Collision Cross Section Measurements for Biomolecules within a High-Resolution FT-ICR Cell: Theory

Supporting Imformation

Dan Guo,[1] Yi Xin,[1] Dayu Li,[2] Wei Xu[1*]

[1]School of Life Science, Beijing Institute of Technology, Beijing 100081, China

[2]College of Information Science and Engineering, Northeastern University, Shenyang 110819, China

*Corresponding Author:
Wei Xu
School of Life Science
Beijing Institute of Technology
Haidian, Beijing, 100081, China
Email: weixu@bit.edu.cn
Phone: +86-10-68918123

1. The derivation of decay profile

With ion-neutral collisions, the ion motion equation in an FTICR cell can be written as:

$$mv' = qv \times B + qE + f(v) \tag{S1}$$

where m is the mass of an ion, $\boldsymbol{v}$ is the velocity of an ion, q is the charge an ion possesses, $\boldsymbol{B}$ is the magnetic field strength, $\boldsymbol{E}$ is the strength of the radio frequency electric field and $f(v)$ is the collision damping term. When neglecting the electric trapping potential, Eqn. S1 becomes:

$$mv' = qv \times B + f(v) \tag{S2}$$

The Langevin collision model:

For the Langevin collision model, the calculated collision cross section is inversely proportional to velocity and has an expression as:

$$\delta_1 = \frac{q\sqrt{\frac{\alpha(M+m)}{mM}}}{2\, v\, \varepsilon_0} \tag{S3}$$

The ion motion equation with the Langevin collision model can be written as:

$$v' = qv \times B/m - c_1 v \tag{S4}$$

in which $c_1 = \frac{q\sqrt{\frac{\alpha(M+m)}{mM}}}{2\varepsilon_0} \frac{p}{Tk} \frac{M}{m+M}$.

Eq. (4) becomes a scalar differential equation when multiplied by vector v and the term $q(v \times B).v$ equals zero. Solve the scalar equation of Eq. (4), the expression of velocity with respect to time was obtained.

$$v = v_0 e^{-t\, c_1} \tag{S5}$$

The hard sphere collision model:

The hard-sphere collision model treats an ion as a sphere and ignores the polarization force between the ion and neutral molecules. In this situation, the damping term is proportional to the square of ion velocity and the ion motion equation becomes:

$$v' = qv \times B/m - c_2 v \mid v \mid \tag{S6}$$

in which $c_2 = \sigma \frac{p}{Tk} \frac{M}{m + M}$. Transform Eqn. S6 into a scalar equation

$$v^{'} = - c_2 v^2 \tag{S7}$$

The solution of Eqn. S7 has an expression as:

$$v = \frac{v_0}{t\, v_0\, c_2 + 1} \tag{S8}$$

2. Fourier transform of the hard-sphere collision time-domain signal

For the hard-sphere collision model, the calculated Fourier transform expression of Eqn. S8 with Mathematica 9.0 is:

$$M(w) = M_0(sqrt((Cos[\frac{2\omega_0}{B}]Re[CosIntegral[\frac{w-\omega_0}{B}]] - Cos[\frac{2\omega_0}{B}]Re[CosIntegral[\frac{(1+B\tau)(w-\omega_0)}{B} \ldots + (Cos[\frac{2\omega_0}{B}]Im[CosIntegral[\frac{w-\omega_0}{B}]] - Cos[\frac{2\omega_0}{B}]Im[CosIntegral[\frac{(1+B\tau)(w-\omega_0)}{B}]] - Im[C \ldots))$$

(1)

where $A = v_0$, $B = v_0\, c_2$, τ is the signal acquisition time, ω_0 is the ion secular frequency.