The Important Peak Index of the Registry of Mass Spectral Data

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John Wiley and Sons, Inc., New York
[Phone: (800) 526-5368; Fax: (201) 302-2300],
3 Volumes, 4,057 pp.,
ISBN #0-471-55270-4, 1991, $750.00

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This is a three-volume set of books containing a tabulation of the six "most important" peaks of the 136,141 different mass spectra of 115,917 compounds contained in the *Wiley/NBS Registry of Mass Spectral Data*. Spectra are listed by the mass-to-charge ratio of each of the three "most important" peaks in a manner similar to that of the *Eight Peak Index*. What differentiates these volumes from its parent publication and from the *Eight Peak Index* is that the peaks listed have been chosen on the basis of their statistical importance rather than just on their relative abundance. To determine the statistical importance of the peaks, the authors have used the same algorithms as they have employed in their "Probability Based Matching" system. This approach reduces the reliance on relatively common ions, such as m/z 43, for identification.

To determine the "most important" ions, both the statistical importance of the mass as well as the relative abundance is considered. The statistical importance or uniqueness, U, of an ion is based on the inverse of the probability of occurrence of the peak in the Registry database. Thus, an ion such as m/z 43, which has a high probability of occurrence, will have a low (zero) U value while ions with low probability of occurrences will have high U values. The relative abundance of a mass, A, is factored in on the basis of the inverse of the probability of occurrence of an ion with that relative abundance. Thus, ions of high relative abundance occur much less frequently than do ions of low relative abundance and, therefore, receive a higher A value. The ions with the highest $A + U$ values are defined as the most important ions. Each page of the volume has a listing of the U and A values to be used in determining a peak's importance. Although, at first glance, it appears that this approach may be difficult to get used to, the "important peaks" tend to be those peaks that a trained mass spectrometrist would pick. I found the system to be relatively simple to use after only a few applications.

The utility of the volumes, however, must rest on how well unknowns can be identified. I tested this by trying to identify a number of spectra that were in my files, including some that have been reported and some that have not appeared in the literature or a data-base. The identity of compounds whose spectra have been published were accurately, rapidly, and easily identified. Not surprisingly, compounds whose spectra have not been reported were more difficult to identify. In some cases, the identities of compounds whose spectra contained similar "most important" ions were of little help in identifying the unknown. In other cases, these identities were quite useful in establishing the general class of compound. Interestingly, the "most important" peaks of steroid metabolites often led to listings in which steroids predominated.

In summary, this index is a useful adjunct to the Registry database, especially as the location in the Registry database is given for the full spectrum of each listing. It will be an important tool for the identification of unknowns based on their mass spectra and can be quite useful in interpreting the spectra of true unknowns. Although the set may be too expensive for individual purchasers, I expect that these volumes will be found in most laboratories that deal with the interpretation of spectra.

Mass Spectrometry

E. Constantin and A. Schnell
Ellis Horwood Ltd., Chichester, UK
[Phone: 0442 231555; Fax: 0442 275115].
184 pp., ISBN #0-13-555525-6 [hardcover, $79.95],
#0-13-553363-5 [paperback $29.95], 1991.

Book review by M. M. Bursey,
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This textbook is a translation by Dr. M. H. Chalmers of a French text first published in 1986. It includes a whirlwind tour of the subject. It might be considered as a text for a brief course on the major topics in mass spectrometry, or it might be used by someone trained in another field of the chemical sciences as a way to read into our field. The subjects of the chapters are mass spectrometry; methods of ionization; classical electron impact ionization source; methods for sample introduction; the mass analyser; methods of display, recording, and processing of signals; types of ions, peaks, and mass spectra; nominal mass and exact mass; analysis of carbon isotopes; metastable ions; ion-molecule reactions; ion clusters; special sources; applications of mass spectrometry in atmospheric investigations; theory of spectra; ion fragmentation mechanisms; isotopic analysis; and recent developments. The average chapter is nine pages long.

As a course textbook, it is too condensed. (Interpretation of mass spectra is covered in half a page, for example.) However, as it flits from topic to topic, it spends just enough time on most topics to make stu-

1044-0305/93/$5.00

dents aware of the existence of ongoing intellectual activity in each area. In addition to the references cited for each chapter, suggestions for further reading are given for the last ten chapters, and there are a one-page general list of reviews and articles of interest and a two-page general bibliography.

To my knowledge this book is unique as an introduction to so many topics for a survey course. So it might be used, for example, in conjunction with a more thorough introduction to spectral interpretation, together with distributed notes to fill out the teacher's own preferences for detailed consideration. The section on special sources would have to be amplified on the developments in matrix-assisted laser desorption and in electrospray that have occurred since 1986, for example.

There are just enough typographical errors to notice.