Supplemental Material

for

Operation and Performance of a Mass-Selective Cryogenic Linear Ion Trap

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1. **Pressure profile in the vacuum chamber after injecting Helium into the cryoLIT**
2. **Determination of A_2 via fitting of the multipole expansion**
3. **Calculating the thermal contraction of the radius in the cryoLIT**

1. Pressure profile in the vacuum chamber after injecting Helium into the cryoLIT

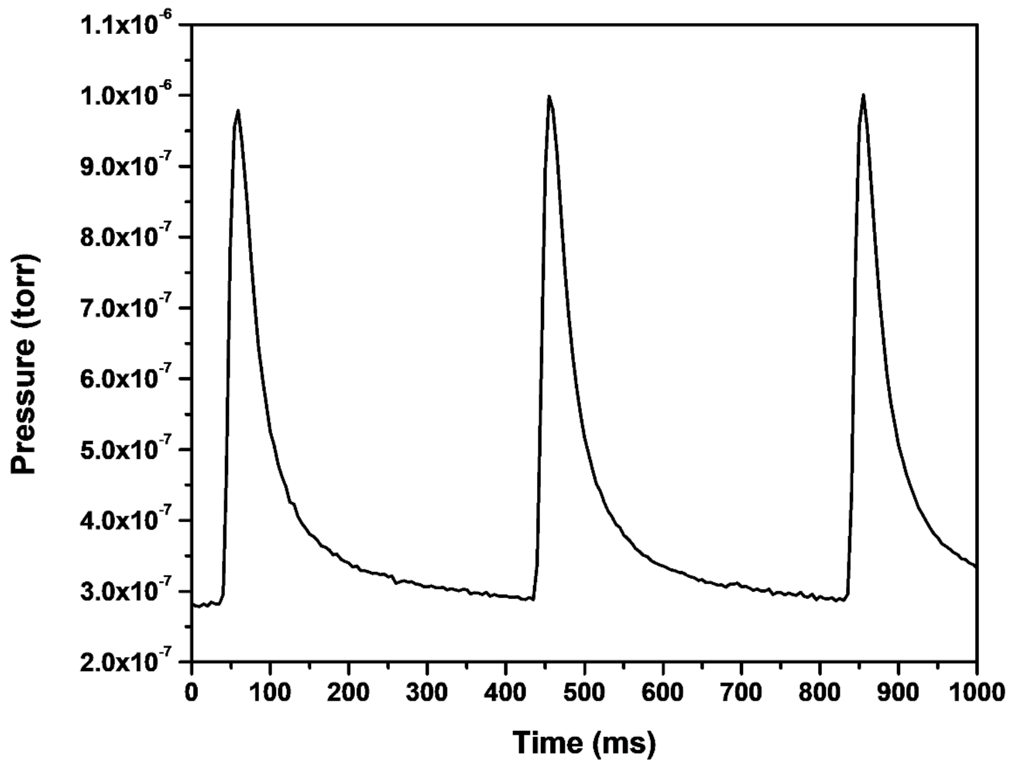

Figure S1. Pressure inside of the vacuum chamber during 3 Helium gas pulses into the cryoLIT, as monitored by an Extorr XT100 residual gas analyzer.

2) Determination of A_2 via fitting of the multipole expansion

For a two dimensional linear ion trap, the electric potential, ϕ, at any point inside of the trap can be approximated by a multipole expansion [1]:

$$\phi(r,\theta) = \phi_0 \sum_{n=0} \left(\frac{r}{r_N}\right)^n (\mathrm{A_n}\cos(n\theta) + B_n \sin(n\theta)) \qquad \text{Eq. S1}$$

Where r and θ are the distance and angle from the center of the trap, r_N and ϕ_0 are the normalization radius of the trap and the field-free potential of the trap, and n is the index of multipole (*i.e.* quadrupole, hexapole, etc.). A_2 can be obtained by fitting Eq. S1 to the trap potential using the method described by Barlow [2]: Using SIMION 8.0, a set of potentials are sampled from a ring of 40 points, 1 mm away from the center of the trap. Since *r* is fixed at 1mm and r_N is the y-radius of the trap, 0.20" (5.08 mm), the potentials only vary as a function of θ. As an initial guess, ϕ_0 is estimated to be the average of the 40 potentials. Using Excel's Data Analysis Toolpak to minimize the square differences between the sampled potentials and Eq.S1, ϕ_0 , A_n, and B_n are found. An additional constraint can be placed by setting all B_n values to 0, but this was not used in this paper. This method calculates the cryoLIT's A_2 to be equal to 0.866. All other calculated A_n values are tabulated in Table S1.

Table S1. Calculated A_n values for the cryoLIT using the multipole expansion fitting method.

A_0	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8
0.261	0.000860	0.866	0.000165	-0.164	-0.0370	0.0517	0.238	2.75

3) Calculating the thermal contraction of the radius in the cryoLIT

To calculate the change in radius in either the x or y direction of the cryoLIT, the thermal contraction, $\frac{\Delta L}{L}$, of both the rf electrodes and the DC endplate must be considered. The rf electrodes undergo thermal contraction, and thus increase the trap radius, by $\frac{\Delta L}{L} * \frac{L_{rf}}{2}$, where L_{rf} is the thickness of the rf electrode in either the x or y direction; the factor of $\frac{1}{2}$ comes from the fact that only the interior side of the electrode contributes to the trap radius. While the rf electrodes shrink, the DC endplate mounting holes, which keep the rf electrodes in place, contract towards the center of the trap by $\frac{\Delta L}{L} * L_m$, where L_m is the distance from the center of the mounting hole to the center of the cryoLIT. Thus the change in the cryoLIT radius can be calculated with the following equation:

$$\Delta r = \frac{\Delta L}{L}\left(L_m - \frac{L_{rf}}{2}\right) \quad \text{Eq. S2}$$

Note, $\frac{\Delta L}{L}$ is a negative number, so the trap radius does in fact decrease as L_m is greater than L_{rf}.

The calculations for the change in radius in the x and y directions are shown below:

$$\left(\frac{\Delta r}{r}\right)_x = \frac{\frac{\Delta L}{L}\left(L_{m_x} - \frac{L_{rf_x}}{2}\right)}{r_x} = \frac{-0.00202 \times (0.353\text{ in} - \frac{0.230}{2}\text{ in})}{0.240\text{ in}} \times 100\% = -0.200\% \quad \text{Eq. S3}$$

$$\left(\frac{\Delta r}{r}\right)_y = \frac{\frac{\Delta L}{L}\left(L_{m_y} - \frac{L_{rf_y}}{2}\right)}{r_y} = \frac{-0.00202 \times (0.313\text{ in} - \frac{0.230}{2}\text{ in})}{0.200\text{ in}} \times 100\% = -0.200\% \quad \text{Eq. S4}$$

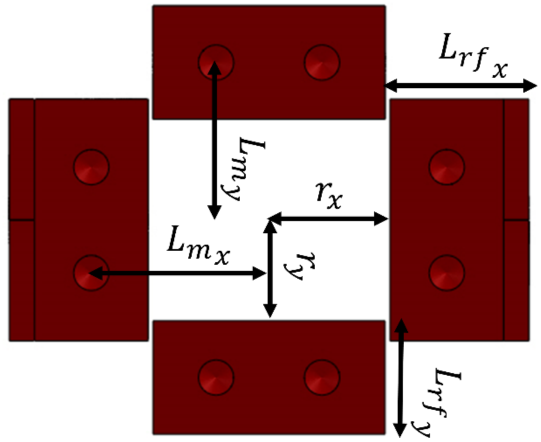

Figure S2. Dimensions used in the calculation of trap shrinking.

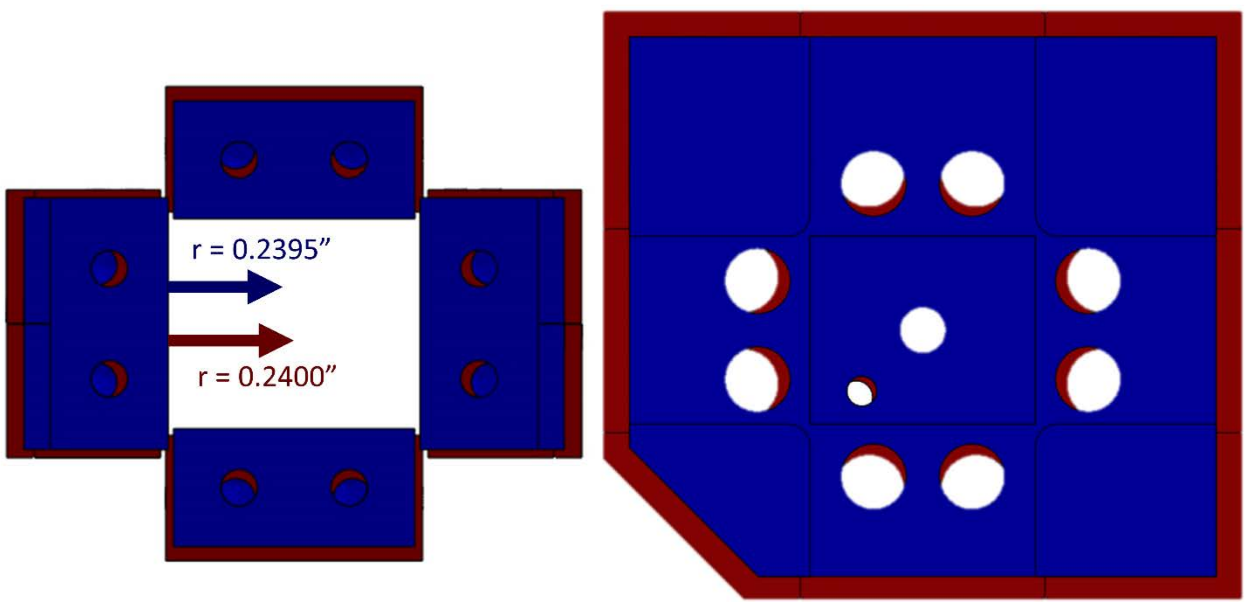

Figure S3. Illustration of the thermal contraction undergone when the cryoLIT is cooled. The contraction of the mounting holes of the DC endplate (right), at cryogenic temperature, causes the rf rods (left) to move inwards, decreasing the trap radius. Note the contraction here is magnified 20 fold.

Bibliography

1. Krishnaveni, A., Verma, N.K., Menon, A.G., Mohanty, A.K.: Numerical observation of preferred directionality in ion ejection from stretched rectilinear ion traps. Int. J. Mass Spectrom. Ion Process. 275, 11–20 (2008). doi:10.1016/j.ijms.2008.05.011
2. Barlow, S.E., Taylor, A.E., Swanson, K.: Determination of analytic potentials from finite element computations. Int. J. Mass Spectrom. Ion Process. 207, 19–29 (2001). doi: 10.1016/S1387-3806(00)00452-8