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Supplementary Information

Characterization and Optimization of Ion Discrimination in a Mini Ion Funnel for Miniature Mass Spectrometer

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Calculation of Collision Coefficient (C)

In general, there are two models – the hard-sphere collision model and the Langevin collision model – applicable to the collision between ions and neutral gas molecules[1, 2]. The Langevin collision model takes into account the induction of dipoles in neutral gas molecules by ions and can better estimate the low-energy collision between small-molecule ions and neutral particles[3]. In the Langevin collision model, the collision cross-section (CCS) between ions and neutral gas molecules can be calculated as follows[2, 4, 5]:

$$\sigma_D \approx \frac{2\pi e}{u}\sqrt{\frac{\alpha_p(M+m)}{\varepsilon_0 Mm}} \qquad (1)$$

where u is the relative speed of ions to gas molecules; α_p: electric polarizability of the gas molecule; ε_0: permittivity of vacuum; M: mass of gas molecule; m: mass of ion; e: ion charge. The collision coefficient (C) is estimated as follows, based on Equation (4) in the main part of this paper:

$$C = \frac{c}{\Omega} = \frac{eP}{KTf_{RF}}\sqrt{\frac{\alpha_p(M+m)}{\varepsilon_0 Mm}} \qquad (2)$$

However, in application, the neutral background gas in the miniature ion trap mass spectrometer is air. We use N_2 to estimate the molecular electric polarizability[6], $\alpha_p = 1.76$ Å^3; the relative mass of gas is 28, the air pressure in the first chamber P = 500 Pa; the temperature is 25 °C; and the RF frequency of the funnel $f_{RF} = 860\ kHz$. For ions with an M/Z of 500 Th, the collision coefficient under these circumstances is about 48. In the experiments the collision coefficients calculated by Langevin collision model for reserpine and roxithromycin are 47.85 and 47.56, respectively. Although the mass-to-charge ratio of reserpine is lower than roxithromycin, reserpine has a larger collision coefficient under the same condition.

It should be mentioned that the Langevin collision model does not consider the actual size of ions, while the ion–molecule collision coefficient is apparently related to ion size and its spatial structural form. As a result, we only provide an estimate of the collision coefficient (C) herein as the reference for setting the parameters for theoretical calculations.

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