Experimental Validation of an Analytical Model for Trapped Ion Mobility Spectrometry

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Background:
A new type of ion mobility method termed, trapped ion mobility spectrometry (TIMS), has been recently shown to offer many attractive features including: rapid (ms) gas phase separations, a compact design enabling efficient integration with time of flight mass spectrometry, the ability to tune the experimental parameters in accordance with the analytical challenge (1-2), and resolving power exceeding 250 (3). Here, we experimentally validate an analytical model (see poster #690 for derivation) that predicts the transient time and the resolving power.

Theory:
Resolving power is given by:
\[ R = \frac{m/z_{2} - m/z_{1}}{2 \sqrt{v T}} \]

where:
- \( v \): gas velocity
- \( t \): time across plateau
- \( m/z \): mass to charge ratio
- \( T \): temperature

In so far as \( v \) and \( t \) represents the Lagrangian path length, eq. [2] reduces to the familiar resolving power expression for drift tube IMS:

\[ R = \frac{m/z_{2} - m/z_{1}}{2 \sqrt{v T}} \]

Substitutions for \( t \) and \( E_{0} \) followed by rearrangement of eq. [2] yields:

\[ R = \sqrt{\frac{L}{16 L_{2}^{2} T}} \]

Dependence of resolving power on the EFG scan rate

Dependence of resolving power on the ion mobility coefficient

Experimental Results:
- \( m/z = 622 \)
- \( m/z = 922 \)
- \( m/z = 1222 \)
- \( m/z = 1522 \)
- \( m/z = 1822 \)

Conclusions:
- Experimental results are in general agreement with the analytical model.
- The TIMS resolution expression (eqn 2) reduces to the same form as that long used for drift cell IMS (eqn 3).
- Most of the analytically relevant work done on the ions occurs as the ions cross the EFG plateau (eqn 2).
- Rearrangement (eqn 4) shows that TIMS resolution is proportional to gas velocity, \( v \), and square root of ion charge, \( q \), but is inversely proportional to \( K_{0} \), and the fourth root of ramp rate, \( \beta \).

References: