Practical Quadrupole Theory: Rectilinear Quadrupole and Hexapole Ion Guides Operated with Collisional Damping Pressures

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Introduction

At the 2008 ASMS conference our group presented a comparison between round rod quadrupoles, flat rod (rectilinear) quadrupoles, and hexapoles as ion guides in high vacuum (no collisions), demonstrating the utility of rectilinear quadrupoles simultaneously passing ions with a widest range of masses at a single RF amplitude. The optimal RF amplitude for simultaneous ion transmission of a wide range of masses (mass range band pass) was demonstrated to be suitably low, allowing for higher RF frequencies to be used.

This follow-on work repeats that comparison in a conventional collisional damping environment, common to LC/MS systems, with the additional characterization of a rectilinear hexapole ion guide, and a wider range of operating frequencies.

Experimental

A system was configured with an electrospray ion source, ion funnel, and ion guide traversing three differentially pumped regions to a 12 mm quadrupole mass filter with 1,000 amu mass range, with an electron multiplier detector. See Figure 1.

The vacuum chamber was designed to mate to an Edwards Vacuum turbomolecular cartridge pump with booster stage, which was mounted into a custom designed housing with three planar rectangular vacuum ports. These vacuum ports align underneath the three rectangular vacuum ports of the ion guide chamber. The pumping speed on these three ports was 20 L/s, 200 L/s, and 200 L/s respectively, with the booster stage upgrading a 12 CFM mechanical pump to have 26 CFM pumping speed. The chamber configuration utilized the insulating collars as conductance limits between the three distinct pumped regions (~30 millitorr, ~2 millitorr, and ~0.2 millitorr respectively), shaded in light green in the figure below.

The electrospray sprayer allows x, y, and z movement to optimize ion transmission to a four inch long heated stainless steel capillary with 0.020 inch inner diameter. The outlet of the stainless steel capillary exits into an ion funnel whose inner diameter ranges from 1.00 inches at its entrance to 0.070 inches at the ion funnel exit, with a 0.080 (2mm) conductance-limiting exit aperture. The ion funnel was operated at 2.2 MHz for all experiments, powered by an Ardara Technologies model 124 self-oscillating RF power supply, and was operated at a pressure of 1.6 to 1.7 torr for all experiments.

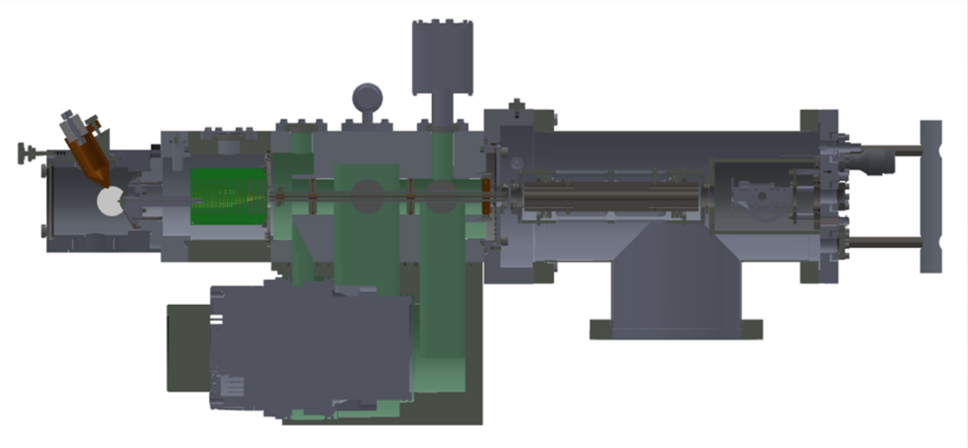


Figure 1. Electrospray quadrupole mass spectrometer system. The three pumped regions for the ion guide are shaded in light green.

Typical ion transmission through the system configured with rectilinear quadrupole ion guide is summarized in the table below.

Element where ion current was measured	Ion current
ESI Needle (@ Front panel meter on ESI PS)	110 nA
Ion Funnel (Preamplifier @ 10^9 gain)	0.77* nA
Ion Guide (Preamplifier @ 10^9 gain)	0.79 nA
Faraday Plate downstream of Ion Guide (Preamplifier @ 10^9 gain)	0.76 nA

*Some ions may pass through the ion funnel exit aperture instead of contacting the electrodes, and therefore are not accounted for in this measurement

Three separate ion guides were designed, each having an inscribed diameter of 5 mm, with the insulating collars that support the rods designed to provide the same conductance limit between the three different pumped stages of the ion guide chamber, since these collars serve as the conductance limits between the three vacuum stages. (Extra holes were added to the hexapole ion guide and round rod collars to increase the gas conductance to match the rectilinear quadrupole.) All ion guides had the same overall length (10.896 inches).

100 mL of a solution of trimethyl glycine (5μM), caffeine(5μM), , and reserpine (5μM), in a 25:25:50 mixture of methanol, isopropanol, and water was prepared for use in all of the following experiments. This solution was used to provide a large mixture of ions from ~m/z 50 to m/z 610.

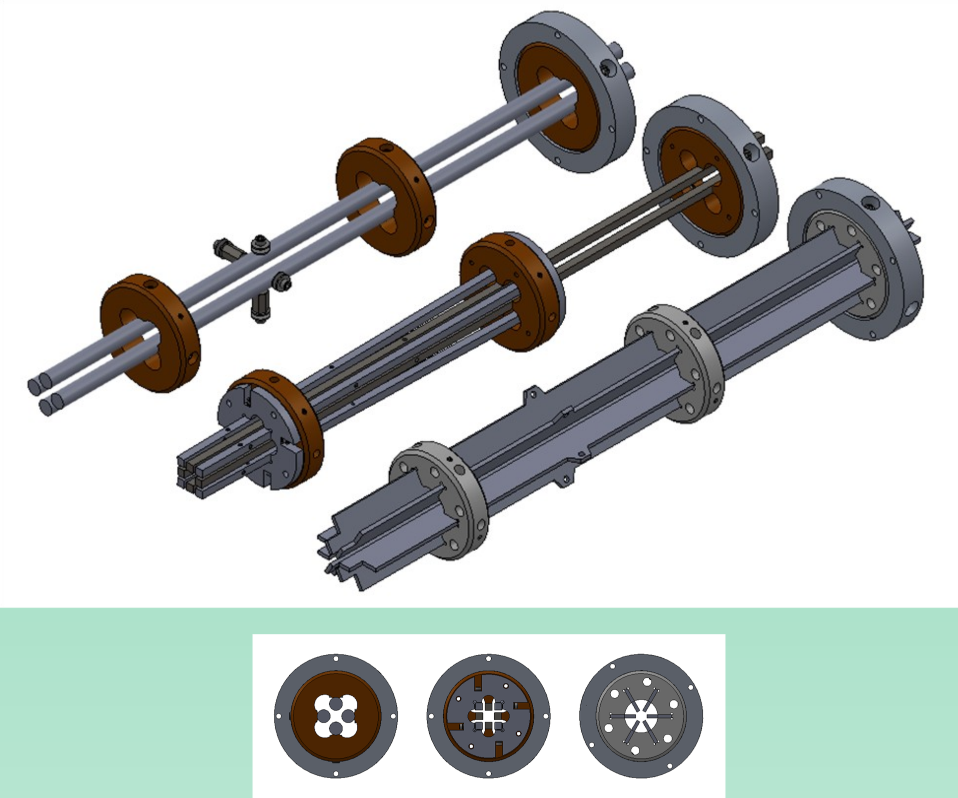


Figure 2. Ion Guides from left to right, 6 mm diameter round rods, 5 mm inscribed diameter rectilinear quadrupole with asymptotic field shaping electrodes, and 5 mm inscribed diameter rectilinear hexapole.

A special RF power supply was created to allow selection of any of 255 resonant RF frequencies applied to the ion guide from 600 kHz to 6.78 MHz, tunable to any capacitive load, by series inclusion of eight pairs of inductors whose inductances were a sequence of binary multiples of each other, from 1 microHenry to 128 microHenries per side, allowing a total inductance range of 2 to 510 microHenries. A high voltage variable capacitor was added across the RF outputs to fine tune frequency selection.

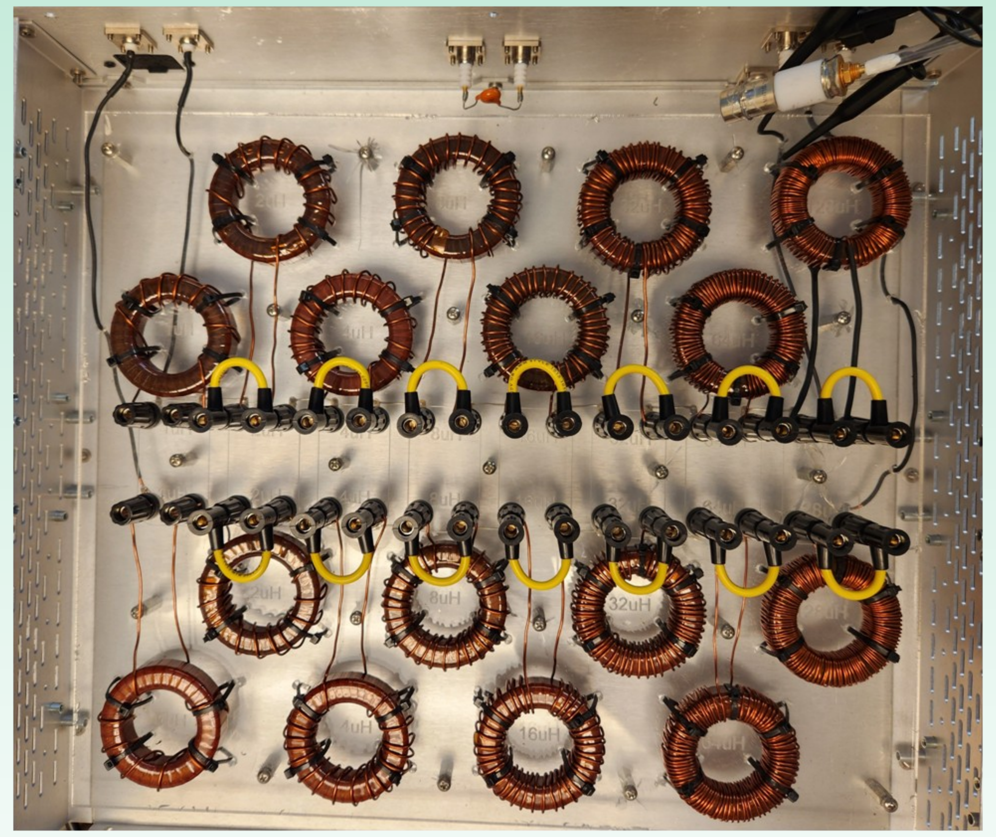
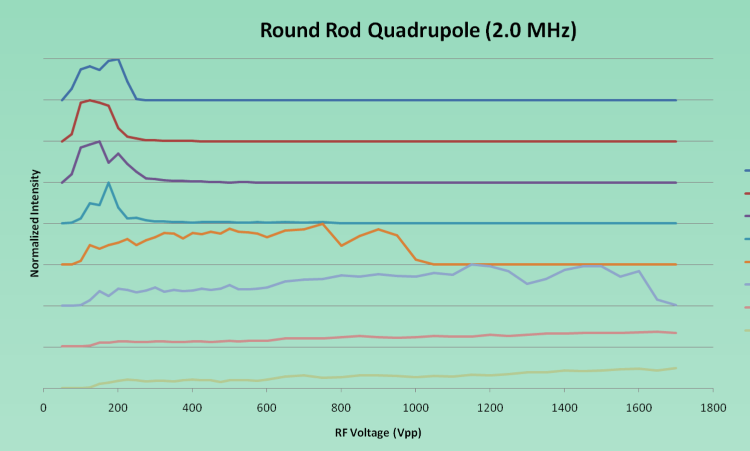
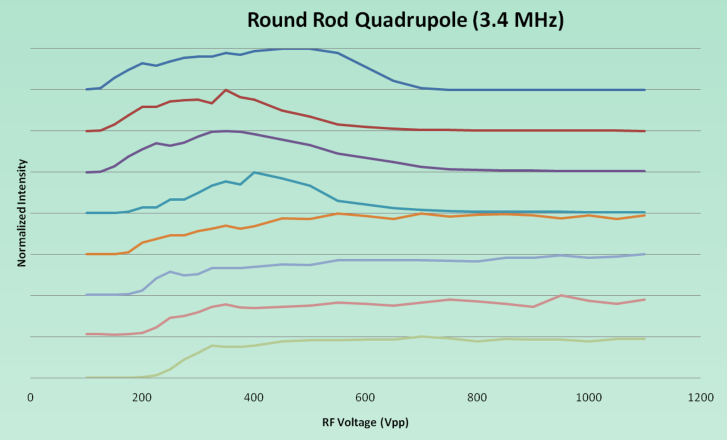


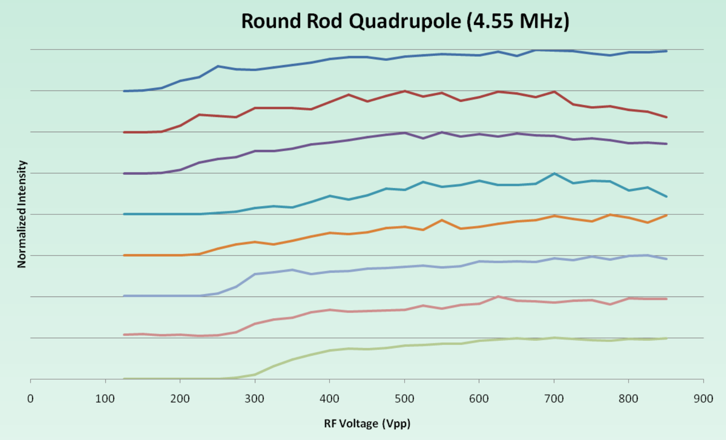
Figure 3. Custom toroidal inductor assembly, which places between 1 and 8 inductors in series per side, providing 255 potential combinations of RF frequency. Inductors had inductances of 1, 2, 4, 8, 16, 32, 64, and 128 microhenries respectively, Yellow jumper wires are used to short the individual inductors, effectively taking them out of the circuit.

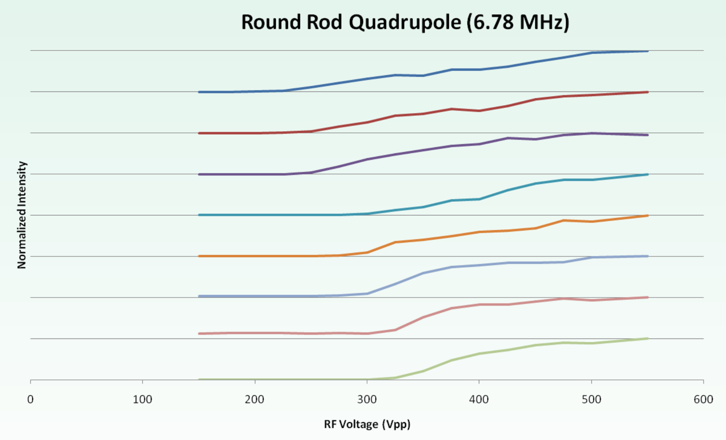
Results and Discussion:

For each ion guide configuration, it was demonstrated that the flatness of the 'transfer function' (plot of ion intensity as a function of RF amplitude) improved as RF frequency was increased, demonstrating an effective reduction in mass discrimination when using higher RF frequencies. Maximum available RF amplitude was ultimately limited by either the efficiency of the RF power supply or maximum voltage without discharge due to the Paschen curve.

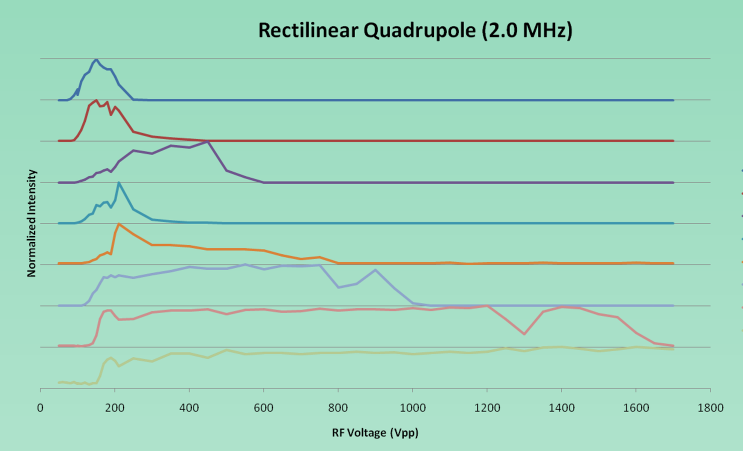


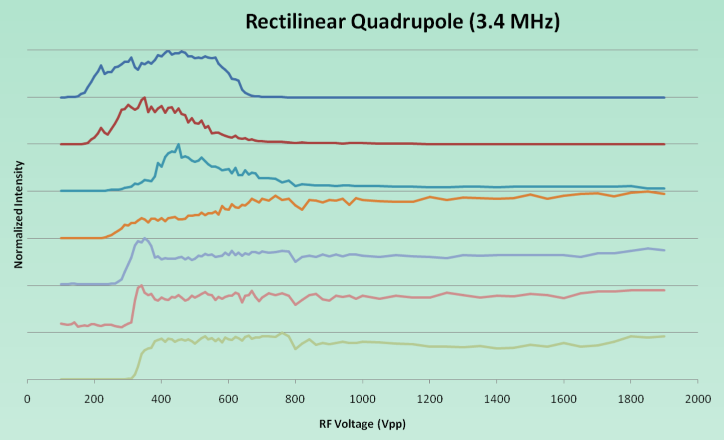


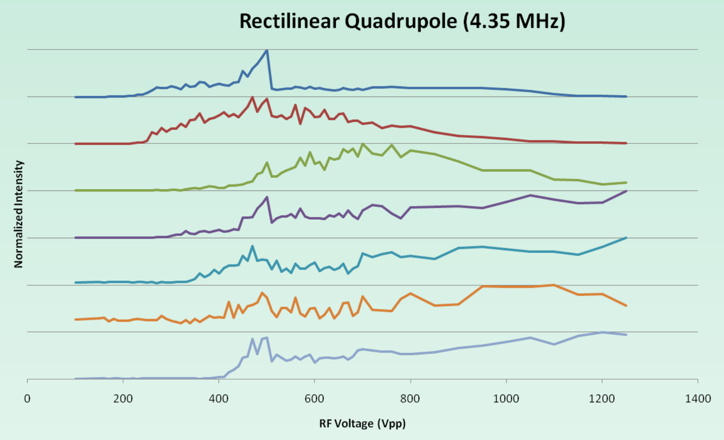


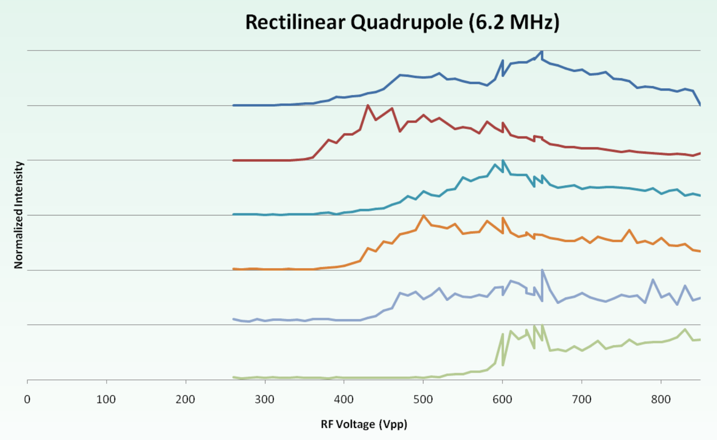


As demonstrated in the 2008 work, the rectilinear quadrupole provided superior mass range band pass to a similarly dimensioned round rod quadrupole. Collisional damping helped reduce the noding effects previously seen in round rod quadrupoles without collisions. At higher RF amplitudes the transfer functions are flat and close to the maximum of each curve.

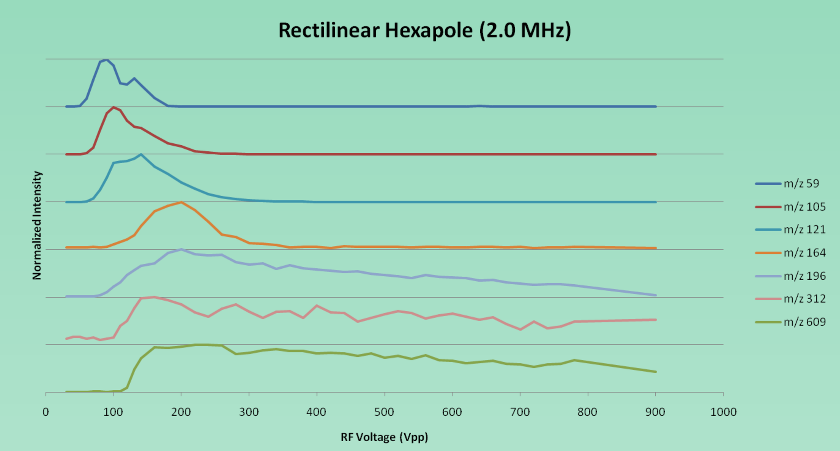


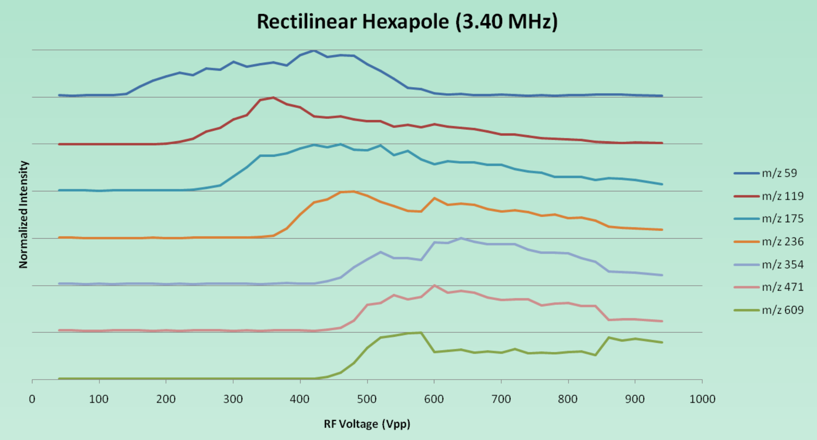


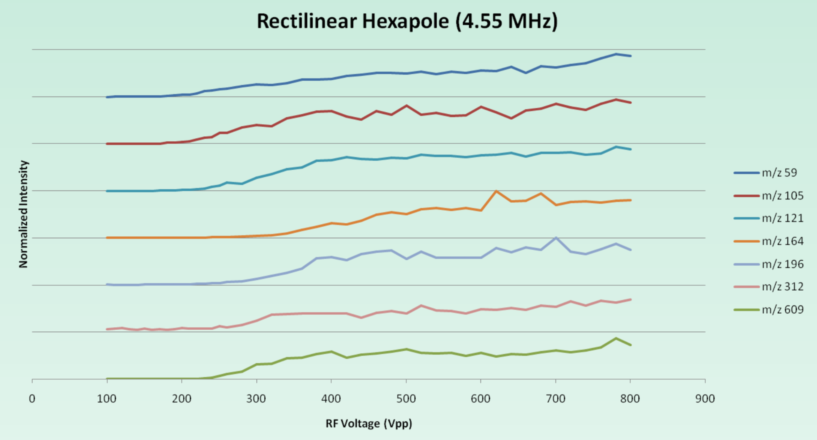


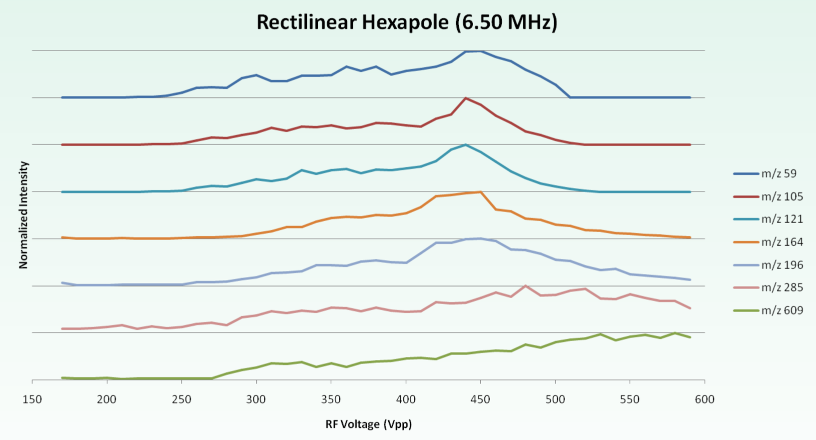


The rectilinear hexapole did not appear to benefit from the higher order fields imparted by the planar faces, presumably because the flat faces aren't wide enough to deviate much from the ideal field, since the dimensions were limited by the requirement to maintain a minimum distance between electrodes to avoid discharge. The transfer functions are not as flat as seen with the higher frequency rectilinear quadrupoles.









Conclusions:

- The rectilinear quadrupole passed the broadest range of masses at a single RF amplitude.
- The optimal RF frequency for the rectilinear quadrupole ion guide in this study was 3.4 MHz for the mass range studied. For higher mass range, a slightly lower RF frequency is recommended (2.0MHz).
- The rectilinear hexapole ion guide used in this study performed better than the round rod quadrupole, with flatter response as a function of RF voltage for a given mass, but not quite as well as the rectilinear quadrupole ion guide. The increase in the number of rods for the same inscribed 'circumference' required the gaps between adjacent rods to become smaller, limiting the RF voltage available without discharge in the first pumped region, due to the Paschen curve.
- The round rod quadrupole as a collisional damping ion guide showed the most mass discrimination, potentially requiring mass programming of the ion guide as the mass resolving quad is set to pass different masses. At higher RF frequencies (greater than 3.4 MHz), there existed a range of RF voltages, where a wide range of ions are passes with moderate mass discrimination for given RF level.
- For these experiments, a custom resonant-circuit RF power supply was used to supply the same RF frequencies to ion guides of varying capacitances. The standard model of our self-oscillating power supply (Model 124) can be configured from 500 kHz to over 4 MHz for a specified capacitive load.

References:

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