Improved Performance Obtained On The Toroid Ion Trap Mass Analyzer Using Asymmetric Electrodes

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A novel ion trap mass spectrometer based on a toroidal ion storage geometry has previously been reported.(1) The analyzer geometry is based on the rotation of the quadrupolar trapping field into the shape of a torus. Initial performance of this device was poor, however, due to the significant contribution of non-linear fields introduced by the rotation of the symmetrical ion trapping field. These non-linear resonances contributed to poor mass resolution and sensitivity as well as erratic ion ejection behavior. More recently, the geometry of the toroid ion trap analyzer has been modified in an attempt to correct for these non-linear fields. Computer simulation programs suggested an asymmetric electrode design that, when implemented, resulted in a significantly improved performance.

Commercial ion trap mass analyzers produce essentially linear quadrupolar trapping fields. A slight positive deviation from linearity is intentionally introduced by stretching the endcap distances (or asymptote angles) in order to improve mass analysis performance. The toroid geometry was optimized using POISSON (a trapping field analysis program developed at Los Alamos National Laboratory) and ITSIM (an ion trap trajectory simulation programs developed at Purdue University). These programs revealed that the original, symmetric toroid analyzer trapping field had a significant, negative non-linear component. Using the Poisson field analysis programs, the field faults were corrected by intentionally skewing the cross-sectional symmetry of the device. In this case, the angle of the asymptotes that correspond to the outer ring electrode was decreased while the angle of the asymptotes corresponding to the inner ring electrode was increased (Figure 1) until a slight, positive non-linear field was achieved. Ion trajectory calculations using ITSIM indicated that the mass resolution and sensitivity of this asymmetric analyzer should be dramatically improved. Based on these simulations, an asymmetric ion trap analyzer has been constructed (Figure 2) and integrated into a modified Finnigan ITMS ion trap instrument. Samples (including n-butylbenzene, benzene and perchloroethylene) as well as the helium buffer gas were introduced directly into the vacuum chamber using a leak valve. Performance characteristics (mass resolution and signal intensity) were then monitored as a function of sample/helium pressure, ejection q-value, and analyzer storage times.

Indeed, improved performance has been realized using the newly constructed asymmetric toroidal ion trap analyzer as is demonstrated in the mass resolution obtained on benzene, n-butylbenzene and other samples. Figure 3 shows the spectrum for benzene with strong signal intensity and unit resolution at a sample pressure of 9×10^{-7} torr and an ionization time of 25 milliseconds. The data system's mass scale was not corrected for the difference in trapping field dimensions, trapping frequency (1034 kHz vs. the expected 1100 kHz) or the reduced β_{eject} (0.88). Although storage capacity and linearity appear promising, current ITMS data system prevents measurement of the analyzer's linear dynamic range. To circumvent this, measurements were made at two different sample pressures and within each pressure range, ion intensity linearly increases with ionization time over two orders of magnitude without significant evidence of space charging. Figure 4 demonstrates the improved mass resolution obtained on the m/z 91 and m/z 92 fragment ions from n-butylbenzene between the original symmetric (Figure 4a) and the new asymmetric (Figure 4b) geometry. A strong dependence of the mass resolution and sensitivity on the β_{eject} value still exists as peak splitting and decreased signal (presumably due to increased radial ejection) is observed at particular values of β_{eject} (especially those corresponding to the non-linear resonances at $\beta_{eject} = 1/2$ and $\beta_{eject} = 2/3$).

References

1. “Development of an Ion Trap Mass Spectrometer with an Alternate Trapping Geometry”, Stephen A. Lammert, Marcus B. Wise, and Cyril V. Thompson, Presented at the 46th ASMS Conference on Mass Spectrometry and Allied Topics, Orlando, FL, 31 May- 4 June 1998.

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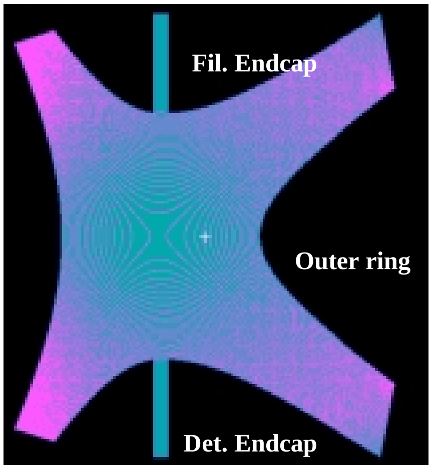

Figure 1

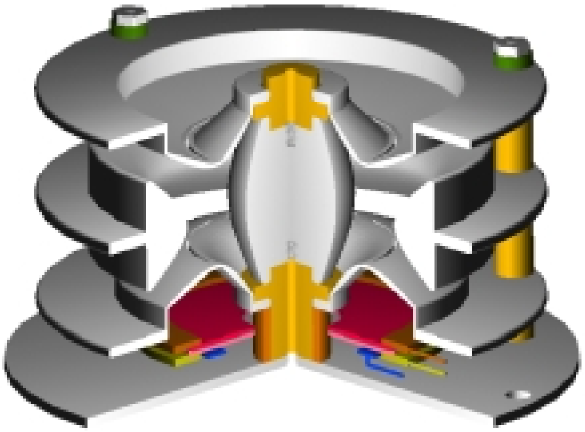

Figure 2

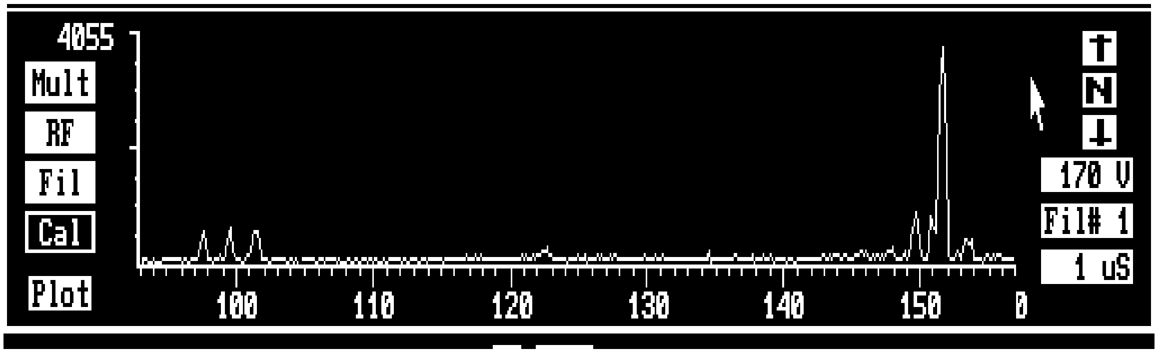

Figure 3

(a)

(b)

Figure 4