Fourier Transform Ion Cyclotron Resonance Mass Resolution and Dynamic Range Limits Calculated by Computer Modeling of Ion Cloud Motion

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Results and Discussion

We simulate FT-ICR experiments, based on efficient and accurate calculation of the forces acting on each ion in an ensemble (cloud), including Coulomb interactions (space charge), the electric field of the ICR trap electrodes, image charges on the trap electrodes, the magnetic field, and collisions with neutral gas molecules.[1] Ion resonances that are closely spaced in *m/z* coalesce into one resonance if the ion number (density) exceeds a threshold that depends on magnetic field strength, ion cyclotron radius, ion masses and mass difference, and ion initial spatial distribution. Transitions between independent and coalesced motion were observed in a series of experiments that systematically varied ion number, magnetic field strength, ion radius, ion *m/z*, ion *m/z* difference, and ion initial spatial distribution (the present simulations begin from elliptically-shaped ion clouds with constant ion density distribution). Our simulations show that mass resolution is constant at a given magnetic field strength with increasing ion number until a critical value (N) is reached. N dependence on magnetic field strength, cyclotron radius, ion mass, and difference between ion masses was determined for two ion ensembles of different *m/z*, equal abundance, and equal cyclotron radius. We find that N and dynamic range depend quadratically on magnetic field strength in the range 1-21 Tesla (see **Figure 1**). Dependences on cyclotron radius and $\Delta m/z$ are linear. N depends on *m/z* as $(m/z)^{-2}$. Empirical expressions for mass resolution as a function of each of the experimental parameters are presented. Here, we provide the first exposition of the origin and extent of trade-off between FT-ICR MS dynamic range and mass resolution (defined not as line width, but as the separation between the most closely resolved masses).

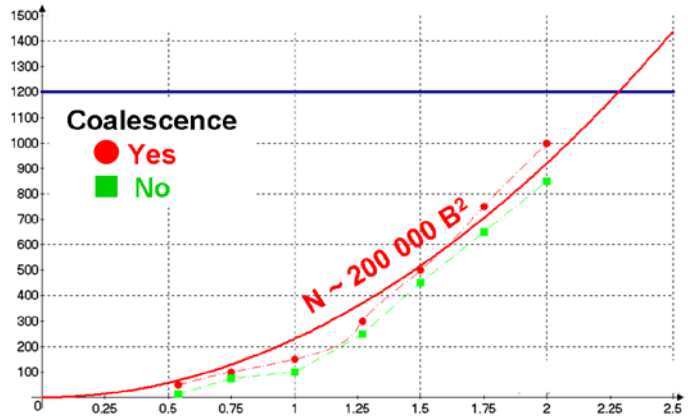

Figure 1. Minimum number of ions at which FT-ICR peak coalescence takes place as a function of magnetic field strength, for equally abundant ions of *m/z* = 100 and 100.3 in a 25.4 mm cubic ICR cell. The smooth curve represents an analytical formula that approximately matches the simulated onsets.

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References

[1] Vladimirov, G., *et al.*, J. Am. Soc. Mass Spectrom. **23**, 375-384 (2012).