

InfiTOF™

Analysis of a Gas Mixture Containing Ammonia and Methane by Using a Compact High-Resolution Multi-Turn Mass Spectrometer

Overview

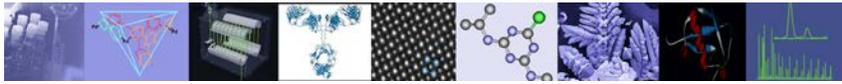
Analysis of a chemical ionization reagent gas consisting of a 5% mixture of ammonia in methane is demonstrated by using the JEOL InfiTOF™ compact high-resolution mass spectrometer. The InfiTOF's high mass-resolving power clearly separates and identifies isotope peaks and trace water contamination with excellent mass accuracy.

The InfiTOF Compact High-Resolution Mass Spectrometer

The InfiTOF™ is a compact time-of-flight mass spectrometer that is ideal for the high-resolution analysis of gases. The entire InfiTOF system (Figure 1), including the vacuum pumps, is approximately the size of a personal computer tower. Unique multi-turn ion optics (described in the following section) provide detection of ions from m/z 1 (H^+) to m/z 1000 with mass resolving power adjustable from unit resolution to greater than 30,000.



Figure 1. The InfiTOF™ Compact High-Resolution Mass Spectrometer System.



Multi-turn mass spectrometers

Although increasing the length of the flight tube can improve the resolving power of a time-of-flight mass spectrometer, this can result in an impractically large system. Multi-turn ion mass spectrometers^[1] with Perfect Focusing ion optics^[2] solve this problem by using compact “figure-8” ion optics. The flight path can either be an “open-loop” series of figure-8 segments (Figure 2, left side) as in the JEOL *SpiralTOF* MALDI-TOF/TOF mass spectrometer or a closed-loop flight path with a single figure-8 segment as in the *InfiTOF* (Figure 2, right side).

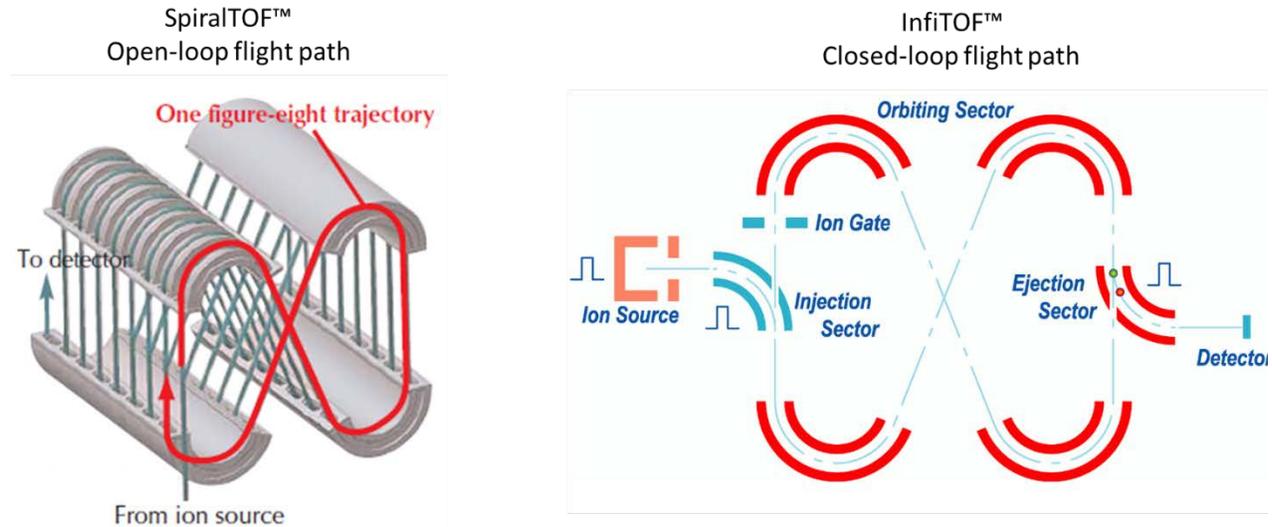


Figure 2. Two multi-turn mass spectrometer configurations.

A variable-resolution time-of-flight mass spectrometer

The InfiTOF’s closed-loop configuration provides a variable-length flight path depending on how many turns (“laps”) the ions make around the figure-8 “racetrack.” The InfiTOF’s control system provides timed ejection pulses that eliminate the overtake problem (fast ions catching up with slow ions after several turns) by ejecting ions outside the programmed m/z ranges. Mass spectra can be measured in three modes: (1) low-resolution full-scan mass spectra, (2) multiple high-resolution segments, and (3) a continuous set of segments to provide full-range high-resolution mass spectra.

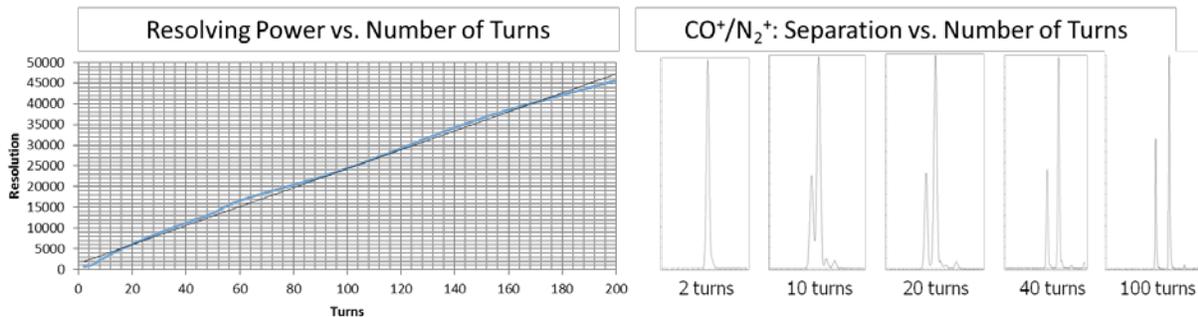
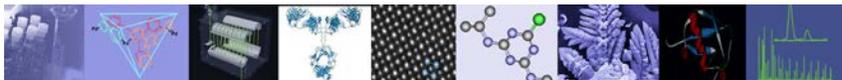


Figure 3. Mass resolving power increases with multiple turns around the InfiTOF ion optics.



Ammonia/methane gas mixture

Mixtures of ammonia in methane are easier to handle than pure ammonia and provide improved sensitivity for ammonia chemical ionization.^[3-5] However, the electron ionization (EI) mass spectra of methane and ammonia contain a number of isobaric peaks that cannot be distinguished by low-resolution mass spectrometry alone.

In the absence of gas chromatography, characterization of low levels of ammonia in methane requires high-resolution mass spectrometry. Figure 4 shows the NIST Mass Spectral Database electron ionization (EI) mass spectra of ammonia (Figure 4A) and methane (Figure 4B) and a summed mass spectrum for 5% ammonia in methane (Figure 4C). Except for slight increase in the relative abundance of the peak at m/z 17, the mass spectrum of 5% ammonia in methane is almost indistinguishable from the methane mass spectrum. Smaller ammonia concentrations would be indistinguishable from pure methane.

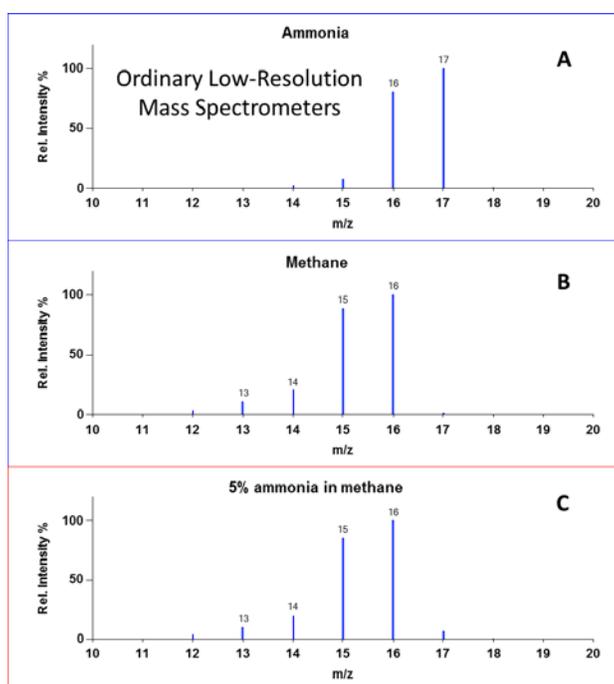
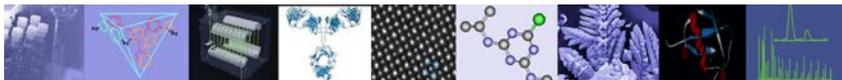


Figure 4. Low-resolution electron ionization (EI) mass spectra of ammonia (1A) and methane (1B) and a 5% mixture of ammonia in methane (1C).

Here we demonstrate the use of a compact, high-resolution mass spectrometer with unique multi-turn ion optics to separate isobaric peaks in a sample of 5% ammonia in methane.

Experimental

Mass spectra were acquired by using the InfiTOF compact multi-turn high-resolution mass spectrometer. The ionizing electron voltage was set to 70 eV. High-resolution mass spectra were acquired in multi-segment mode (20 turns) to give a resolving power of approximately 6000 (FWHM) at m/z 16. The gas mixture was introduced directly into the mass spectrometer through a deactivated fused-silica capillary tube.



Results

Figure 5 shows that the InfiTOF has clearly resolved the isobaric ammonia and methane peaks, including the isotopic peaks and trace water peaks. Trace peaks corresponding to protonated methane (CH_5^+) and protonated ammonia (NH_4^+) from ion-molecule reactions are well separated from the $^{13}\text{CH}_4^{++}$ and H_2O^{++} respectively. Accurate mass measurements were all within 0.001 u, providing unambiguous elemental composition assignments.

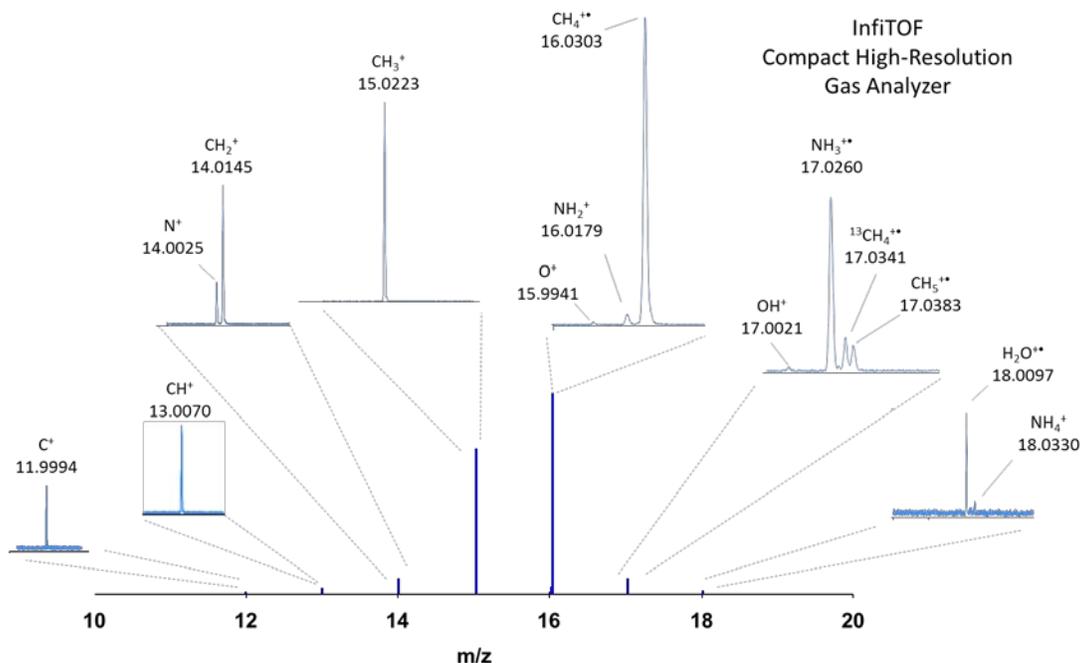


Figure 5. High-resolution InfiTOF mass spectrum of 5% ammonia in methane

Conclusion

Trace peaks in gas mixtures are easily separated and identified without chromatography by the high mass-resolving power of the InfiTOF compact multi-turn mass spectrometer.

References

- [1] M. Toyoda, D. Okumura, M. Ishihara, I. Katakuse. Multi-turn Time-of-Flight Mass Spectrometers with Electrostatic Sectors. *J. Mass Spectrom.*, **2003**, 38, 1125.
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