A Study of Resonance Ejection at Beta values > 1 for Helium and Air Buffer Gases in Ion Trap Mass Spectrometers

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Ion trap field portable mass spectrometers typically require the use of a helium buffer gas. The ability to substitute air for helium as the buffer gas significantly impacts the portability of ion trap mass spectrometers since compressed helium cylinders are not needed. Previous studies [1,2] using air as the buffer gas in ion traps manufactured by Finnigan-MAT have demonstrated the utility of this approach. While helium remains the preferred and superior buffer gas, conditions exist where similar performance in both sensitivity and mass resolution can be achieved on Finnigan ITMS instruments using air as the buffer gas. Teledyne (San Jose, CA) 3DQ ion trap mass spectrometers have similar analyzer dimensions as the Finnigan ion traps however early versions used a resonance ejection frequency which corresponds to ejection qz-values which are higher than the stability boundary value of 0.908 (β=1). This study attempts to find the optimum operating conditions for the Teledyne 3DQ Discovery for both helium and air buffer gases as a function of the frequency of resonance ejection.

Mass peak width (solid line) and intensity (dotted line) data for the ejection of m/z 69 from PFTBA at various values for β_{eject} when using helium as the buffer gas is shown in **Figure 1.** There is an observed symmetry around the β=1 axis. Note especially, the slight enhanced performance at exactly β_{eject} =1 over the immediately neighboring values. The β-value for a resonance ejection frequency of 540 kHz (the default for the Discovery II) is shown by the solid vertical line. The corresponding "Mathieu sideband"[3] frequency (in this case 360 kHz) is shown by the dashed vertical line. As can be seen, these positions are in the middle of a range of frequencies that provide the narrowest peak widths with FWHM values between 0.2 and 0.3). The local maxima/minima of the peak intensities varies more widely than does the peak width in these two optimum ranges ($0.7<\beta_{eject}<0.95$ and $1.05<\beta_{eject}<1.3$). Some of these local minima and maxima correspond to known non-linear resonances[4] in the ion trap (β= 0.5, 0.67, 0.71). A steep peak width increase (not observed at low values of β_{eject}) is also observed as β_{eject} approaches a value of 1.5. In addition, no measurable signal is detected at β_{eject}-values > 1.5.

When air is substituted for helium as the buffer gas, the overall peak intensities for all mass-to-charge values is dramatically reduced by a factor of more than 10. This performance is also in contrast to previously reported performance using air buffer gas in direct air monitoring[5]. Differences also occur in the general appearance of the data for peak width and intensity as a function of β_{eject}-value. The slightly enhanced performance seen for helium at exactly β_{eject}=1 is a dramatic reduction in performance when using air especially for m/z 69 (**Figure 2)**. In addition, the local maxima/minima in the range of $0.7<\beta_{eject}<0.95$ and $1.05<\beta_{eject}<1.3$ are not as extreme. This implies that the non-linear resonances are less important to consider when using air as the buffer gas. Also,in contrast to the helium results, the optimum performance occurs at β_{eject}-values <0.5 or >1.2. Finally, the plot asymmetry (especially at β_{eject}-values approaching 1.5) observed for helium is absent . Only small differences are observed at the extremes of these two plots and measurable signal is still present when using air at β_{eject}-values > 1.5.

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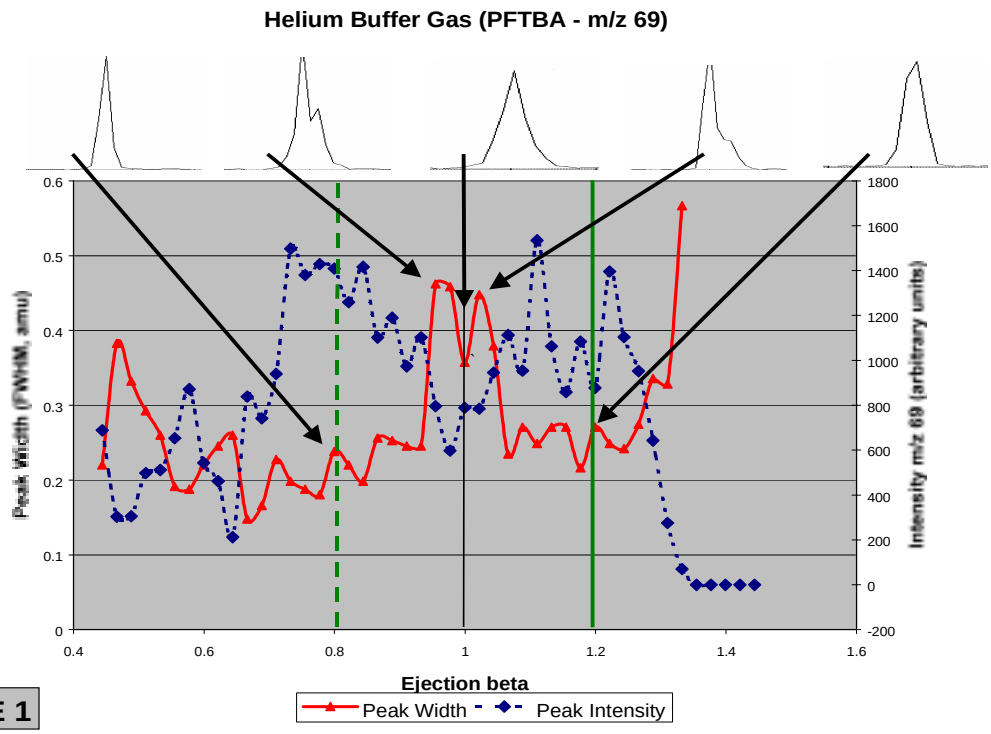

FIGURE 1

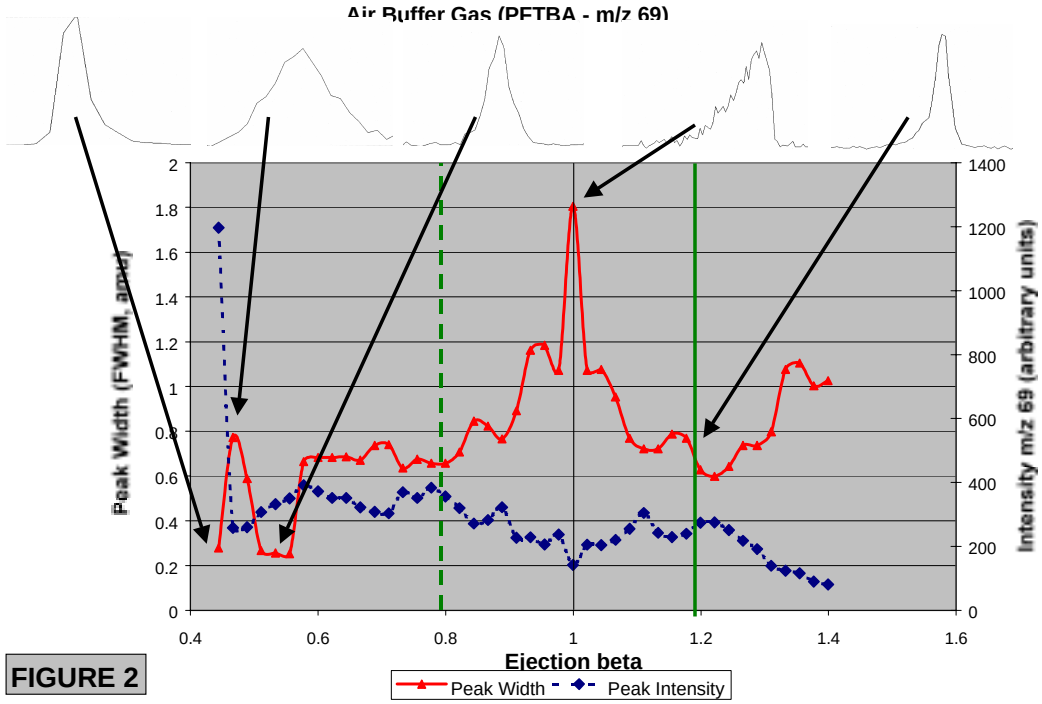

FIGURE 2