

Fundamental Studies Involving Collision-Induced Dissociation Of Strongly Bound Metal Oxide Ions In Quadrupole Ion Traps

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Historically, studies involving collision-induced dissociation (CID) in quadrupole ion traps (QIT) have focused on the fragmentation and structural elucidation of organic and biological ions. To better understand collisional activation in the QIT we have focused much of our attention at ORNL to the opposite extreme of the mass range, viz, diatomic ion dissociation.¹ The use of helium as the collision bath gas (as is most common) restricts the strength of a bond that can be dissociated via CID. This limit² is around 400 kJ mol⁻¹ and stems from a combination of the maximum ion kinetic energy that can be reached and the limited collision energy that can be converted to internal energy with the light collision gas, helium. Recently, conditions have been elucidated in which very strongly bound species can be dissociated in QITs via CID.³ Using neon as the collision (bath) gas and high q_z trapping conditions the CID rate for strongly bound metal oxide ions has been as large as 100 sec⁻¹ with complete retention of the product metal ions where required.³

These fundamental studies recently allowed the determination of absolute bond dissociation energies from the dissociation rate of metal oxide ions.⁴ For these small diatomic systems mass is found to greatly influence the rate of CID, such that two isotopes of a given metal can have measurably different CID rates at the same excitation voltage. It is the ability to correct for these mass effects that makes possible the determination of bond dissociation energies from the CID rates.

When operating at high q_z (0.67) considerable kinetic energy can be imparted into an ion without any observed scattering. This has enabled experiments to be performed whereby strongly bound metal oxide ions are dissociated via CID while atomic metal ions at the same nominal mass are kinetically excited but not scattered. We provide evidence that the CID of diatomic ions in the presence of atomic ions can be highly beneficial in plasma source mass spectrometry where isobaric interferences often hamper quantitative analyses. With an understanding of the conditions that are optimal for conversion of kinetic energy to internal energy we have been able to implement a mass scan function that allows CID to be deliberately performed while the mass spectrum is being acquired.

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