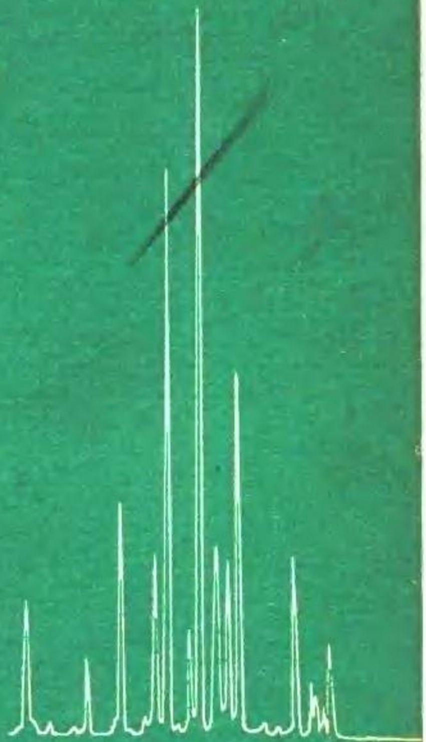

DEVELOPMENTS IN APPLIED SPECTROSCOPY

Volume 2

Proceedings of the
Thirteenth Annual Symposium on Spectroscopy
Held in Chicago, Illinois
April 30 - May 3, 1962

edited by

J. R. Ferraro and J. S. Ziomek

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PREFACE

For the last thirteen years, the Chicago Section of the Society for Applied Spectroscopy has sponsored a symposium in the spring of each year. In this span, the symposia have shown a steady increase in attendance, in the number of papers presented, in the number of sessions, and in the number of days the conference lasted. The duration of the most recent symposium was four days, with sessions devoted to molecular spectroscopy, including infrared, Raman, ultraviolet, and visible, and to X-ray, NMR, emission, and flame spectroscopy, respectively, with a special session devoted to gas chromatography because of its growing interest in applied spectroscopic work.

Another feature of this last symposium was the attempt on part of the Symposium Committee to establish and maintain the scientific level at that of applied physics. This should place the present symposium at a level somewhere between that of the Ohio State symposium and that of the Pittsburgh meeting, thus approaching the level of applied chemical physics.

In addition, the symposium was designed to offer to scientists from other disciplines and students an opportunity to attend introductory panels and lectures and at the same time the mature investigators a meeting ground and the chance to keep abreast of the latest developments in spectroscopy. How well these aims have been accomplished is best attested to by the phenomenal growth of the symposium.

In 1961 the first attempt was made to publish the proceedings of these symposia. The result was Volume 1 of "Developments in Applied Spectroscopy." This book is Volume 2 in this series and contains 41 papers in the various areas of spectroscopy discussed at the 1962 symposium. The contributors to this volume are some of the country's leading spectroscopists. The distribution of the topics is based on the organization of the symposium program.

The symposium and the proceedings would not have been possible except through the tremendous effort of the Symposium Committee. We wish to acknowledge the contributions of Jay A. Sheinkop, William J. Driscoll, Edward A. Piotrowski, John Danaczko, John P. Kapetan, Elma Lanterman, John E. Forrette, Robert J. Manning, Stuart Armstrong, and Miles Schwartz. In particular, we wish to give special thanks to Dr. Lanterman and Mr. Forrette for reviewing several of the manuscripts pertaining to X-ray spectroscopy and gas chromatography that appear in these proceedings.

John R. Ferraro
Argonne National Laboratory
Argonne, Illinois

Joseph S. Ziomek
Martin-Marietta Corp.
Orlando, Florida

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INFRARED AND RAMAN SPECTROSCOPY

WORLD-WIDE COMMUNICATION OF SPECTROSCOPIC INFORMATION

Forrest F. Cleveland
Illinois Institute of Technology
Chicago, Illinois

There are hundreds of thousands of spectroscopists in the world, and they carry out tens of thousands of investigations and obtain hundreds of thousands of dollars worth of results, but the potential value of all this effort is largely lost because of an archaic and ineffective means of communication of these results.

If spectroscopy is to make its maximum contribution, efficient and effective methods must be devised for the rapid diffusion of new information throughout the domain of spectroscopy, and for the retrieval of the older information buried in the literature.

THE LANGUAGE PROBLEM

The first difficulty encountered is, of course, the language problem. According to a study made by UNESCO, scientific results are published in at least 34 languages, but half of the value is lost because half of the scientists cannot read the articles in the language of publication; for example, 50% of the results are published in English, but 50% of the world's scientists cannot read English.

At first thought, translations might seem to be the answer. But translations are slow, costly, often erroneous, and for the most part unobtainable. In fact, most of the articles are never translated, and it would obviously require enormous effort and expense to translate material from each of the 34 languages into each of the other 33.

What is needed is an interlanguage which would be the common denominator of those half dozen European languages in which the scientific vocabulary largely originated, and which would be readable at sight by any scientist who has a knowledge of one or more of these languages. Since the scientific vocabulary has now spread throughout the world, such an interlanguage would be quite suitable for world-wide communication. Fortunately, an interlanguage of this type already exists in Interlingua, which appeared in 1951 after 27 years of research and development.

"SPECTROSCOPIA MOLECULAR"

Impressed by the ease of reading Interlingua and convinced of the necessity of doing something to improve the transmission of spectroscopic information beyond the language barriers, I decided to begin the publication in Interlingua of a small periodical, called "Spectroscopia Molecular," in my own field of research. The first issue was mailed, by a strange coincidence, exactly 10 years ago today, on May 1, 1952. The use of Interlingua assured the easiest readability by the greatest number of spectroscopists.

"Spectroscopia Molecular" now goes to 400 spectroscopists, laboratories, and libraries in 31 countries. The periodical has supported itself by subscriptions and advertisements, and now has a reserve sufficient to guarantee publication for a year in advance. If more than this is received, it is used to improve the periodical.

"Spectroscopia Molecular" contains brief reports of new research results, summaries of significant articles, reports of spectroscopic meetings, reviews of new books, a calendar of future spectroscopic events, details of new instruments, news about spectroscopists, and other news and information of interest and value to workers in this field. The emphasis is on new developments and on keeping the spectroscopists up to date.

Experience with this periodical during its first ten years of monthly publication provides convincing proof of the usefulness of Interlingua for world-wide communication.

THE CENTRAL LIBRARY

The Society for Applied Spectroscopy itself, through the dedicated effort of Theodore H. Zink, Chairman of its International Activities Committee, is using Interlingua in its Central Library for Spectroscopy (212 Chestnut Hill Drive, Ellicott City, Md., U. S. A.). This library, as one of its services, publishes twice a month the periodical, "Titulos Spectroscopic," a complete list of titles of current spectroscopic books or articles. These titles are sent to the library by spectroscopists in all parts of the world. They are then translated into Interlingua by the Interlingua Division of Science Service (80 E. 11th St., New York 3, N. Y., U. S. A.) and are published within one month after their appearance in the original journal. The language of the article is indicated. If the spectroscopist can read the language, a reprint may be obtained from the author, or a photographic copy of the article can be obtained from the library. If not, an Interlingua translation of the abstract or complete article can be obtained. For faster service, the library is collecting reprints of all spectroscopic articles, and expects soon to be able to prepare lists of references on specific topics.

This service enables the spectroscopist to know what articles are being published and to obtain quickly a copy of any article in a language he can read. Keeping up to date is thus no longer such a formidable task. Spectroscopists are indebted to the Society of Applied Spectroscopy for providing this useful service.

MULTILINGUAL DICTIONARY

Another use of Interlingua is in a "Multilingual Dictionary for Spectroscopy" I am preparing in collaboration with Associate Editors Bonino (Bologna), Dupeyrat (Paris), Matossi (Freiburg), Morcillo (Madrid), Stammreich (São Paulo), and Wolkenstein (Leningrad); Advisory Councilors Herzberg (Ottawa) and Mulliken (Chicago); and Linguistic Editor Gode (New York). In this, a complete list of spectroscopic terms will be given, each one followed by a concise and correct definition in Interlingua. Under this will be given the corresponding terms in English, Spanish, French, German, Italian, Portuguese, and Russian.

The dictionary will be the equivalent of 21 bilingual dictionaries, and its existence will have a tendency to standardize international usage, which in turn will facilitate world-wide communication in spectroscopy. (Dr. F. O. Holmes, of the Rockefeller Institute for Medical Research, is preparing a similar dictionary for virology.)

ABSTRACTS IN INTERLINGUA

Next to the medical workers, who are using Interlingua for abstracts in 25 of their journals and who have used this interlanguage in the programs of a dozen international meetings, the spectroscopists are the ones who have shown the greatest initiative in the improvement of communication in their field. A natural next step would be the use of Interlingua in the programs of international spectroscopic meetings and for abstracts in the spectroscopic journals. This would extend the range and usefulness of the programs and journals.

CONCLUSION

The spectroscopist can now read about new developments in "Spectroscopia Molecular" and read the titles of all recent articles in "Titulos Spectroscopic." If any article is important for his work, he can quickly get a copy of it, in a language he can read, from the "Central Library for Spectroscopy."

Soon he will be able to find the exact meaning of any unfamiliar term, and the corresponding expression in eight languages, by reference to the "Multilingual Dictionary for Spectroscopy."

Soon, too, he will be able to extract the essence of programs and articles in unfamiliar languages by reading the accompanying Interlingua abstracts.

When these instruments have been developed to perfection, long strides will have been made toward the improvement of world-wide communication in spectroscopy.

METHODS OF STORING, RETRIEVING, AND CORRELATING INFRARED SPECTRAL DATA

Freeman H. Dyke, Jr.

Jonker Business Machines, Inc.
Gaithersburg, Maryland

For analytical chemists, retrieval and correlation of data has always been a major problem. Finding a real solution could greatly reduce the amount of valuable time now necessary for qualitative and quantitative analyses, and enable the correlation of spectral data with chemical, physical, and biological properties. In other words, an effective data retrieval and correlation technique would make analytical chemistry an even more valuable research tool.

The purpose of this paper will therefore be to examine more closely both the problem and the currently used or available solutions for the retrieval of infrared spectral data. This examination will consist of:

1. Defining the ideal data processing equipment for meeting the needs of the analytical chemist.
2. Examining the four methods now most widely used.
3. Describing a fifth and entirely new technique known as "Termatrex."
4. Summarizing a trial evaluation of Termatrex equipment for handling infrared spectral data, conducted by the American Society for Testing Materials.
5. Describing the Termatrex index for X-ray diffraction data as authored by the American Society for Testing Materials and produced by Jonker Business Machines.

Examining the parameters of the ideal retrieval system for spectral data, we find it should tell the chemist exactly which compounds are present and furnish a quantitative analysis of an unknown. To date, however, the ideal equipment has not been developed. Nevertheless, we may reasonably expect to find in equipment today at least the following features:

1. Speed in output—A search of collections of up to 250,000 compounds should take only a few minutes.
2. Flexibility of vocabulary—The system should be able to absorb an unlimited number of characteristics. This feature would enable the chemist to search by combinations of functional groups, by analytical data of all types, and by chemical, physical, and biological properties.
3. Flexibility in output—The searcher should receive instantaneous feedback from his data retrieval equipment. Only when he does can he employ the detective-like technique of question—answer, question—answer, question—answer so often necessary in a search of spectral data.
4. Immediate availability—The chemist should have direct access to his data retrieval systems, preferably by having the equipment located right in the laboratory.
5. Direct access to information—After completing a search, the chemist needs direct access to the detailed information on those chemical compounds found to meet the requirements of the search questions.
6. Low cost—The equipment should be priced within the means of most analytical laboratories around the world.

The four data retrieval techniques currently in use are the manual index, the edge-notched card, the punched card, and the computer. Let us now examine the advantages and disadvantages of each of these techniques individually.

Probably the oldest of the data processing methods is the manual index. Examples are the "Sadtler Spectra Finder" for infrared data and the "Fink Index" for X-ray diffraction data.

The manual index is generally an inverted system, in which all data on those compounds having a given characteristic are grouped on a page dedicated to that characteristic. The advantages of the manual index can be summed up as follows:

1. At present, this is the least expensive means of organizing and disseminating an index.
2. After completing a search, the chemist has direct access to the name, and as a rule to some summary information on the compounds meeting the requirements of the search questions.
3. The manual index can be kept in the laboratory where it is immediately available for use.

There are, however, some disadvantages of using a manual index for retrieving and correlating data. Among these disadvantages are:

1. The limitation of having to restrict the search to one or possibly two characteristics at a time. Even when the data are organized in a table format, it is relatively difficult to search for even as few as four characteristics in one operation.
2. The difficulty of performing a search when there are a large number of items to be scanned and a great many items listed under each characteristic.
3. The impossibility of performing negative searches, a screening technique recognized as one of the most valuable methods of conducting a search.
4. The difficulty of keeping the index current. When new compounds are added to the manual index, the entire system must be updated.

The second method currently in use for storing and retrieving data is the edge-notched card. At one time or another, this system has been applied to most forms of spectral data.

In this system, a separate edge-notched card is allotted to each item in the data collection. These cards may vary in size from three inches to two feet on each edge. The characteristics of the item are coded around this edge by notching.

A search of the system is performed by slipping long needles through the area of the card edge representing the characteristics in the search question and shaking the needles. Those cards which fall off the needles are the items meeting the requirements of the search question. The advantages of the edge-notched card system for data retrieval are as follows:

1. Direct access can be supplied to a microfilm or reduced copy of the spectrum itself as well as to summary information on the compound. This direct access is the major advantage of this method of retrieval.
2. Updating the system is quite simple because new cards can be disseminated to use whenever new compounds are added to the data collection.
3. Direct availability to the chemist is possible because the edge-notched card index can be kept in the analytical laboratory.