

Figure 5. Mass chromatograms for m/z 82 in: (a) standard drug mixture; (b) cocaine.

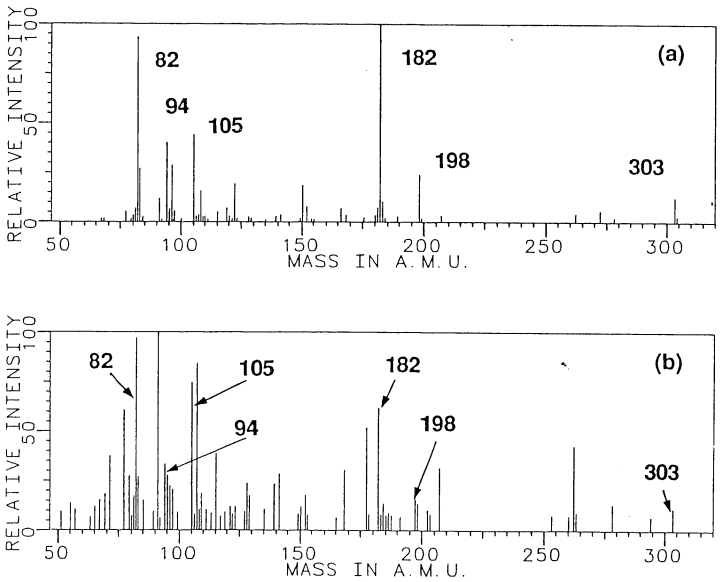

Figure 6. (a) Mass spectrum of cocaine standard; (b) Mass spectrum of component in urine extract eluting at 15 minutes (unsubtracted).

significant ions in the two spectra, mass measurement differences (based on 32K data points, and without internal calibrant) averaged only 8 ppm, adding an additional degree of confidence to the assignment of the unknown as cocaine.

Supercritical Fluid Chromatogaphy/FTMS. Supercritical fluid chromatography (SFC) has experienced a recent growth in popularity as an alternative approach to liquid chromatography, due to its increased resolution and faster analysis times. SFC is particularly attractive as a chromatographic method for coupling with FTMS, due to the reduced gas burden, in comparison with HPLC. We have performed preliminary experiments coupling SFC with the dual-cell Fourier transform mass spectrometer to demonstrate the capability of the dual-cell geometry to deal with the gas load imposed by SFC. These experiments indicate that both high mass spectrometric resolution and accurate mass measurements are possible with SFC/FTMS [19].

For this work, a 5 meter x 50 micron ID fused silica column, coated with a 0.25 micron polydimethylsiloxane film was introduced directly into the source chamber through the transfer line normally used for GC/FTMS. A restrictor was created at the end of the column by using a microflame to draw out the end of a 1 meter portion of deactivated but uncoated column to an inside diameter of approximately one micron. Details of the instrumentation used for SFC have been described elsewhere [19]. With the SFC interface in place, pressures in the source chamber were approximately 5 x 10^{-5} torr. Despite this high source cell pressure, we were able to obtain relatively high quality mass spectral data with analyzer side detection at 5 x 10^{-7} torr.

Figure 7a shows a total ion chromatogram of the separation of two model compounds, caffeine and methyl stearate, by SFC/FTMS. The isopentane CI spectra (Figures 7b and 7c) of each of these compounds shows only the $[M+H]^+$ peaks and the carbon 13 isotope peaks for each of the two compounds. Though crude, these results demonstrate the feasibility of coupling SFC with FTMS.

The high resolution obtainable for SFC/FTMS is shown in Figure 8, which shows the molecular ion region of caffeine, taken under self-CI conditions (no reagent gas). Separation of the molecular and pseudomolecular ions is shown at a resolution of 8,000. It must be emphasized that this resolution was obtained for a direct mode spectrum, over the mass range 50 amu up to the highest mass measured, using a data collect of 128K data points. This resolution is only data point limited, and does not reflect the maximum attainable at the working pressures of SFC/FTMS. We expect that resolutions in excess of 10,000 should be readily attainable [55]. Accurate mass measurements in the low ppm range for caffeine taken in the EI mode are shown in Table II.

Laser Desorption/FTMS. Laser desorption (LD)/FTMS [20] has been applied to a variety of chemical problems, ranging from fundamental studies of ion-molecule reactions [21,22], to the analysis of pharmaceuticals [4,23-29], to polymers [7,30-35], to organometallics [6-39], and to surface analysis [4,40]. The large number of papers being generated from the few laboratories working

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SFC/FTMS separ
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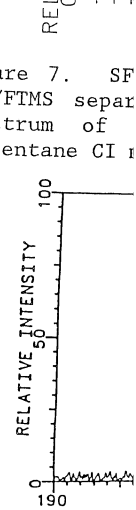

Figure 8. Mole
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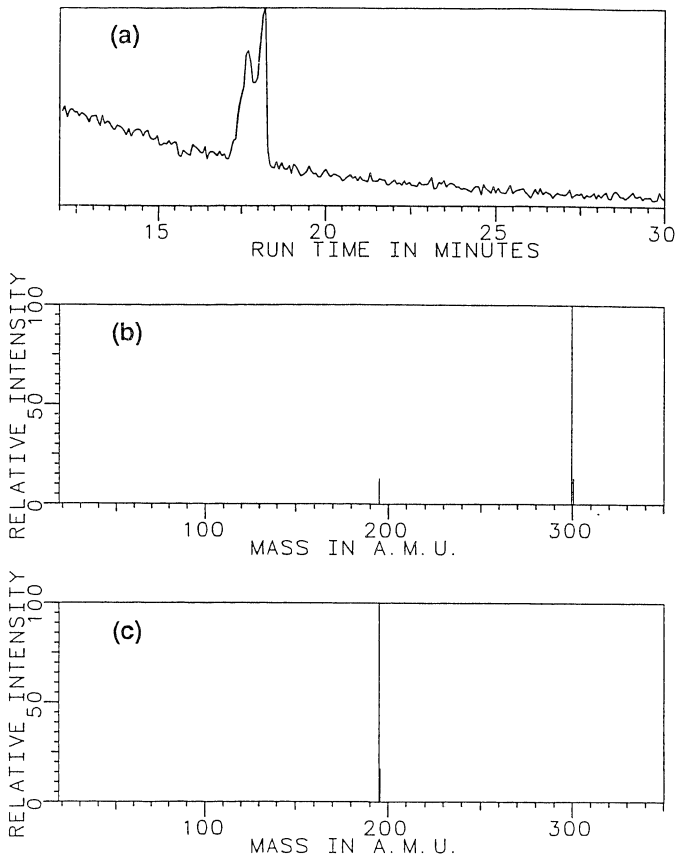

Figure 7. SFC/FTMS feasility study: (a) total ion current for SFC/FTMS separation of methyl stearate; (b) isopentane CI mass spectrum of methyl stearate (with trace of caffeine); (c) isopentane CI mass spectrum of caffeine.

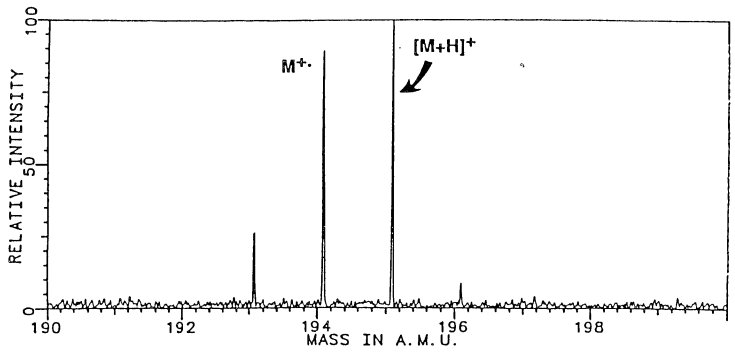

Figure 8. Molecular ion region of SFC/FTMS spectrum of caffeine under self-CI conditions, detected at a resolution of 8,300.

with LD/FTMS should serve to indicate the growing importance of the methods. In this article, we present two specific applications of LD/FTMS to surface and inorganic analysis.

A simple example of the use of LD/FTMS for surface analysis may be found in the analysis of blue stain on the surface of a copper part. In order to determine the nature of the stain, we obtained LD/FTMS spectra for samples of both stained and unstained copper. Both samples were mounted on the automatically rotated sample insertion probe on the FTMS-2000. The samples were rotated after each laser shot to expose a fresh surface at the laser focus. Approximately twenty-five laser shots were signal averaged for each spectrum, in order to increase signal-to-noise, and to provide a spectrum which would represent the averaged composition of the surface.

This approach was employed, since spectra of single spots on the surface might have local variations in composition which would hinder a comparison of the two samples. The spot size at the focal point was approximately 150 microns in diameter. The instrument was operated in dual-cell mode, with ions detected in the analyzer side immediately after the laser was fired, in order to minimize undesirable ion-molecule reactions which might occur at the higher pressures in the source cell. Both positive and negative ion spectra were collected for each sample.

Positive ion spectra were not particularly helpful, showing only Cu^+ and trace alkali metal ions (Na^+, K^+). However, the negative ion spectra were more complex, and a comparison between the spectrum of the stained copper (Figure 9a) with the unstained copper (Figure 9b) shows several additional peaks in the spectrum of the stained copper. Examination of these peaks revealed them to result from contamination of the surface by sulfur, with prominent peaks identified as:

$$S^-,\ HS^-,\ S_2^-,\ CuS_2^-,\ CuS_2H^-,\ Cu_2S_2^-,$$
$$Cu_2S_2H^-,\ \text{and}\ Cu_3S_3^-$$

These ions were identified by mass measurement as well as their isotopic abundances. Resolution for these spectra was approximately 5,000 which was adequate to separate CuS_2^- from traces of I^- present on the surface as a contaminant in both samples. The analysis was confirmed by Auger spectroscopy, which clearly showed the presence of sulfur on the surface. The contamination was later found to have resulted from vulcanized rubber that had come in contact with the stained copper parts.

Another example is found in the analysis of the mineral zircon. We had previously published [4] a spectrum of a positive ion laser desorption spectrum of a sample of the mineral zircon (zirconium silicate) showing uranium as $^{238}U^+$, present in the sample at a level of approximately 15 parts-per-million [41]. The spectrum, which showed mixed zirconium oxides and hydroxides as the most intense peaks in the spectrum, was taken with a four second delay between the laser pulse and ion detection, in order to allow neutrals to be pumped out of the cell. These conditions had been found adequate for analysis of organic compounds. However, it was found that the reactivity of zirconium was such that the mixed oxides and hydroxides were produced as ion-molecule reaction products during the long trap period.

Table II. SFC-

COMPOSITION
$C_8H_{10}N_4O_2^+$
$C_8H_9N_4O_2^+$
$C_4H_6N_2^+$

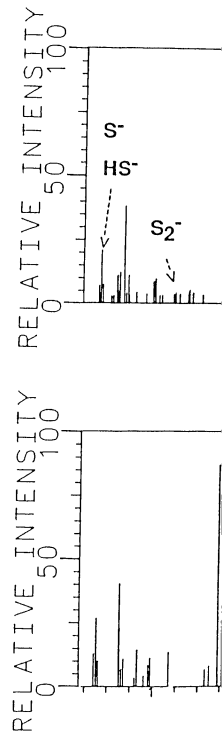

Figure 9. Analys
sulfide contamina
standard.

Table II. SFC-FTMS, Electron Impact Measured Masses for Caffeine

COMPOSITION	CALCULATED	MEASURED	DIFFERENCE (ppm)
$C_8H_{10}N_4O_2^+$	194.080376	194.080307	-0.36
$C_8H_9N_4O_2^+$	193.072551	193.072597	-0.23
$C_4H_6N_2^+$	82.053098	82.052900	-2.4

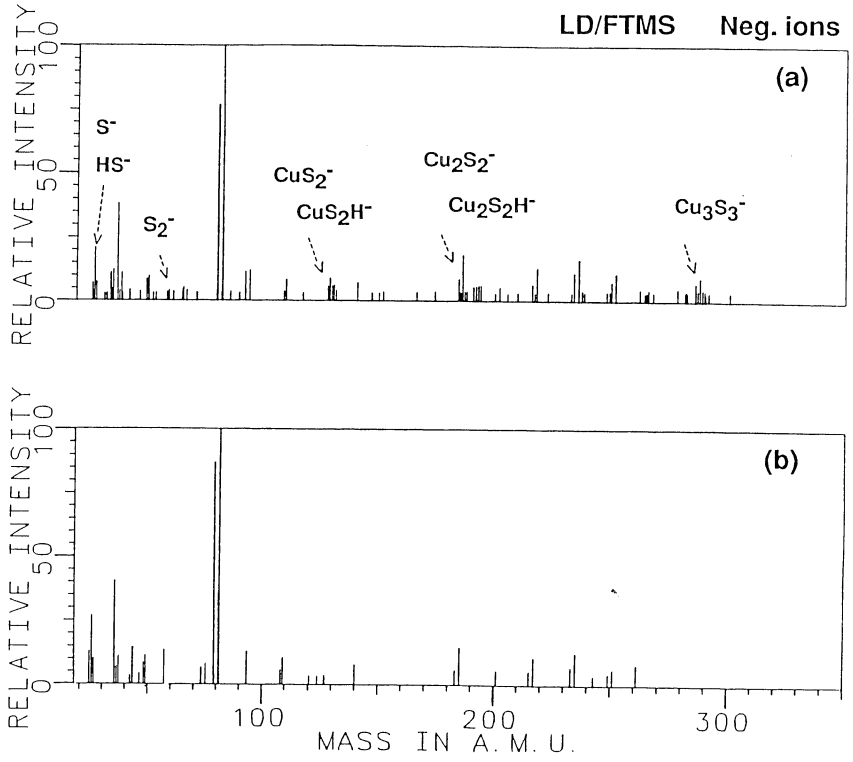

Figure 9. Analysis of a surface stain on copper showing copper sulfide contamination: (a) stained copper; (b) "clean" copper standard.

By reducing the delay time from four seconds to 100 milliseconds, we find that the ion-molecule reaction products are significantly reduced, and that the base peak is now due to Zr^+. A laser desorption spectrum of a sample of zircon containing approximately 100 times more uranium than the previous sample is shown in Figure 10. This spectrum shows the presence of lead resulting from the radioactive decay of uranium, as well as uranium and uranium oxide peaks. Trace rare earths are also evident, giving peaks due to Er^+, Yb^+, Y^+, and Hf^+. Unlike the previously published example, no ejection was required in order to see the uranium. The ratio of ^{238}U to its radioactive decay product, ^{206}Pb, may be used to date the mineral. The ratios for this sample gave a calculated age of 1.5 million years, which agreed with the age determined by standard geological methods.

MS/MS. The capability of trapping ions for long periods of time is one of the most interesting features of FTMS, and it is this capability that has made FTMS (and its precursor, ion cyclotron resonance) the method of choice for ion-molecule reaction studies. It is this capability that has also lead to the development of MS/MS techniques for FTMS [11]. FTMS has demonstrated capabilities for high resolution daughter ion detection [42-44], and consecutive MS/MS reactions [45], that have shown it to be an intriguing alternative to the use of the instruments with multiple analysis stages. Initial concerns about limited resolution for parent ion selection have been allayed by the development of a stored waveform, inverse Fourier transform method of excitation by Marshall and coworkers [9,10] which allows the operator to tailor the excitation waveform to the desired experiment.

In addition, several approaches to ion activation that are not well-suited to conventional types of mass spectrometers, are very well-suited for use with FTMS. These include photodissociation and ion-electron collisions [46-49]. In this paper, we would like to present some applications of ion-electron collisions to MS/MS, and show that the method may be a suitable alternative to collisional activation for some applications. We will also discuss some of the desirable characteristics of the dual cell geometry, as applied to MS/MS experiments.

Positive ions may be trapped by electrostatic attraction in the ionizing electron beam, if the electron beam current is sufficiently high [50]. Ion-electron collisions may cause enough energy to be deposited in the trapped ions to result in further ionization [51], or activation resulting in bond breaking [52]. Activation of ions by ion-electron collisions results in fragmentation which may be compared to collisional activation, and which may be used to obtain breakdown curves [53]. The ion-electron collisional activation approach has been given the tongue-in-cheek name, "Electron Impact Excitation of Ions from Organics", or, "EIEIO".

We have recently shown that it is possible to perform MS/MS experiments by making use of the ion-electron collisions in a Fourier transform mass spectrometer [54]. Parent ion selection, which could not easily be achieved in the previous experiments, is accomplished by gating off the electron beam for a short period of

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time, in order to permit ion ejection. The high field of the superconducting magnet helps keep the ions from drifting out of the electron beam, allowing them to undergo collisions with electrons when the beam is gated on again.

An example is shown in Figure 11, which shows the method applied to a synthetic mixture, containing acetyl acetone, N-methyl aniline, isophorone, and acetophenone. After ions have been formed by electron impact, they are confined in the source cell and allowed to undergo ion-molecule reactions ("self-CI") for a period of 100 milliseconds (Figure 11a). The electron beam is left on during this reaction period at a low electron energy (3 eV) in order to help confine ions in the electron beam. Following the reaction period, the electron beam is gated off for approximately 3-5 milliseconds, during which two swept-frequency ion ejection events select out the $[M+H]^+$ ion (and some molecular ion) for acetyl acetone, which has a relative abundance of only 1-2 percent due to the high proton affinity of the N-methyl aniline. The electron beam is then gated back on, and the conductance limit is grounded for a period corresponding to one trapping oscillation for the ions. This has the effect of transferring virtually all of the $[M+H]^+$ ions into the analyzer cell (Figure 11b). The ions remain trapped in the electron beam for a period of 100 milliseconds, at a low electron energy, (4 eV) and a high electron current (25 microamperers). During this period, the ions undergo activation and fragmentation, resulting on the formation of daughter ions at m/z 42 and m/z 85 (Figure 11c). Selection of the M^+ and $[M+H]^+$ ions for N-methyl aniline and the EIEIO spectrum for this component is shown in Figures 12a and 12b.

In addition to the EIEIO experiments, the dual cell has also been employed for collisional activation (CA) experiments. Selected parent ions may be transferred to the analyzer cell for CA. With pulsed valve introduction of the collision gas (argon) into the analyzer cell, it is possible to obtain very high daughter ion resolution. Figure 13 shows a $C_6H_5CO^+/C_8H_9^+$ doublet from CA of acetophenone and mesitylene, detected at a resolution of 500,000.

A major difficulty in using FTMS for complex mixture analysis by MS/MS techniques has been the tendency of daughter ions to react with neutral species from the sample. These unwanted ion-molecule reactions can complicate the interpretation of MS/MS spectra, or even prevent the observation of daughter ions altogether. However, we may use the dual-cell geometry to transfer selected parent ions into the analyzer cell, where they are isolated from reactive neutral species. If this is done, then the use of FTMS with collisional activated dissociation (CAD) for complex mixture analysis is greatly facilitated. As an example, we consider the determination of which of three possible isomers is present in an epoxy resin extract. For one component of the extract, diamino-diphenylsulfone (DADPS), it has been shown using a hybrid instrument of BEQQ geometry [55] that CAD spectra are substantially different for different isomers.

We have repeated this work to demonstrate the use of the dual-cell FTMS to distinguish isomers in a mixture. Figure 14a shows an electron impact spectrum of the epoxy resin extract introduced via the direct insertion probe. Figure 14b shows the 50 eV CAD

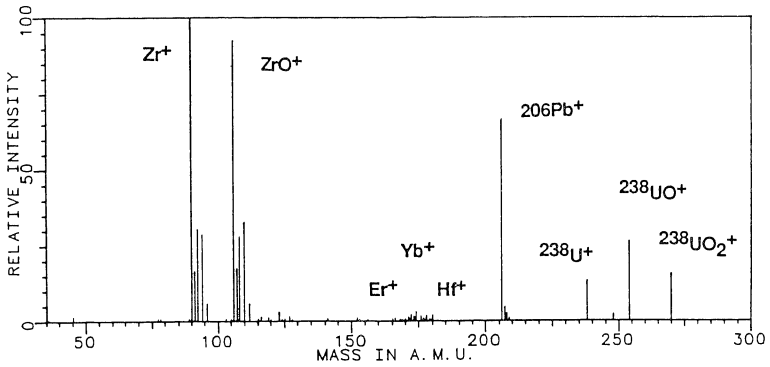

Figure 10. Mass Spectrum of zircon mineral (sample courtesy of M. Harrison and S. deLong, SUNY, Albany).

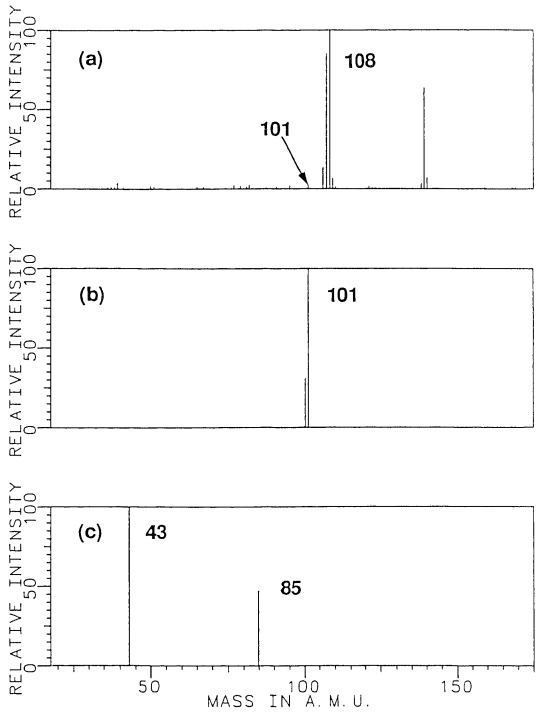

Figure 11. Identification of acetyl acetone in a synthetic mixture by EIEIO: (a) Self CI mass spectrum showing acetyl acetone at ~2%; (b) Selection of acetyl acetone (M^+ and $M+1^+$); (c) EIEIO fragments from acetyl acetone in mixture.

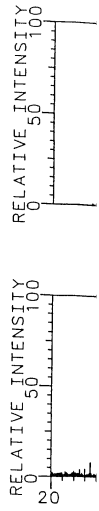

Figure 12. Id
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fragments of N-

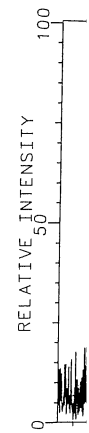

Figure 13. Is
mesitylene, det

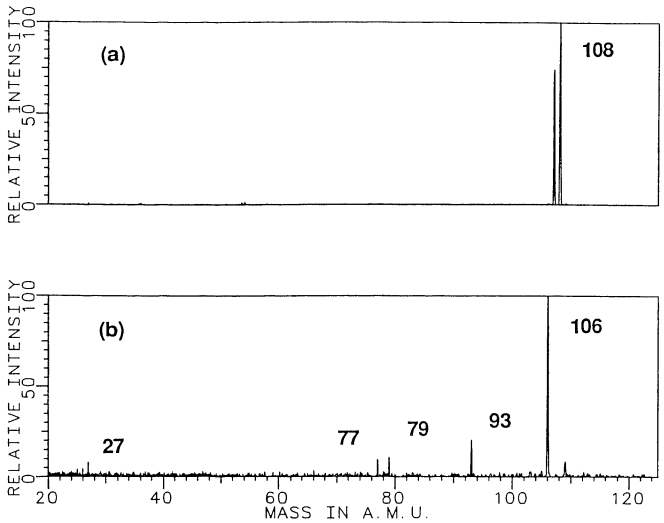

Figure 12. Identification of N-methyl aniline in the synthetic mixture by EIEIO: (a) Selection of N-methyl aniline; (b) EIEIO fragments of N-methyl aniline in the mixture.

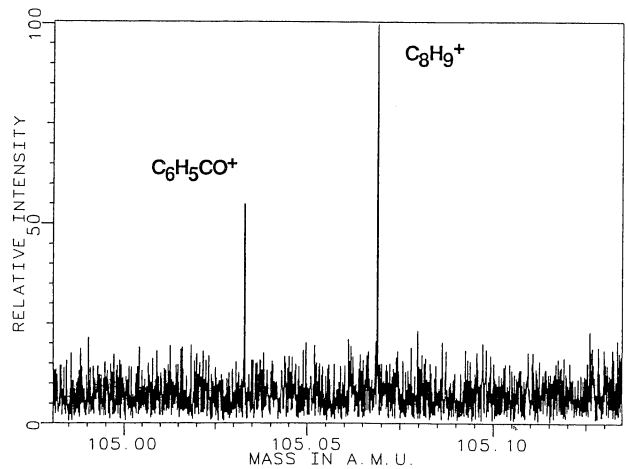

Figure 13. Isobaric daughter ions from CAD of acetophenone and mesitylene, detected at a resolution of 500,000.

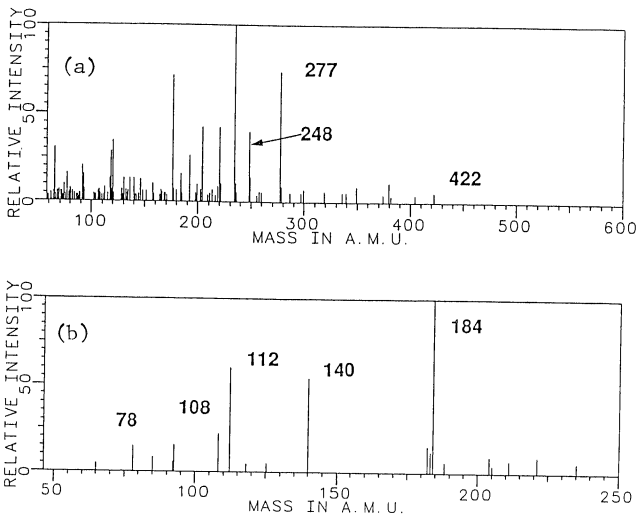

Figure 14. (a) EI spectrum of epoxy resin extract: (b) 50 eV CAD spectrum of m/z 248 component in epoxy resin extract.

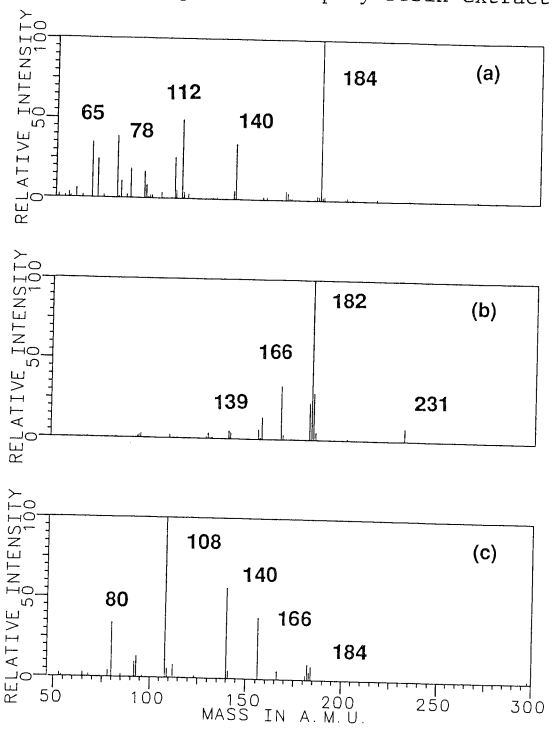

Figure 15. 50 eV CAD spectra of pure diaminodiphenylsulfone isomers: (a) 3,3′-diaminodiphenylsulfone; (b) 2,4′-diaminodiphenylsulfone; (c) 4,4′-diaminodiphenylsulfone.

spectrum of the m/z 248 ion, using argon as the collision gas. A comparison of this spectrum with the 50 eV CAD spectra obtained for three different isomers of DADPS (Figures 15a, 15b, and 15c) clearly shows that the component in the epoxy resin extract is the 3,3′ isomer. While there are some differences observed in comparing the FTMS-CAD spectra to those reported for the hybrid instrument, this work verifies that FTMS-CAD provides a viable approach to this type of analysis.

Conclusion

The dual cell geometry has been employed to overcome difficulties resulting from high gas loads associated with coupling both gas chromatography and supercritical fluid chromatography with FTMS. For laser desorption and MS/MS experiments, the dual cell geometry has allowed us to separate ions from reactive neutrals, thus eliminating unwanted ion-molecule reactions. These developments have enabled us to apply FTMS to a variety of analytical problems, as evident from the examples in this report.

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