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In situ collisional dissociation in a selected-ion flow tube: a novel, inexpensive SIFT–CID operation

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Abstract

A selected-ion flow tube (SIFT) apparatus has been adapted for collision-induced dissociation experiments. Ions selected from an ion source upstream in a flow tube, or generated by chemical reaction midstream, and then thermalized to 294 $\pm$ 3 K by collisions with He or Ar buffer gas atoms at 0.35 $\pm$ 0.01 Torr are subjected to multi-collision-induced dissociation (CID) with He or Ar atoms just before sampling. CID is achieved by raising the potential of the sampling nose cone from 0 to -80 V. This simple and inexpensive, yet novel, CID operation has been tested on a wide range of molecular ions ranging in complexity from simple diatomic and polyatomic ions to multiligated and solvated ions and even to doubly charged derivatized C_{60} cations. The bond energies of the dissociated ions were as large as approx. 100 kcal mol^{-1}. The CID technique was found to be useful for the determination of bond connectivities in reactant and product ions, for distinguishing between isomeric ions and for the elucidation of dissociation and reaction mechanisms involving doubly charged derivatized fullerene ions. Although an attempt was made to correlate measured CID thresholds with known bond energies, the CID technique was found to have only limited application in the determination of absolute or relative bond energies, given our current understanding of its theory of operation.

Keywords: Bond connectivities; Cations; Collision-induced dissociation; Selected-ion flow tube

1. Introduction

Since its inception in 1976 by Adams and Smith [1], the selected-ion flow tube (SIFT) has provided a powerful and marvellously versatile mass spectrometric technique for the investigation of the kinetics and energetics of reactions of ions with molecules. The versatility of this technique has been advanced further by various modifications designed to probe the structure and stability of reactant and product ions using collision-induced dissociation (CID). For example, in 1992, Squires [2] added a triple-quadrupole mass spectrometer after the sampling nose cone for CID studies of sampled ions. More recently Lindinger and his colleagues [3] have operated a conventional selected-ion flow drift tube (SIFTDT) for the determination of rate coefficients for collisional dissociation. Here we propose a new and inexpensive mode of operation of a conventional SIFT apparatus [4,5] for multi-collision CID studies of ion structures and energetics. It involves simply biasing the

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