I. SIMULATION OF IONS IN A PENNING TRAP

Ions are confined radially by a magnetic field $\mathbf{B}$, with an ideal quadrupolar trapping potential of V_T. The potential and field near the centre of the trap is approximated as

$$\Phi_T(x,y,z) = V_T(\gamma' - \frac{\alpha'}{2l^2}(x^2+y^2-2z^2)) \qquad \mathbf{E} = -\nabla\Phi_T(x,y,z) = \frac{\alpha}{l^2}(-x\mathbf{i} - y\mathbf{j} + 2z\mathbf{k}) \tag{1}$$

where $\gamma' = 1/3$ and $\alpha' = 2.77373$ are geometric factors for the cubic trap, and l is the edge length[1]. The force experienced by an ion in the trap is

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v}\times\mathbf{B}) \tag{2}$$

Charges and mass are simulated in atomic units, lengths in nm and time in ns.

A. Integration scheme

The code uses the Boris integrator[2] as formulated in Birdsall and Langdon[3]. This is a modified leapfrog scheme in which positions are calculated at times $..., n-1, n, n+1, ...$ and velocities at times $..., n^{-1/2}$, $n^{+1/2}, ...$

$$\mathbf{v}^- = \mathbf{v}^{n-1/2} + \frac{q\mathbf{E}}{m}\frac{\Delta t}{2} \tag{3}$$

$$\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t} \qquad \mathbf{t} = \frac{q\mathbf{B}}{m}\frac{\Delta t}{2} \tag{4}$$

$$\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}'\times\mathbf{s} \qquad \mathbf{s} = \frac{2\mathbf{t}}{1+t^2} \tag{5}$$

$$\mathbf{v}^{n+1/2} = \mathbf{v}^+ + \frac{q\mathbf{E}}{m}\frac{\Delta t}{2} \tag{6}$$

B. Ion motion

The cyclotron frequency ω_c is predicted by $\omega_c = \frac{qB}{m}$[1]. To achieve 1% phase error in simulated cyclotron frequency requires $\Omega\Delta t \lesssim 0.3$[3], [4]. The cyclotron radius r is predicted by $r = \frac{mv}{|q|B}$ and is measured for a single particle simulation by the distance between maxima in the x dimension.

In a quadrupolar trapping potential of V_T, the modified cyclotron frequency ω_+ is predicted by

$$\omega_+ \equiv \frac{\omega_c}{2} + \sqrt{\frac{\omega_c^2}{4} - \frac{\omega_z^2}{2}} \qquad \omega_z = \left(\frac{2\alpha q V_T}{ml^2}\right)^{1/2} \tag{7}$$

The modified cyclotron frequency is measured by peaks in the Fourier transform of the induced current time signal.

C. Induced current

FTICR-MS measures the current induced between detector plates on walls of the cube parallel to the magnetic field. In the simulation, current is induced by the movement of the 'image' $\mathbf{E}_{image}(r)$ associated with each ion, that is, a charge equal in magnitude to the potential that would be produced at the ion position due to a unit potential applied to the detector electrode[1].

$$I = q\mathbf{v}\cdot\mathbf{E}_{image}(\mathbf{r}) \qquad \mathbf{E}_{image} = -\frac{\beta'}{l}r_j \qquad \beta' = 0.72167 \tag{8}$$

D. Simulation results

TABLE I
REPLICATING: HAN AND SHIN[5]. INPUT, PREDICTED AND MEASURED SIMULATION PARAMETERS

$B = 0.7646T, V_T = 1.0V$											
				predicted		**measured**		**error: timestep**			
species	**charge**	**mass**	v_0 **(m/s)**	$\omega_c/2\Pi$ **(Hz)**	r **(nm)**	$\omega_c'/2\Pi$ **(Hz)**	r' **(nm)**	Δt **(ns)**	$\epsilon : \Delta t$	$\epsilon : \Delta t$ **/ 10**	$\epsilon : \Delta t$ *** 10**
HCO^+	1	29.02	10	404,618	3,933	404,531	3,933	118			
CH_3CO^+	1	43.04	10	272,770	5,835	272,777	5,835	175			

TABLE II
REPLICATING: LEACH ET AL.[6]. INPUT, PREDICTED AND MEASURED SIMULATION PARAMETERS

$B = 7.0T, V_T = 1.0V$											
				predicted		**measured**		**error: timestep**			
species	**charge**	**mass**	v_0 **(m/s)**	$\omega_c/2\Pi$ **(Hz)**	r **(nm)**	$\omega_c'/2\Pi$ **(Hz)**	r' **(nm)**	Δt **(ns)**	$\epsilon : \Delta t$	$\epsilon : \Delta t$ **/ 10**	$\epsilon : \Delta t$ *** 10**
Cs^{+}	1	132.9	2700	808,792	5,313	807,812	5,319	59			
$?(\frac{\mathsf{m}}{\mathsf{q}} = \mathsf{150})$	1	150.0	2700	716,618	5,996	715,937	5,997	67			

TABLE III
CONVERSION FACTORS

property	**unit**	**SI unit**
mass	amu	$1.660538921(73) \times 10^{-27} kg$
charge	e	$1.60217653(14) \times 10^{-19} C$

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