

An Empirical Study of MS/MS Systems: Transmission Efficiency, Fragmentation Efficiency and RF Only Mass Discrimination of Various Collision Cells

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MS/MS systems are used in a variety of configurations. With the use of different ion sources, concerns may arise due to the “brightness” of the source. Because of this, it is imperative that the best collision cell be used for a given application. Some collision cells exhibit high-mass discrimination. Others may offer excellent throughput, but require high gas loads and/or RF power to obtain good collisional data. In this work, we have evaluated quadrupole, hexapole, and octupole collision cell configurations with various entrance and exit lens aperture sizes. These results provide the user information from which the best possible TQMS system may be designed for a given application.

Introduction:

Ion transmissions of TQMS systems were compared to a mass spectrometer with a single quadrupole mass filter. The same size quadrupole and ion source design were used on the single mass filter system as the mass-selecting quadrupole mass filters of the TQMS systems. Transmission data taken without collision gas compares the efficiency of each multi-pole device as an ion guide. Spectral data were taken at varying amounts of collision gas and different aperture sizes on the collision cells. These spectral data compare how each multi-pole device performs as a collision cell.

Experimental:

The Merlin Automation Data System from Extrel CMS performed all data acquisition and instrumentation control. Perfluorotributylamine (PTA) was leaked into the front portion of a differentially pumped chamber at a rate of 5×10^{-6} Torr and ionized with an Axial EI ionizer. 19mm Quadrupoles fitted with pre and post filters (Tri-Filter™) were used for mass filtering in Q1 and Q3. 1.2 MHz, 300 W, model 150QC quadrupole power supplies, controlled both mass selecting quads. All spectra were collected on a Faraday plate.

The same tuning (voltage settings for ion optics) needed for optimum collision in an MS/MS system was used for all hardware configurations. Since Collision Induced Dissociation (CID) depends upon the collision energy, which is dependent upon:¹

1. The incident ion energy
2. The mass, density and structure of the target gas
3. The mass of the parent ion

The tuning of the ionizer and optics utilized relatively high ion energy. This may not be optimum for best looking peaks, but it does afford the best fragmentation in a collision cell. Optics tuning was also optimized for the best Q1MS ion current intensity.

Data was taken using a single quadrupole for comparison to all other configurations. An RF Only device was added to investigate the throughput transmission efficiency of a Hexapole and an Octupole at different frequencies.

MS/MS data was obtained using different collision cells. A Hexapole with 2mm rods and an inscribed diameter of approximately 3mmmm was compared to a 3mm Octupole with an inscribed diameter of approximately 6mm. Inter-quad lenses with aperture sizes of 8mm were compared to 13mm apertures on the Octupole. The Octupole was also operated at different frequencies for comparison, 1.7 MHz, 2.1 MHz and 2.9 MHz.

Our previous studies have shown that the use of a quadrupole as an RF only device shows low mass and high mass cut-off at various RF levels². Therefore, most of the focus on this discussion is on higher order RF devices such as the Hexapole and Octupole.

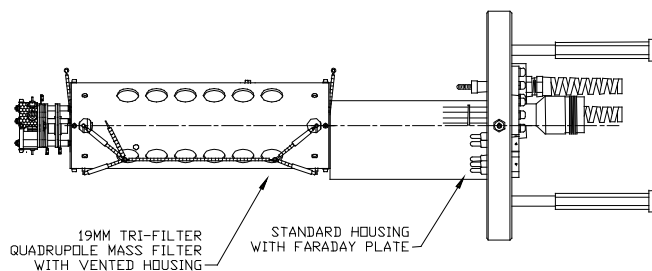


Figure 1: The "Standard" configuration for single quad comparison; Axial EI Ionizer, 19mm Tri-Filter™ quadrupole mass filter, Faraday plate detector.

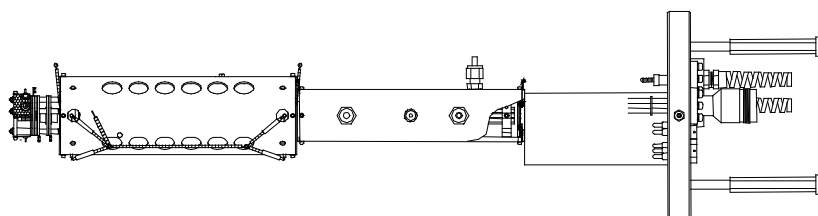


Figure 2: Configuration for Quadrupole-Hexapole and Quadrupole-Octupole transmission studies; Axial EI Ionizer, 19mm Tri-Filter™ quadrupole, RF Only device, Faraday Plate detector.

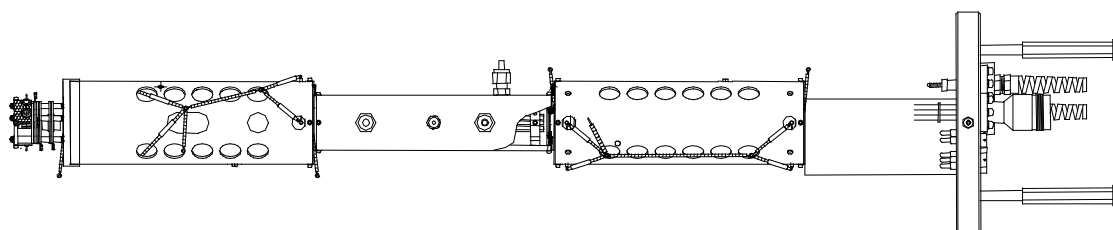


Figure 3: Configuration for ms/ms studies; Axial EI Ionizer, 19mm Tri-Filter™ quadrupole, RF Only device, 19mm Tri-Filter™ quadrupole, Faraday Plate detector.

Results and Discussion:

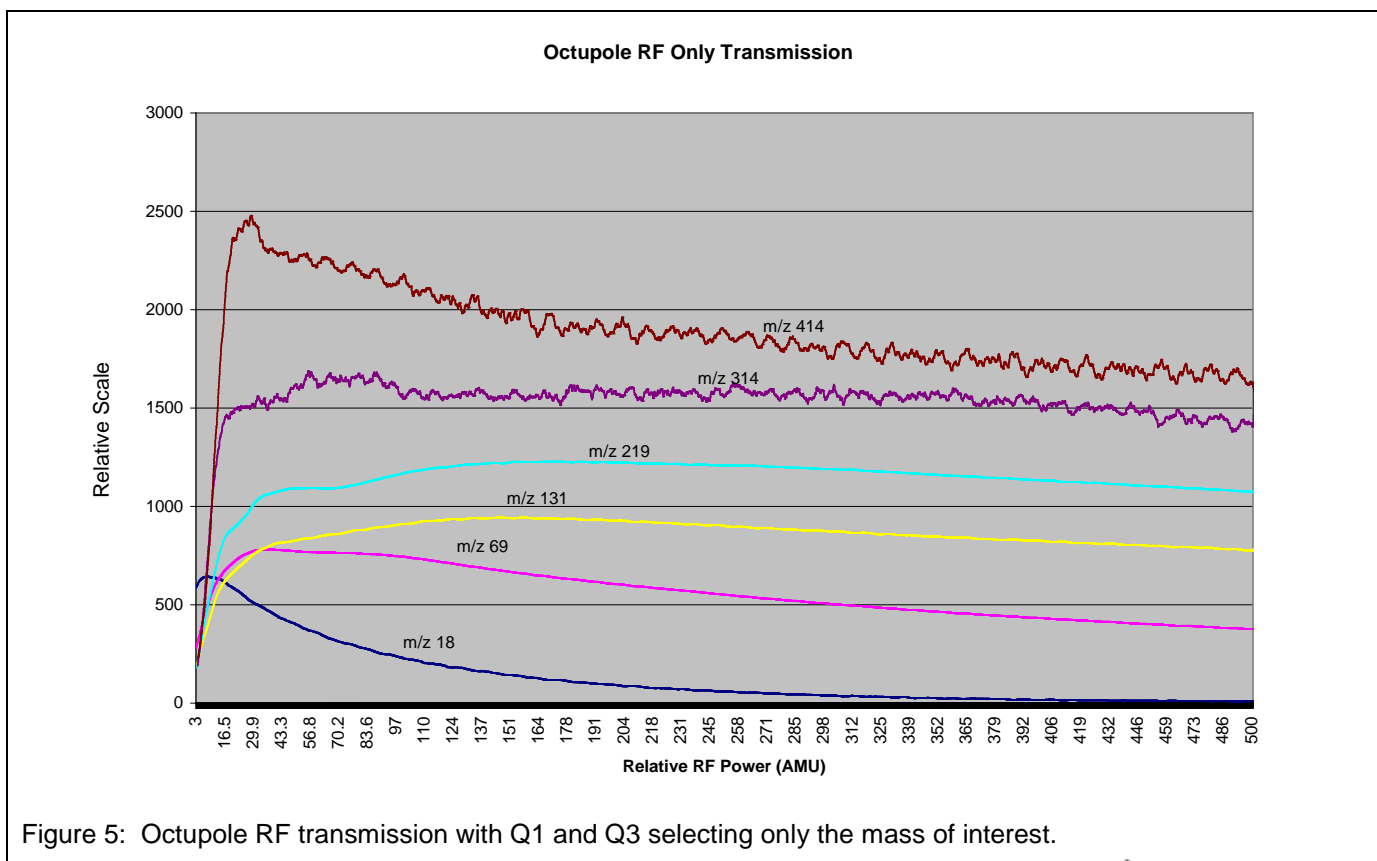
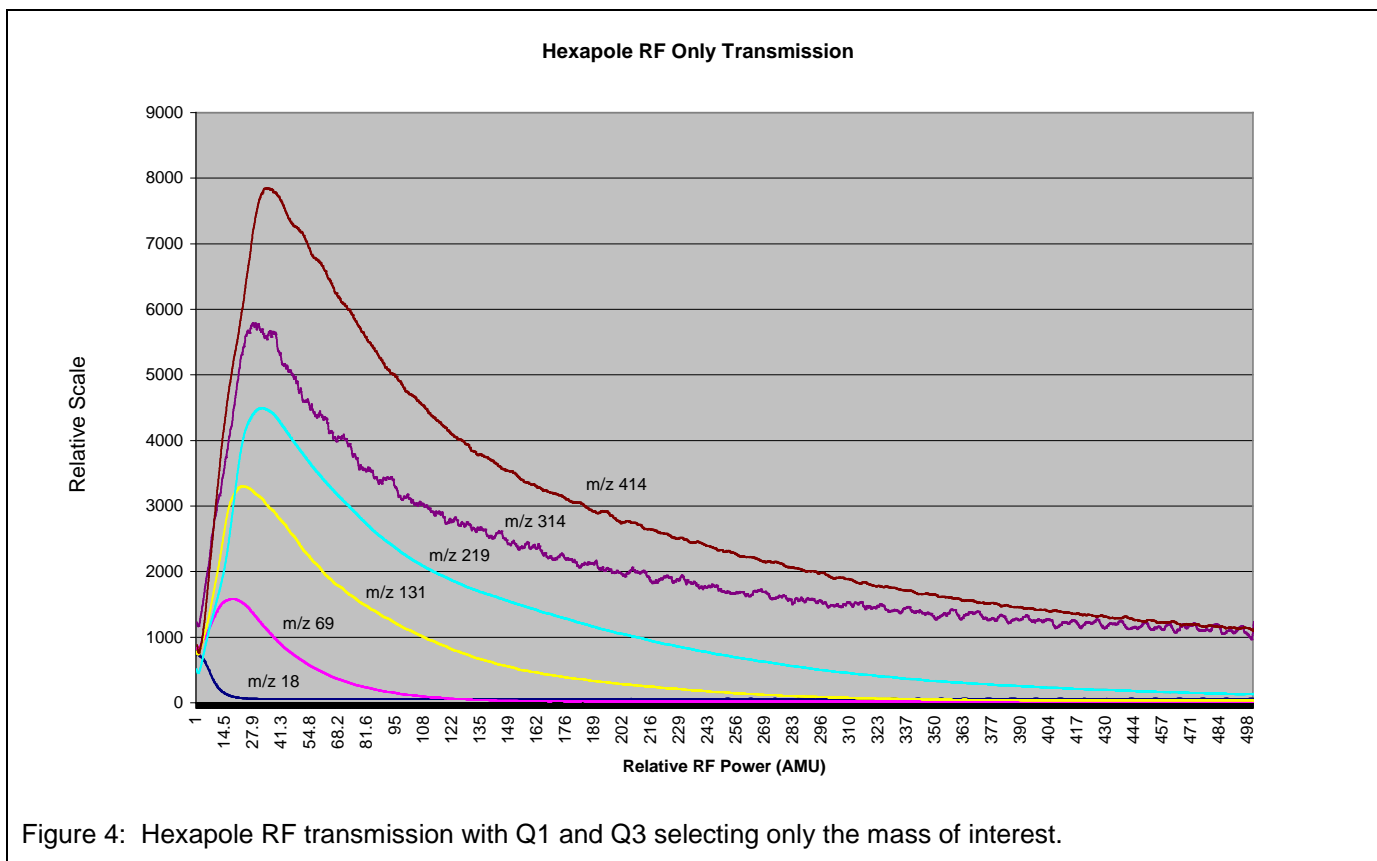
Figure 4 shows the Hexapole transmission operating at 2.1 MHz. Since the previous work was done using 9.5mm mass filters, the Octupole transmission studies were repeated for consistency. The octupole transmission results are shown in Figure 5. In these tests, the resolving quadrupoles, Q1 and Q3, allowed only the selected mass of interest to pass through. The RF level on the collision cell was ramped from

low mass to high to represent the full range of RF amplitude.

It can be seen in Figure 5 that the Octupole's ion transmission extends to higher RF levels. This is consistent with the previous work shown. The efficiency of the Octupole as a collision cell was tested with different size apertures as is shown in Figure 6 below.

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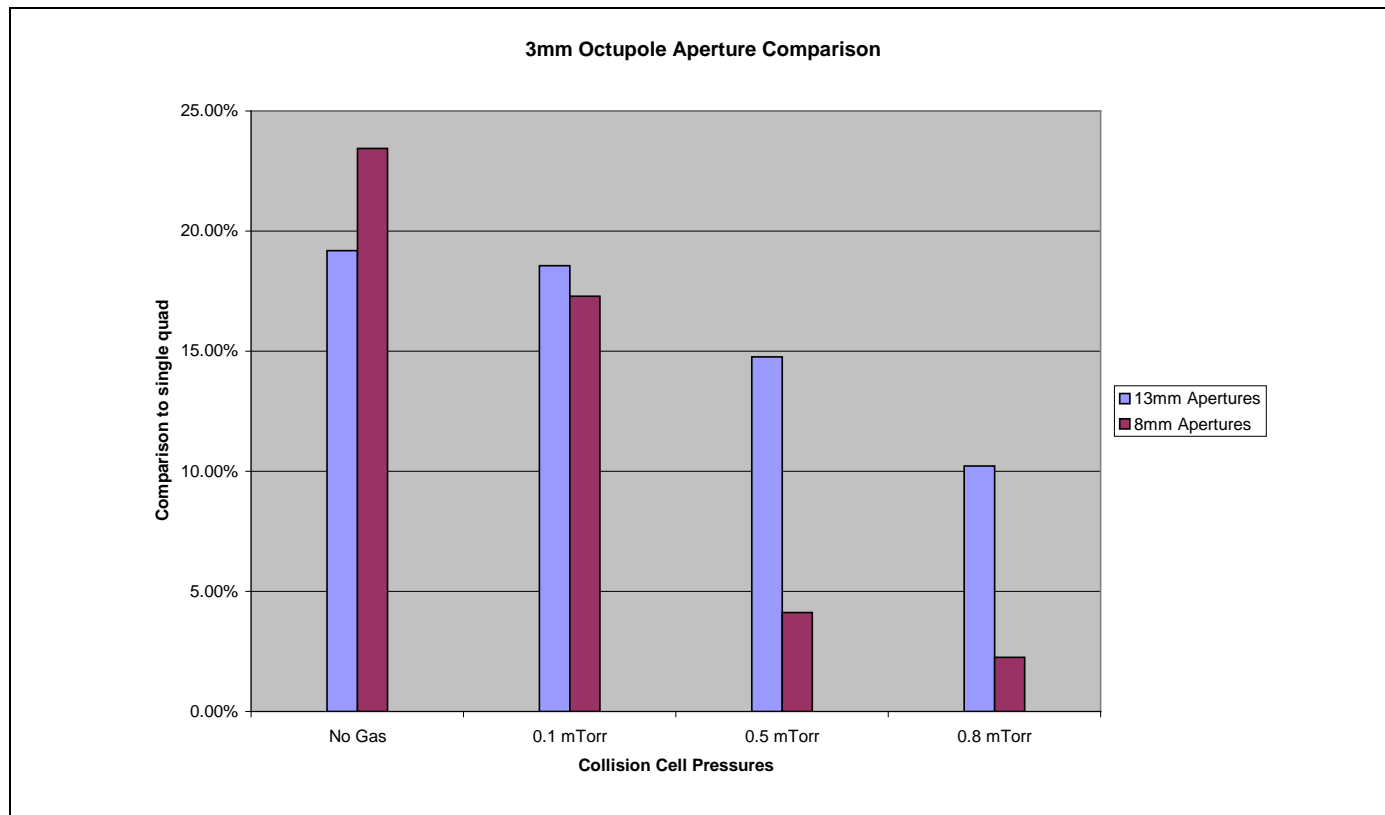


Figure 6: 3mm Octupole collision cell with different sized apertures, transmission shown at various pressures.

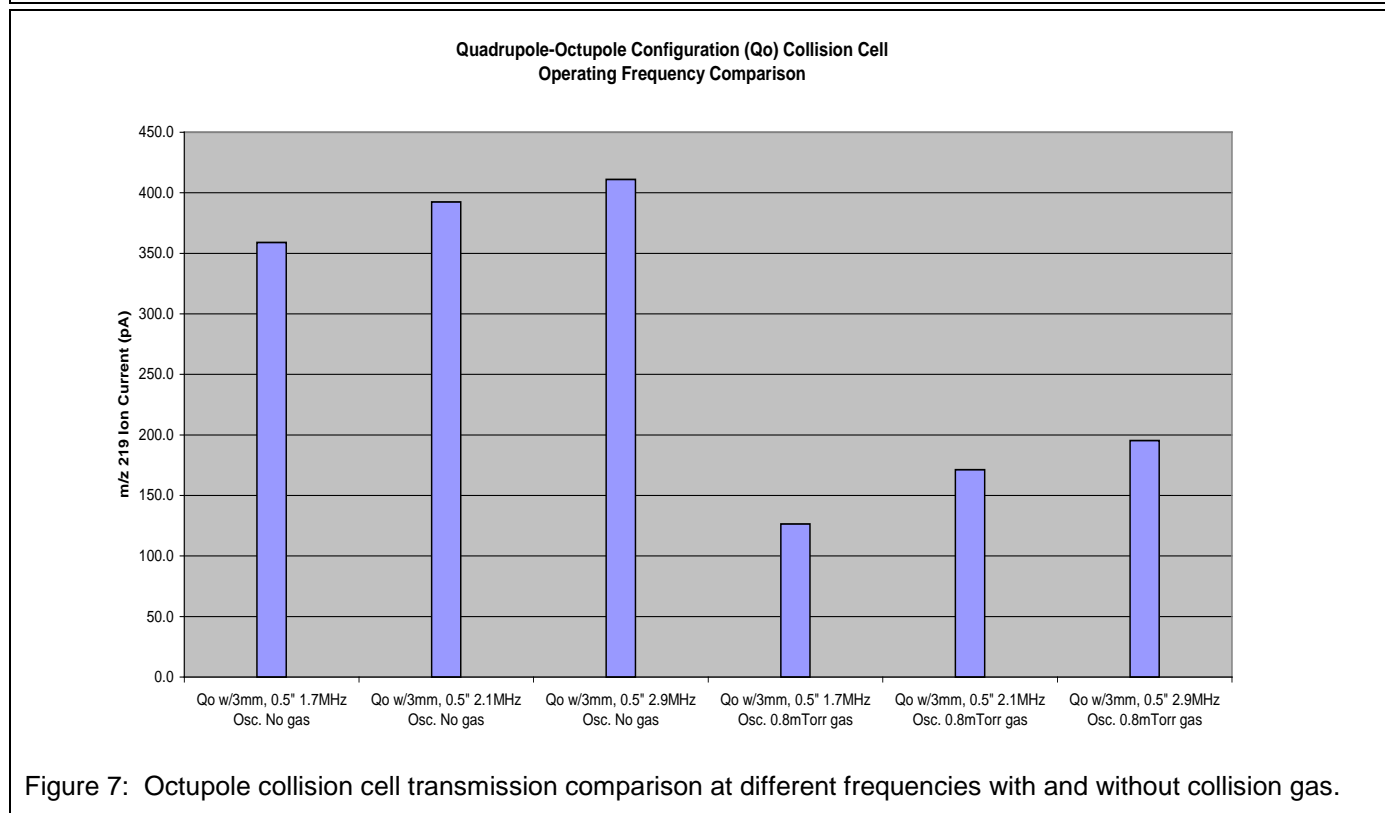


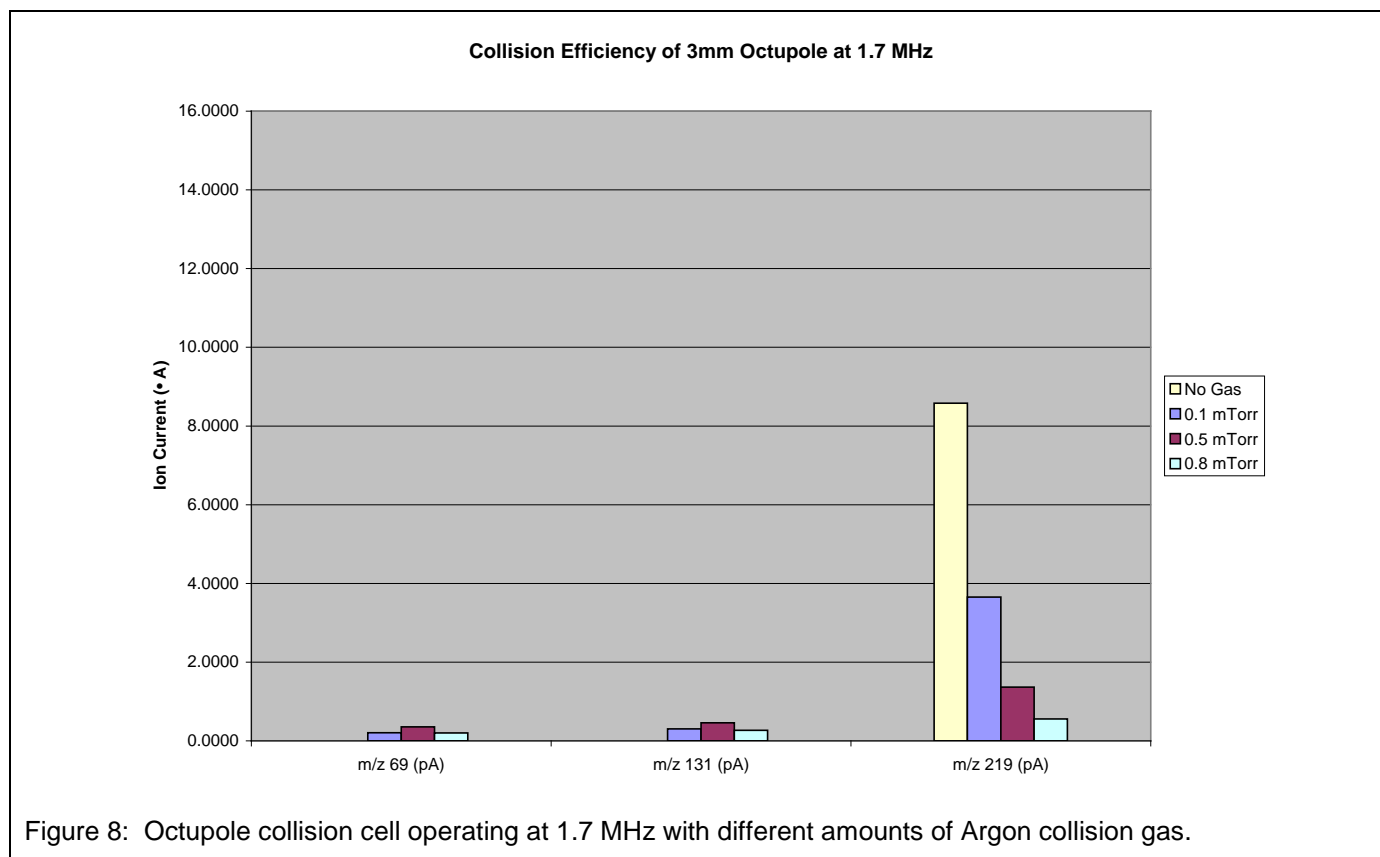
Figure 7: Octupole collision cell transmission comparison at different frequencies with and without collision gas.

It can be seen from Figure 6, that the 3mm Octupole with 13mm apertures afforded the best ion efficiency of the Octupole as a collision cell was tested with different size apertures as is shown in Figure 6 above.

Building on this information, Ion transmission was investigated on the Octupole as an ion guide and as a collision cell operated at different RF frequencies: 1.7 MHz, 2.1 MHz & 2.9 MHz. The tests were performed as a Quadrupole-Octupole configuration first as an ion guide, then 0.8mTorr Argon collision gas added to the collision cells. For these tests, m/z 219 was selected in Q1. The Octupole was operated at one-tenth the RF power applied when compared to the corresponding mass of Q1. This is consistent with results shown earlier that the Octupole can pass

higher masses at lower RF levels. These comparisons are shown in Figure 7 below.

It can be seen in Figure 7 that if the Octupole is operated at a higher frequency (2.9MHz), transmission efficiency is increased both as an ion pipe (no gas) and as a collision cell (0.8 mTorr gas). To investigate this phenomenon further, the Octupole was tested as a Quadrupole-Octupole-Quadrupole configuration with 13mm apertures. The following charts show ion peak intensities of both the parent ion, m/z 219 and the product ions, m/z 69 and 131. It should be noted that for direct comparison, the Y-Axes are the same for the charts shown in figures 8, 9 and 10.



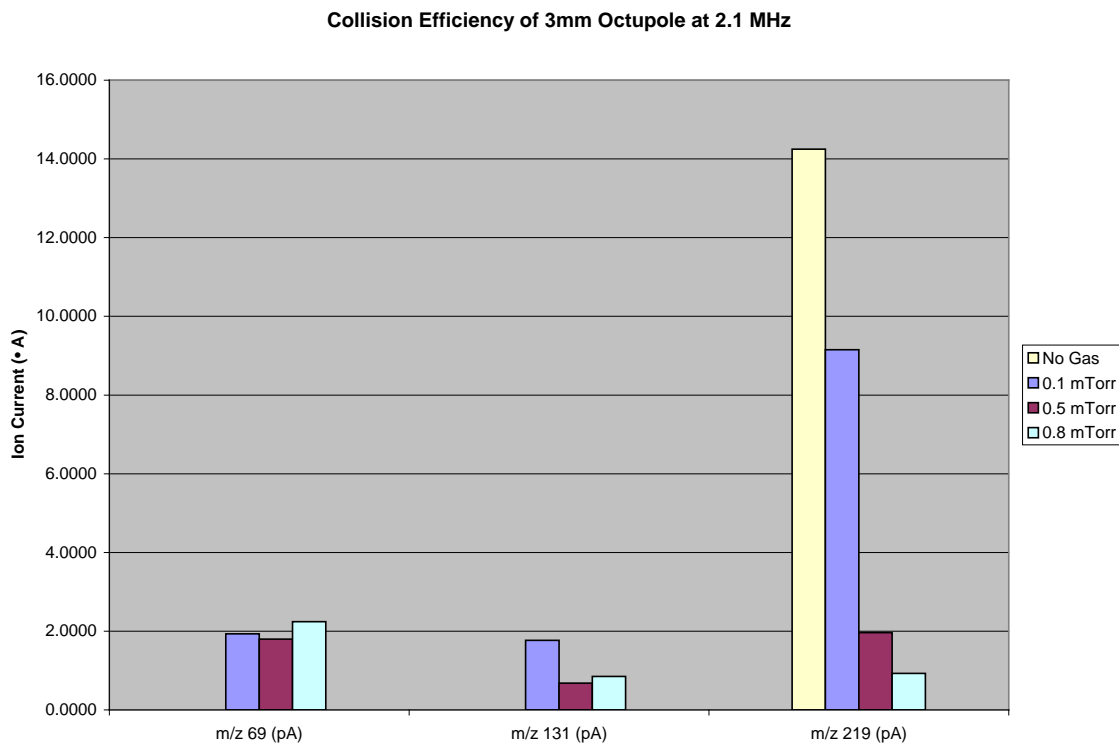


Figure 9: Octupole collision cell operating at 2.1 MHz with different amounts of Argon collision gas.

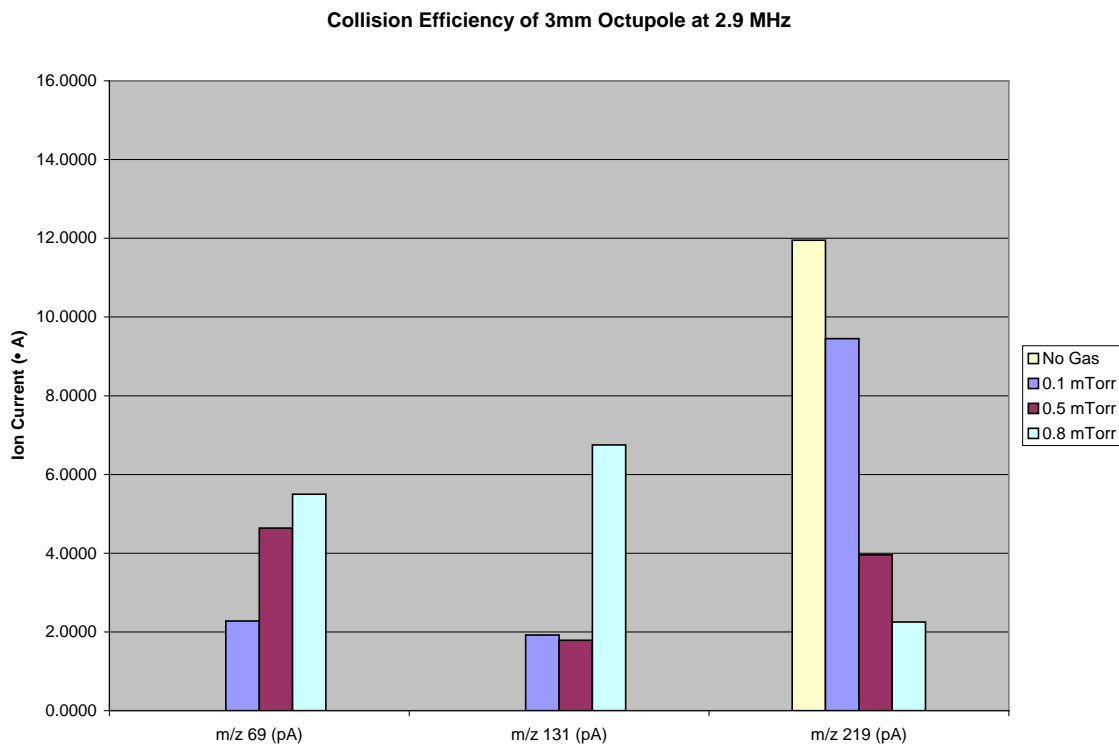


Figure 10: Octupole collision cell operating at 2.9 MHz with different amounts of Argon collision gas.

It can be seen in the three previous charts that the Octupole operating at 2.9MHz not only improved the abundance of ion transmission, but the higher frequency also improved fragmentation efficiency.

Conclusions:

1. Some RF devices afford better ion throughput efficiency than others: Octupole > Hexapole > Quadrupole

2. Some RF devices pass a broader range of masses for a give RF level: Octupole > Hexapole > Quadrupole
3. The Octupole tested showed better transmission with 13mm apertures than with 8mm apertures as entrance and exit lenses
4. Frequency matters! The Octupole tested showed not only better throughput transmission as an ion pipe and as a collision cell, but also showed better fragmentation at all collision cell pressures used.

References:

¹ McLafferty, F.W., *Tandem Mass Spectrometry*, Wiley Interscience, New York, 1983. Chapter 6: "Collisionally Activated Dissociation of Low Kinetic Energy Ions", Pages 125-146.

² Pedder, Randall E. and Wei, Jian, *Transmission Characteristics of RF-Only Devices: Quadrupoles and Octupoles as Ion Pipes*, Extrel Application Note RA_2005C, Poster presented at the 46th ASMS Conference on Mass Spectrometry and Allied Topics, Orlando, FL, 1998