

**MODELING COLLISIONAL ACTIVATION IN THE QUADRUPOLE ION TRAP:
FROM DIATOMIC IONS TO HIGH MASS PROTEINS**

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The dissociation of particularly stable ions, such as strongly bound diatomic ions, and high mass ions, such as those derived from proteins, is being effected via multiple ion/neutral collisions in a wide variety of instrument types. One such example is collisional activation in the quadrupole ion trap whereby a parent ion is subjected to acceleration in a bath gas present at about 1 mtorr. In this instance, collisional activation proceeds over the time frame of at least ten milliseconds to as long as one second and involves hundreds to many thousands of collisions. Under these conditions, an ion population assumes a distribution of internal energies, which ultimately determines the macroscopic dissociation rate and the appearance of the product ion spectrum.

We have been developing a model to describe the relatively complex situation represented by ion trap collisional activation. It involves modeling both the ion acceleration process and collision inelasticity. The theory of ion transport in gases applies and can be used to develop a picture that allows for the prediction of the rates of dissociation as a function of experimental conditions and, in favorable cases, the appearance of the product ion spectrum. Under some conditions, rapid energy exchange conditions prevail such that Arrhenius activation parameters can be determined directly from the measured dissociation kinetics. In other cases, dissociation rates are largely determined by the collisional activation rate. This talk will summarize our model and compare it with data acquired with parent ions that range from tantalum oxide ions to protonated leucine enkephalin. The data include activation via conventional resonance excitation, whereby the parent ion is accelerated at its fundamental z-dimension secular frequency, activation by bringing ions close to a stability boundary (i.e., the so-called boundary-activated dissociation experiment), and ions activated by heating the bath gas. The latter experiment represents a case in which ion activation is effected by accelerating the bath gas rather than electrically accelerating the ion. The two approaches are equivalent in terms of activating the parent ion but can have important differences in the appearance of the final product ion spectrum. A variety of interesting and significant implications regarding optimal means for activating relatively small, highly stable ions and for activating very large ions have become apparent from this work and will be discussed.