

# Classical Kinetic Theory of Electric Field Excitation in Quadrupole Ion Traps

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We are developing a rigorous kinetic theory of electric field excitation of ion motion under multiple collision conditions in quadrupole ion traps based on the Boltzmann equation, an integro-differential equation describing the effect of applied forces and collisions on the time-dependent ion distribution function in six-dimensional (spatial and velocity) phase space. Because numerical values for physical quantities of particular interest and importance in an ensemble of ions (such as kinetic energy and effective temperature along the coordinate axes) emerge from integration of their distribution function, the procedure allows *a priori* prediction of their relationship with experimental parameters. The theory is not dependent on any special assumptions about electric field strengths or ion-neutral interactions and mass ratios, and it provides a microscopic definition for the ion-neutral collisional damping force which was previously added *ad hoc* to the Mathieu equation. The model also gives damping force corrections that are equivalent to the random force previously introduced when using a phenomenological, Langevin equation to replace Newton's equations of motion. The theory is similar to that developed by Viehland *et al.* to describe ion cyclotron resonance (ICR) collision broadening, but a more recent method of weighted residuals for solving the Boltzmann equation is used in this case. As such, the model promises to improve upon the results obtained from the phenomenological equations developed analytically by Goeringer and McLuckey using simple momentum transfer theory. Furthermore, such a detailed investigation of the underlying principles for such phenomena is prerequisite to successful development of a comprehensive theory for the ion trap collision-induced dissociation process. In depth understanding of the process, in turn, will likely indicate directions for improving ion trap-based approaches to solving molecular measurement problems, for novel instrument development, and, possibly, for altogether new fundamental chemical measurements.

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