An Ion Guide Study: Quadrupoles, Rectilinear Quadrupoles, Hexapoles, and Octopoles

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There are a variety of different kinds of RF-only devices currently in use as ion guides and collision cells, including quadrupoles, rectilinear quadrupoles, hexapoles, and octopoles. Quadrupoles and hexapoles are known to have better collisional focusing properties than octopoles, allowing for phase space compression of ion beams into narrower cross sectional areas when a buffer gas is present. Octopoles are known to simultaneously transmit a wider range of masses than quadrupoles, with hexapoles having a mass range bandpass somewhere between quadrupoles and octopoles. Rectilinear quadrupoles are used as ion guides, both as pre-filters and as collision cells, promising the collisional focusing of quadrupoles with some octopolar character to minimize noding effects when focusing through a restricted exit aperture.

I. OVERVIEW

The goal of efficiently transporting ions from one ion optics device to another with and without collision gas present has lead to the use of a variety of different RF-only devices, including quadrupoles, hexapoles and octopoles. Each device has shown to have different characteristics to be beneficial in a specific experiment. In the case of passing the widest mass range without noding there has not be a definitive comparision of the devices.

Individually, it has been shown that quadrupoles and hexapoles have provided better collisional focusing while the octopole provides a wider mass range band pass. The rectilnear quadrupole has been shown to compare more closely to the hexapole. To determine the best overall device with regards to noding, band pass, and complexity, the transmission curves are examined at different frequencies and ion energies.

It was deteremined that the wide rectilinear and hexapole provide the smoothest transmission functions with a wide mass range band pass. The wide rectilinear showed to have the optimal band pass at low ion energy while the hexapole proved best at higher energies. It is predicted that with collisional dampening, the wide rectilinear will provide the smoothest transfer function along with a wide mass range band pass compared to the other RF-only devices

II. EXPERIMENTAL

Five different types of ion guides were tested; round rod quadrupole, narrow rectilinear quadrupole, wide rectilinear quadrupole, hexapole, and octopole (no results shown). All of the test ion guides were 6.0 inches long with an inscribed diameter of 4 mm.

The experimental test setup for each configuration included an axial molecular beam ionizer followed by the ion guide in question with the same 4 mm entrance and exit apertures, followed by a 9 mm rod diameter round rod analytical quadrupole, and the same flange mounted electron multiplier detector. All of the ion guides were tested in high vacuum operation without collision dampening gas. Each ion guide was tested with varying frequencies and ion energy. RF frequencies were applied to the devices with using an Ardara Technologies RF Power Supply. The ion energy was changed by increasing the pole bias on the RF-only device. The transfer functions were then examined as a function of mass, ion energy and RF frequency.

III. RESULTS AND DISCUSSION

Each device was tested at different frequencies between 1.5 MHz and 2.0 MHz and at different ion energies at each frequency.

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Figure 1. An array of 4mm inscribed diameter ion guides: quadrupole, wide rectilinear quadrupole, narrow rectilinear quadrupole, hexapole, and octopole.

The round rod quadrupole had a traditional resolving quadrupole geometry, ~4.6 mm rod diameter, with a 4 mm inscribed diameter to best approximate a pure hyperbolic quadrupole (1.148:1 r to rzero)[1].

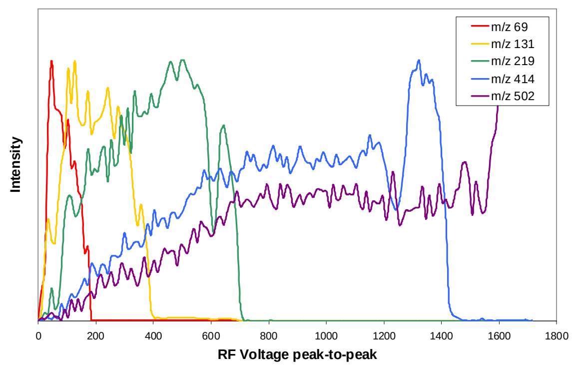

Figure 2. Round rod quadrupole transmission curve at 2.02 MHz and -20 V pole bias.

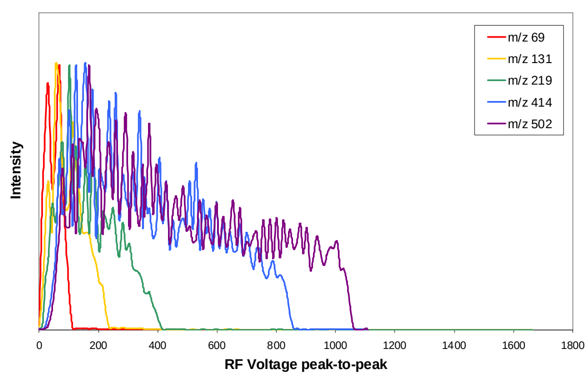

Figure 4. Narrow rectilinear quadrupole transmission curve at 1.67 MHz and -70 V pole bias.

For the round rod quadrupole, a large noding effect was observed for all masses which increased with ion energy. The mass range band pass (overlap of the various ion intensity transfer functions at a given RF level) was narrow at low RF voltage, and did not appear to get wider as the RF voltage was increased.

The narrow rectilinear quadrupole had a 1.35 mm wide flat portion facing the inside of the ion guide, with 45^{o} angle corners. The width of the flat portion of the rod was 33.7% of inscribed diameter, a profile predicted by Sakudo and Hayashi[2] to be equivalent but slightly better than having 40.9% of inscribed diameter with 90^{o} steps, for approximating a hyperbolic quadrupole.

Frequencies of 1.67 and 1.95 MHz were applied to the narrow rectilinear quadrupole and higher ion energies were required for good transmission. Similar to the round rod quadrupole large noding effects were observed, but a wider mass range pand pass was achieved.

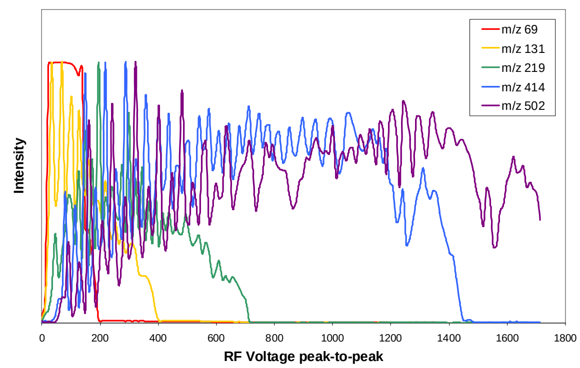

Figure 3. Round rod quadrupole transmission curve at 2.02 MHz and -60 V pole bias.

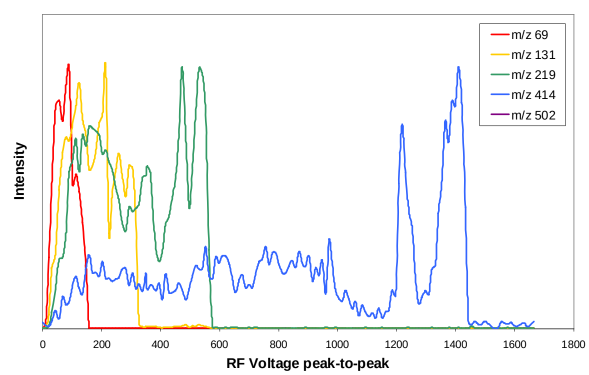

Figure 5. Narrow rectilinear quadrupole transmission curve at 1.95 MHz and -20 V pole bias.

Since Pierce and Halsall[3] demonstrated that the rectilinear quadrupole works passably as a resolving quadrupole although with marginal performance as compared to a round rod or hyperbolic quadrupole, it is no surprise that the two devices have similar behaviors.

For the round rod and the narrow rectilinear quadrupoles, the severe noding effect with ion energy as well as poor overlap of the transform functions for the different masses makes these two devices less than desirable for a general ion guide in the absence of collisional dampening gas.

The wide rectilinear quadrupole has a 3.28 mm wide flat with 90° angle steps (81.9% of inscribed diameter). The width was arbitrarily chosen to be twice the width of the optimum width with 90° angle step. Frequencies of 1.67 and 1.95 MHz were applied to the qudrupole and transmission curves were obtained at low ion energies.

The RF only spectra gathered using the wide rectilinear quadrupole rank among the smoothest transmission curves of the ion guides tested. There was also an increased overlap of the intensity maxima across the mass range. The sweet spot in optimum RF voltage yielded the highest sensitivity for the widest range of masses. The wide rectilinear quadrupole exhibits the largest overlap of the widest range of masses, across a wide range of RF voltages.

The wide rectilinear quadrupole ion guide did unfortunately exhibit noding effects with higher ion energy, although not as prominent as the round rod and narrow rectilinear quadrupoles.

The hexapole consists of six evenly spaced rods[4] and a 2 mm effective rod diameter. Frequencies of 1.7 and 2.0 MHz were applied to the hexapole and transmission curves were obtained at high ion energies.

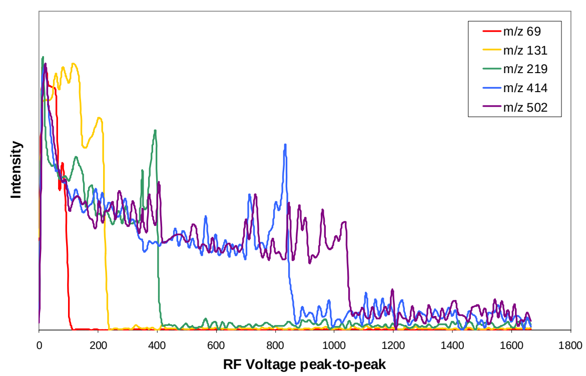

Figure 7. Wide rectilinear quadrupole transmission curve at 1.67 MHz and 0 V pole bias.

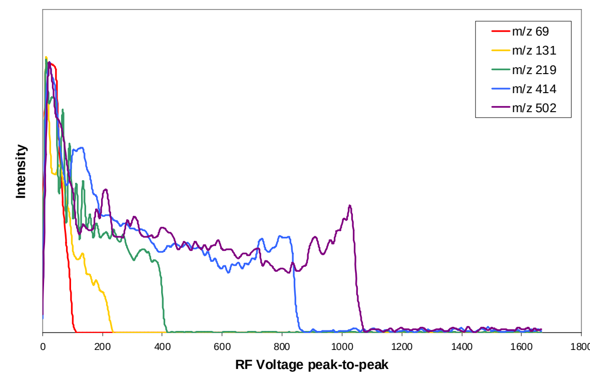

Figure 8. Wide rectilinear quadrupole transmission curve at 1.67 MHz and -10 V pole bias.

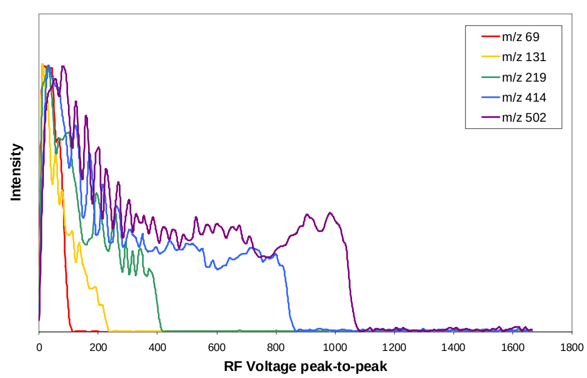

Figure 9. Wide rectilinear quadrupole transmission curve at 1.67 MHz and -20 V pole bias.

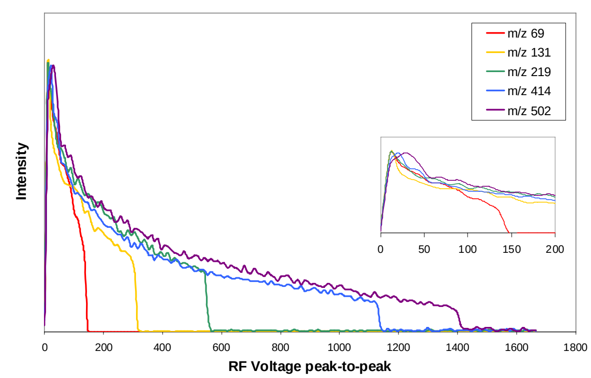

Figure 6. Wide rectilinear quadrupole transmission curve at 1.95 MHz and 0 V pole bias. Insert is a close up of the RF voltage from 0 to 200 volts peak-to-peak.

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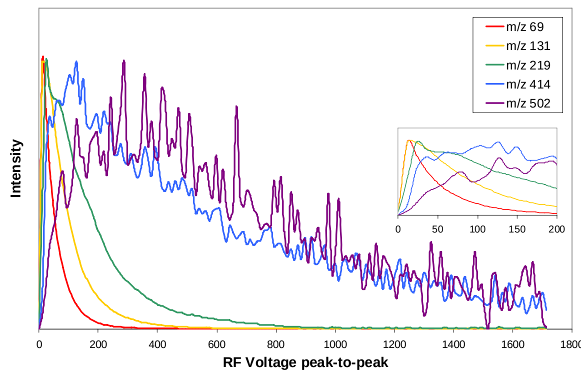

Figure 10. Hexapole transmission curve at 1.71 MHz and -20 V pole bias. Insert is a close up of the RF voltage from 0 to 200 volts peak-to-peak.

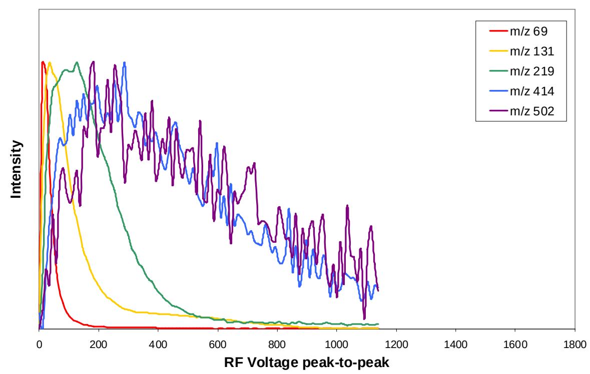

Figure 11. Hexapole transmission curve at 1.71 MHz and -60 V pole bias.

IV. CONCLUSIONS AND FUTURE WORK

For low ion energy ion transfer, the wide rectilinear quadrupole offers the highest transmission for the widest range of simultaneous masses with smooth transfer functions.

For high ion energy ion transfer the hexapole offers the smoothest transfer functions across a reasonably wide mass range bandpass, although for a given RF voltage there is a wide range of relative transmission for the various masses (mass discrimination).

The results from the hexpole ion guide provided smooth curves with good overlap of the maximums for the different mass, but the optima did not overlap as well as in the wide rectilinear quadrupole (poor mass range bandpass). The hexapole ion guide also shows minimal ion energy noding effects as compared to the quadrupole ion guides. Compared to the wide rectilinear quadrupole, the hexapole provides smoother transmission curves when higher ion energies are required.

The octopole has evenly spaced 8 rods[3] and a 1.35 mm effective rod diameter. Due to time constraints, no transmission curves were obtained due to poor signal strength. The setup for the octopole must be reevaluated before any conclusions can be drawn on it.

With collisional dampening, it is predicted that the ion energy related noding effects of the rectilinear quadrupole would diminish dramatically, making the wide rectilinear quadrupole the ion guide with the optimum transmission characteristics (smooth transfer function with optimum transmission across a wide mass range bandpass).

V. REFERENCES

1. Dennison, R. D. *J.Vac. Sci. Tech.* **1971**. 8, p.485.

2. Sakudo, N and Hayashi, T.; "Quadrupole Electrodes with Flat Faces"; *Rev. Sci. Instrum.* **1975**. 46. p. 1060.

3. Pearce, C.G. and Halsall, D.;"A Quadrupole Mass Filter with Flat Electrodes"; *International Journal of Mass Spectrometry and Ion Physics*, **1978**, 27, pages 31-41.

4. Gerlich, Dieter. In *State-Selected and State-to-State Ion-Molecule reaction Dynamics. Part I: Experiment.* Edited by Cheuk-Yiu Ng and Michael Baer. John Wiley & Sons, Inc. 1992.