A Mini mass spectrometer with a low noise Faraday detector

Supporting Information

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Ion-neutral collision model

In the case of small ions, the Langevin collision model is a good approximation of low energy collisions between neutral molecules and small ions[1].

The damping coefficient of Langevin collision model is

$$c = \frac{z}{2\varepsilon_0}\frac{p}{kT}\sqrt{\frac{\alpha_p(m+M)}{mM}}\frac{M}{m+M} \tag{1}$$

where z is the ion charge, ε_0 is the permittivity of vacuum, p is the pressure of buffer gas, α_p is polarizability of the buffer gas, k is the Boltzmann constant, T is temperature, M is mass of the buffer gas molecule, m is mass of the ion.

The effect of mass scan rate on mass resolution

An equation relating mass resolution to the damping and scan rate has been explored theoretically by Douglas et al. Briefly mass resolution of a peak within an ion trap[2],

$$\frac{m}{\Delta m} \cong \frac{q\Omega}{2\sqrt{2}}\left(\frac{1}{\sqrt{3}c + 2scanrate/c}\right) \tag{S2}$$

where q is the ejection q value (0.7847 for all ions in this study), Ω is the RF frequency, c is the damping coefficient of Langevin collision and *scantrate* is scan rate of the instrument.

According to the relationship between mass Δm and scan rate. The duration of FWHM was t_{FWHM},

$$t_{FWHM} = \frac{\Delta m}{scanrate} \tag{S3}$$

From eqn S2 and S3, the relationship between the t_{FWHM} and scan rate could be found,

$$t_{FWHM} \cong \frac{2\sqrt{2}m}{q\,\Omega\left(\frac{scanrate}{\sqrt{3} * c + \frac{2 * scanrate}{c}}\right)} \tag{S4}$$

Similarity, the interval of the two isotope peaks,

$$\Delta t = \frac{dm}{scanrate} \tag{S5}$$

where dm is the mass difference between two isotope peaks. In order to improve mass resolution and the ability to separate isotope peaks. In order to separate ion isotope peaks, regulating scan rate could be an approach to satisfy $\Delta t \geq \quad t_{FWHM}$,

$$\frac{\Delta t}{t_{FWHM}} \geq 1 \tag{S6}$$

Transfer function of the Faraday cup

Due to the high gain of 10^{11}, the bandwidth is limited to 430 Hz, which broadens the peaks of spectra. According to the voltage gain versus frequency characteristic, a second stage transfer model can be obtained through typical TIA Noninverting Gain amplifier circuit. The transfer function of the Noninverting Gain amplifier circuit is,

$$H(s) = -\frac{2R + sCR^2}{1 + 2sCR + s^2C^2R^2} \tag{S7}$$

where *R* is the half of feedback resistor, *C* is the feedback capacitor.

In order to compensate the high frequency of the signal, a reverse transfer function of the $H(s)$ is introduced,

$$H_1(s) = -\frac{2\{1 + sc_1[r_1 + r_1(1 + sc_1r_1) + r_2]\}}{(2 + sc_1r_1)(1 + sc_1r_2)} \tag{S8}$$

where $c_1r_1 = CR$, and c_1r_2 is an introduced polar of the reverse transfer function. In this case, the polar is set at 20 kHz.

From eqn S8, the discrete reverse transfer function is deviated,

$$H_1(z) = \frac{-86.46z^2 + 172.66z - 86.21}{z^2 - 1.94z + 0.94} \quad \text{(S9)}$$

References:

(1) Hou, C.; Xu, Q.; Zhang, F.; Jiang, T.; Xu, W. *Journal of Mass Spectrometry* 2019.

(2) Goeringer, D. E.; Whitten, W. B.; Ramsey, J. M.; McLuckey, S. A.; Glish, G. L. *Analytical chemistry* 1992, *64*, 1434-1439.