and its natural inhibitor are identical within the statistical errors.

Calculation of Hausdorff Mass for Parts of a Surface. In a third series of calculations the contact area of trypsin with BPTI was analyzed along the lines described above. The average Hausdorff mass $\bar{M}$ (see eq 3) was now determined for all surface points of the contact area (as calculated from the structure of the trypsin–BPTI complex). It turned out that the concept of self-similarity holds reasonably well for the surface area of trypsin centered around residue Ser-190 [$D = 2.226 \pm 0.011$ (eq 1)], $D = 2.259 \pm 0.018$ (eq 2) and for the one of BPTI around residue Lys-15 ($D = 2.116 \pm 0.021$ and $D = 2.045 \pm 0.041$, respectively) but that the fractal dimensions of both areas are different. While the fractality of the binding region of trypsin is higher than the average dimension of this molecule, the corresponding value in BPTI is smaller. From this result it seems to be questionable whether the local fractality of a surface area can be used as a guideline for the identification of receptor sites or preferential locations for protein–protein interactions. This latter statement is supported by the fact that there are surface areas of the BPTI (close to residue Ala-40) which have nearly the same D-value [$D = 2.237 \pm 0.007$ (eq 1)] as the trypsin inhibitor site but are far away from the contact area. The same is true for the trypsin molecule. We found an area (close to residue Ser-110) with the low value $D = 2.144 \pm 0.003$ (from eq 1), which is very close to the fractal dimension of the BPTI-binding region.

CONCLUSION

We have demonstrated that the Hausdorff mass approach is well suited for the systematic study of the surface complexity of proteins. Surfaces of proteins do show self-similarity, which is a global statistical information. This fact is relevant for the study of transport phenomena of substrates from the bulk phase to the surface as well as parallel to the surface.[1,2] The concept of fractals can also be applied to the study of selected surface areas (like the trypsin–BPTI interaction site), but it is only of minor importance for the identification of such sites. The biological key and the lock may have different fractality even when there is a highly specific interaction.

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Registry No. BPTI, 9087-70-1; lysozyme, 9001-63-2.

REFERENCES AND NOTES

(1) Pfeiffer, P. *Appl. Surf. Science* **1984**, *18*, 146–164.
(2) Pfeiffer, P.; Welz, U.; Wippermann, H. *Chem. Phys. Lett.* **1985**, *113*, 535–540.
(3) Lewis, M.; Rees, D. C. *Science* **1985**, *230*, 1163–1165.
(4) Aqvist, J.; Tapia, O. *J. Mol. Graphics* **1987**, *5*, 30–34.
(5) Farin, D.; Peleg, S.; Yavin, D.; Avnir, D. *Langmuir* **1985**, *1*, 399–407.
(6) Mandelbrot, B. B. *The Fractal Geometry of Nature*; Freeman: San Francisco, 1982.
(7) Feder, J. *Fractals*; Plenum Press: New York, 1988.
(8) Connolly, M. *J. Appl. Crystallogr.* **1983**, *16*, 548–558.
(9) Mattila, P. *Ann. Acad. Sci. Fenn.* **1975**, *1*, 227–244.
(10) Zachmann, C.-D.; Brickmann, J., manuscript in preparation.
(11) Heiden, W.; Schlenkrich, M.; Brickmann, J. *J. Comput.-Aided Mol. Des.* **1990**, *4*, 255–269.

COMPUTER SOFTWARE REVIEWS

Spectrochimica Acta Electronica[1,2]

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Spectrochimica Acta Electronica is an unusual product, a computer-readable supplement to a printed journal, *Spectrochimica Acta*. Pergamon Press is to be commended for this interesting experiment in electronic publishing. Spectrochimica Acta Electronica, otherwise known as Part B of *Spectrochimica Acta*, contains data or programs that are intimately associated with papers published in the printed section of the Journal.

The first issue of this new section, Volume 46B of *Spectrochimica Acta*, appears as 3 disks which are related to two papers in Part A of the Journal. The first paper, entitled Simulation of Atomic Spectra. I. Profiles and Signal-to-Background Ratios of 350 Prominent Lines Emitted from an Inductively-Coupled Plasma or "Whatever" Customized Atomic Emission Lines appears in hard copy with an appendix and also a $3^1/_2$ in. diskette containing a program, data files, and a manual. The printed text details the purpose of the work, with emphasis on its spectroscopic aspects, and the appendix provides the information needed to access the diskette and make use of the program and data. Additional tutorial guidance is in the manual which is on the diskette.

The program concerns primarily simulation of the 350 prominent lines derived from 65 elements in an inductively-coupled plasma as a function of the spectral bandwidth of the spectrometer and the Doppler temperature of the source. A spectrum is displayed as a function of wavelength in terms of (SBR + 1), where SBR is the signal-to-background ratio. A spectral window of 80 ppm is covered. In addition, the spectral data that are displayed encompass, inter alia, the SBR and background equivalent concentration (BEC) in the maxima of the spectral structure, the full width at half-maximum (FWHM) of the peaks, the standard values of SBR and BEC, and the detection limit. The main purpose of the program that is provided is to facilitate the conversion of data on SBRs, BECs, and detection limits from instruments of different spectral bandwidth and thus to allow unbiased comparisons

between different inductively coupled plasmas or between ICPs and other sources.

The database covers both simple lines and complex HFS composites, and the authors claim a vast improvement in the data as a result of the interactive development of the program and the database. Relevant studies and the development and testing of various models for handling HFS composites are detailed in the hard copy. These studies may be reworked using the program and an additional small dedicated database.

The tutorial section of the manual provides elementary instructions for the practical use of the program and incorporates a variety of instructive examples, as well as a brief "course" on spectral line profiles. the approach leaves many possibilities for the customization of spectral lines because both the data for the individual spectral lines and the "umbrella" files for all lines grouped in a database have a simple, transparent organization. Users may easily add customized files to the existing databases or generate new databases for any purpose.

The second paper, Spectral Data Base for the Identification of Fibers by Infrared Microscopy, is a hard-copy text accompanied by a $3^1/_2$ in. diskette containing data files and the text of the paper, the latter in both WordPerfect 4.2 and ASCII formats. The article discussed the spectroscopic aspects of fibers and explains the purpose of the data files.

The work deals with the infrared spectra of single synthetic fibers, obtained rapidly, and with minimal sample preparation, by infrared (IR) microscopy. An IR spectral library of 53 polymer fibers was constructed, the spectra entered in the format defined by the Joint Committee on Atomic and Molecular Physical Data (JCAMP-DX).[2] The chemical subclass of the fibers which, with the exception of nylon, is unknown can be identified in the first two cases I tried by a computer search which uses an absolute derivative search algorithm.

With both papers I was able to load the disks and use the computer-readable files easily. I was able to install and run the program from the first paper, for example, on my AST 486/33 computer (VGA graphics) with no difficulty.

Overall, I find this a fascinating product, which could lead to an improvement in the quality of papers in this journal and other journals. If authors use this mechanism to submit papers along with supporting data and programs, it will be much, much easier for others to check such research work as well as to extend the findings. Extrapolation of this idea could lead to a much more valuable scientific literature in this age of computerization. Pergamon Press and its senior editorial director for the physical sciences, Dr. Peter Shepherd, have chosen well in using this journal as the harbinger of possible things to come. For those in the field of spectroscopy, this journal is well worth looking at.

REFERENCES AND NOTES

(1) *Spectrochimica* Acta, Pergamon Press plc, Headington Hill Hall, Oxford, OX3 0BW U.K. Telephone 44-865-794-141. The current annual price of the entire journal, including the SAE section, is DM 1560.
(2) McDonald, R. S.; Wilks, P. A. JCAMP-DX: A Standard Form for Exchange of Infrared Spectra in Computer-Readable Form. *Appl. Spectrosc.* **1988**, *42*, 151–155.

BOOK REVIEWS

The Index and Abstract Directory: An International Guide to Services and Serials Coverage. 2nd ed. EBSCO Publishing: Birmingham, AL. 1990. 2784 pp. $179.00. ISBN 0-913956-50-3.

EBSCO is a serials vendor. As have other serials vendors, EBSCO has developed an extensive database of titles which they supply. *The Index and Abstract Directory* provides a reference source to locate all serials in the database that are covered by one or more abstracting or indexing services.

The first major section is a listing of serials (periodicals, newspapers, and monographic series) arranged alphabetically by subject category. (The "Chemistry" section of this part occupies just over 30 pages.) Full bibliographic information is given for each title. The last part of each entry in this section is the list of index/abstract services which include the title in their coverage. The basis on which the titles were selected for inclusion in this section has to be questioned. For example, the "Chemistry" section includes about a dozen titles in the *CA Selects* series of current awareness publications. There are over 200 titles currently in the *CA Selects* series, and all contain abstracts derived from *Chemical Abstracts*. *The Index and Abstract Directory* inaccurately lists *Chemical Abstracts* as covering the titles. On the other hand, the only entry for *Molecular Crystals and Liquid Crystals* is on page 253 with a note that it has ceased. No mention of the current incarnation of the journal is found, despite the fact that we just received a note from the publisher (Gordon & Breach) that the full 1992 subscription for *Molecular Crystals and Liquid Crystals Science and Technology* will cost $7,781.06! One can find such entries as *Revista Cubana de Quimica* and *Vitreous Enameller* in the "Chemistry" section, however.

The second major section is Index and Abstract Service Title Listings, including over 700 services with complete bibliographic information on each service. "A list of all serial titles covered by each service also appears under the index/abstract listing." The Entry for *Chemical Abstracts* occupies about 44 pages with approximately 8500 entries (titles only) for the serials covered by *CA*. A spot check of a number of those titles in the Alphabetical Title Index, the third section of the work, found all of the titles referenced to the pages on which the full bibliographic information is located in the first section. There is also an ISSN Index which leads to the entries in Section 1 and a section which lists Index/Abstract Services by Subject Classification. The "Chemistry" section of the latter includes only 10 services. Not found on the lists are such specialized works as *Chemoreception Abstracts*, *Chromatography Abstracts*, and *Methods in Organic Synthesis*.

For a work of this type to be very useful in a broad range of library settings, some serious analysis of the relative rankings of the primary journals in various disciplines should precede its compilation. The day is long past when librarians will rotely select every title which is included in a given abstracting or indexing service's list of serial titles covered. The EBSCO product is useful for purposes of comparing which titles are included in more than one service's profile. However, most librarians consider many other factors before deciding to place a subscription nowadays. Nevertheless, for a library which cannot afford to buy *Chemical Abstracts Service Source Index* (*CASSI*), *The Index and Abstract Directory* might be a reasonable alternative.

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Technology Transfer: The Role of the Sci-Tech Librarian. Edited by Cynthia Steinke. Haworth Press: Binghamton, NY. 1991. 172 pp. $22.95. ISBN 1-56024-116-0.

The contributors expand the definition of technology transfer to encompass the process of taking technical knowledge, ideas, services, inventions, and products from their originator to a potential user. It is not limited to communication between developed countries and the Third World. Each author provides unique definitions, explanations, and illustrations of the concept. The volume, also published as *Science and Technology Libraries*, Volume 11, Number 2, evaluates the role of the information specialist in the technology-transfer process.

Specific topics considered include information needs and communi-