International Journal of Mass Spectrometry 215 (2002) vii–viii
www.elsevier.com/locate/ijms

Preface

Detectors and the measurement of mass spectra

A glance at many commercial and research mass spectrometers often reveals a wealth of ingenuity, technology and multidisciplinary know-how invested at the detection end of the instrument to enable high efficiency and high data quality. Nevertheless, detectors are frequently the performance bottleneck in mass spectrometry and detector research is an often-neglected multidisciplinary area playing only a supporting role in miscellaneous research projects. This special issue of IJMS should help to consolidate the advances in detector research and show where we came from and where we are going at a time when technology is allowing increased activity in detector development. There are potentially large benefits from a cohesive area of detector research in mass spectrometry. I was very pleased when Gareth Brenton suggested this volume and I was asked to be guest editor.

The detector research community could be divided into two groups:

(a) those whose primary interest is the detectors and the measurements;
(b) those whose primary interest is the science they can do with the detectors.

Both groups are represented in the present volume. The view is taken that detection and measurement involves electron multipliers, all detector instrumentation and data processing on an equal footing. Papers in this volume cover both terrestrial and space applications and include cryogenic detection which offers unique capabilities, for example, in the detection of very heavy molecules or charged particles.

Ionization of molecules makes them both separable and detectable. The function of the detector is to measure the ions but unfortunately all such measurements are imperfect and may not even be easily reproducible. Why are measurements of mass spectra imperfect? The detector itself should ideally do no more nor less than reveal what is incident on it but ‘exact’ measurement of the incident spectrum would require very high resolving power and dynamic range. Detector performance is limited in a way which depends on the specific detector and these are of many types distinguishable by their physical structure (single slit, arrays of various types including one- and two-dimensional arrays, FT-ICR, etc.), sensing strategy (analogue, event counting, integrating, etc.), dispersion coordinate (time, space, frequency), mass range (low mass, very high mass) and other characteristics. Similarly, electron multipliers of various types are a vital part of many detectors in mass spectrometry, and their performances are central to the measurement of mass spectra. In addition, there are important issues connected with the interpretation of measurements made. For example a single ion incident on a MCP may be registered by more than one detector of an array. Is this a problem or an advantage? Should the area under a peak or the peak height be taken? Is the measured spectrum a convolution of the incident spectrum with a single detector function?

At first sight it may appear that the solution to detection and measurement problems lies simply in better

1387-3806/02/$20.00
PII S1387-3806(02)00540-7

quality, more stable, faster electronics, better electron multipliers, etc., but this is only part of the story. There are broad issues of the best operating conditions, intriguing questions in data processing, problems of non-linearity of electron multipliers at high incident intensities or for high mass ions, non-uniformity of detector arrays, etc. Detection and measurement is a highly important multidisciplinary research area since detectors often hold the key to large performance increases, but because no detector can be perfect, the limitations must be understood in order to optimize the measurement conditions and deconvolute the data. There are numerous impediments to the accurate measurement of a mass spectrum and researchers converge on these problems from many directions. Since no detectors are perfect, questions arise of the relation of the measured data to the information required. Modeling and data processing to recover the incident spectrum may therefore be regarded as a vital part of the measurement process. Probabilistic methods and maximum entropy occupy an important place here.

For the present purposes the front-end of the mass spectrometer may be regarded as the part of the instrument which prepares the ions for measurement and as already mentioned the detector consists of all parts of the mass spectrometer from the entrance aperture for a single detector, the MCP front face (for a detector array), the STJ or microcalorimeter of a cryogenic detector, or the ion trap for a FT-ICR ion trap, up to the data acquisition and storage system. The latter must be included since data capture is an essential part of the measurement process. A great deal of effort has resulted in ‘front ends’ which produce spectra with a high information content (highly resolved spectra of high intensity) but this increases the need for more advanced detectors, data acquisition, data processing, etc. If an expensive mass spectrometer has taken many man-years to develop, the value of a detector system which does not limit its performance is evident.

This volume concerns the detection of ions. Research and development of detectors for other particles such as electrons, X-rays and UV frequently overlap since there are similar forces driving detector development in these areas such as the need for parallel detection, increase of the resolving power, dynamic range, uniformity, linearity, robustness, etc. Also the need for instrumentation in space research necessitates low size, weight and power consumption and this can impact on terrestrial instruments. Since detector research is underpinned by similar enabling technologies (e.g., silicon technology, packaging, interconnect), then advances in these technologies tend to influence all areas of detector research. Synchrotron users are currently driving initiatives for more detector support since third generation synchrotrons are being built with large output fluxes placing severe demands on detector performance, particularly in the life sciences. Within this community the needs of those measuring electron energy spectra will be included. To some extent mass spectrometry interests are represented by those measuring electron energy spectra since at least in the case of spatial dispersion the needs are very similar. Some of the technologies which will emerge will be generic and mass spectrometry should benefit, for example, in fast data acquisition and processing methods. Spatial dispersion is only one of the means of dispersing ions in a mass spectrum but in electron energy spectroscopy, and UV and X-ray spectroscopy, the dominant dispersion means is spatial and therefore it can be expected that detector array research will be very active.

An identifiable detector research community in mass spectrometry could minimize the dissipation of know-how, maximize potential and provide support, especially to new research students entering this multidisciplinary area. It is hoped that this volume will help in consolidating the achievements of detector research and raise the profile of this exciting area.

Keith Birkinshaw
Physics Department, University of Wales
Aberystwyth, Ceredigion, SY23 3BZ, UK