example uses, and future course of development of the University of Tokyo Information Retrieval System. It was interesting to learn that the computer centers at the Japanese universities, in contrast to those in the United States, are principally devoted to the support of research and are largely staffed by scientists. S. Fujiwara described potential sources of errors in information retrieval systems. S. Heller (Environmental Protection Agency) and G. W. A. Milne (National Institutes of Health) described the NIH–EPA World-wide Chemical Information System which consists of 18 large databases. Y. Yoneda (Faculty of Engineering, University of Tokyo) described an information retrieval system for the retrieval and correlation of physical properties of organic molecules and the estimation of physical properties of other molecules from similar molecules, component functional group, and the like in the database.

The syllabus, approaches, and educational problems of a short course on computer-based instrumentation were discussed by R. E. Dessey.

Again, all the participants expressed the need for expert technical assistance in computer hardware and software in the chemical laboratory which is common in industrial and governmental laboratories. Several examples were given to illustrate how chemistry departments profit by the addition of full-time computer scientists. It was felt that this need will become more apparent in the future as it is anticipated that computer centers in universities will decentralize as size and costs of the large computers shrink. However, it was again apparent that in most university laboratories, the administration is not enthusiastic about creating such appointments in chemistry, and that the interaction and communication with personnel in other departments and especially computer service groups was difficult.

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The Role of Chemical Information Science in Computer-Assisted Chemical Research†

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The essential role of chemical information science to the design of chemical research via computer is illustrated with subject indexes, notation systems, correlation methods, and on-line databases.

Chemical information science has become an integral component of computer-assisted chemical research planning and design.[8-16] Other components, in addition to mathematics and statistics, include computer science and the application of techniques such as artificial intelligence and pattern recognition.[1-6,18] Whereas computer science is concerned primarily with algorithms, i.e., the design of sequences to be processed in a computer to yield output information from input information, information science is concerned with the obtaining and processing of information and designing its input format so that it may be evaluated, related, correlated, and extrapolated in a variety of output formats.[16]

The above description of information science emphasizes the importance of data and information and, to a degree, deemphasizes the role of the computer. It is certainly true that the major contributions of information science by chemists have been in areas which are peripheral to what computer scientists do. Some of these contributions, which will be discussed in this paper, are indexing systems, notation systems, the correlation of data and information, and the design of on-line databases.

I do not mean to imply by the above that computer science is not important to the work of chemical information scientists. A knowledge of computer science is highly advantageous to the understanding of many disciplines of science in which computers are utilized. Interaction with a computer, such as in the construction, manipulation, or analysis of algorithms,[4] forces one to think through a problem, very much like a teacher does with students. Thus, when linguists attempted automatic translation via computer, they discovered that the process of translating from one language to another was considerably more complex than they had realized. When chemists attempted programmed organic synthesis, in which they were reasonably successful, they could not approach the achievement of the human intellect and intuition. They have gained, however, considerably more insight into how chemists conceive synthetic paths.

INDEXING

Indexing and classification systems are the basic concepts in information science for making data and information available and for arranging data and information in usable and useful formats. Classification and taxonomic concepts, such as those of Mendeleev, Dumas, and Linnaeus, have been of great value in the understanding and teaching of science and in the reduction of many facts to a matrix of knowledge.[16] Work in the area of artificial intelligence could benefit by paying more attention to classification concepts.

Of the variety of indexes in chemistry, such as subject, author, patent number, formula, and ring, the most difficult to achieve is the subject. Because a subject index is based on words, it is fraught with semantic, linguistic, and logic difficulties. To the user of an index, a word does not always mean what an author or indexer thinks it means. An index based on isolated words communicates the least amount of information and is characterized by the maximum amount of noise; it is like a dictionary without definitions, i.e., a simple word list.

Yet the isolated word index, called the uniterm index, was the one that designers of computerized information systems

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opted for in the late 1950s and well into the 1960s. Although it is still used to some extent despite the noise and false drops encountered by the users, it was displaced by the keyword concept. The conceptual differences between the two concepts, i.e., uniterm and keyword, are relatively slight, except for the introduction of links and roles and thesaurus control. With the advent of on-line databases since the late 1960s, the keyword indexing concept has been the overwhelming choice. Although a certain degree of vocabulary control can be exercised, the products from most database producers are based on the keywords in the title of documents.

If an index is to be an efficient and effective tool, one which permits the retrieval of only wanted references, then it must be conceptually oriented. In a conceptually oriented subject index, a subject such as *Methanol* is associated with or related to activity on or by it as a product, reactant, use, property, etc., i.e., the role of the subject as described in a reference. To achieve economy in computer operations, especially for input, sorting, and read/writes, we indicate differentiating roles of terms by the following mnemonics:

A = Analysis
C = Composition
D = Determination
E = Effect
P = Preparation
Q = Quality or Property
R = Reaction
T = Treatment
U = Use or Application

Thus, Methanol -A, Methanol -D, Methanol -P, etc., differentiate documents on the subject Methanol by whether the objective and results are the Analysis of Methanol, the Determination of Methanol in a mixture, or the Preparation of Methanol.

Should the users in our R&D environment require a generic:specific relationship for certain subjects, we denote this as follows:

Alcohol:Ethanol-
Alcohol:Methanol-
Alcohol:Propanol-

The generic:specific relationship is particularly important for relating the literature of polymer chemistry as there are many ways to describe a polymer, such as Polyethylene, Ethylene Polymer, Polymethylene, Olefin Polymer, etc. By using the generic:specific relationship, i.e., Polymer:Ethylene-, like things are placed together as an associated whole in which browsing and the detection of relationships are relatively easy.

To achieve a still greater discrimination among the terms in an index, we combine the terms in what we call a Multiterm,[9] such as in the following example:

Polymer:Ethylene -Q/Degradation/Mechanism//

This Multiterm communicates the information that the document referred to is concerned with "the mechanism of polyethylene degradation". The oblique stroke or virgule (/) following each term is the symbol we use to have the computer wrap around the Multiterm to yield the following additional Multiterms in the alphabetical subject printout:

Degradation/Mechanism//Polymer:Ethylene -Q/
Mechanism//Polymer:Ethylene -Q/Degradation/

The double virgule marks the end of the input Multiterm and indicates in each of the computer-processed Multiterms the logical order of the associated terms.

Possibly the strongest motivation for the adoption of keyword indexing based on titles of documents has been the economic factor, viz., the elimination of the human indexer. But this may be false economy if the product yields unwanted documents with doubtful assurance that all pertinent documents have been retrieved. A retrieval mechanism that adds two hours of unnecessary reading per week for 100 chemists reduces over-all productivity by five chemists per year. Would it not be more economical to assign at least one chemical information scientist to produce a computerized Multiterm index in harmony with the needs and interests of the 100 chemists? An additional advantage of the chemical information scientist is that as the documents are scanned for inclusion and indexing in the information system, each document entered could be coded in the computer relative to classes of chemical interest or relative to specific R&D programs within the environment for special printouts by the codes.[13] This coding mechanism is one activity in which a human brain is far superior to anything yet produced via computers, and at far lower overall costs. It is but one example of the potential value of information science to chemical research.

NOTATION SYSTEMS

In areas such as pattern recognition, programmed organic synthesis, instrumental (x-ray, NMR, IR, and UV) data acquisition and analysis, and correlation of chemical structures with physical and biological data, the preparation and translation of structural information for computer input has been a major stumbling block. A relatively large number of information systems have installed the Wiswesser Line Notation (WLN) and Chemical Abstracts Service (CAS) has based its Registry System on atom-by-atom connectivity tables. Both of these developments are noteworthy, but primarily as indexing systems which were designed to overcome the difficulties of indexing by chemical nomenclature. As WLN expanded among users, its rules for encoding became overly complex and as Woodward and Isenhour[19] stated, "the actual encoding procedure still constitutes a major hurdle". Relative to the CAS Registry System, Woodward and Isenhour pointed out that "the user of such systems must also have the ability to encode. . .to interrogate the system". Thus Woodward and Isenhour have been working toward the development of generating automatically connectivity tables in computer compatible format by television scanning of stylized chemical structures coupled with on-line computerized pattern recognition.

On the introduction of the Dyson notation system in 1946 and others which followed, such as Wiswesser's, Silk's, Gruber's, Hayward's, and Fugmann's, I tried to apply them in my work on chemical structure storage and retrieval and on correlations of chemical structures with their properties and uses. Although I found each system to have merit, particularly in yielding unambiguous and unique designations, they required major modifications for computer processing; they were too prone to encoding, decoding, and input errors; they were over-complicated with rules and exceptions, and yet unable to handle important areas of chemical structures, such as polymers and resins; and they were particularly weak in relating moieties and functionalities in correlation work. Consequently, I worked out a new notation system, one in which each symbol would designate a carbon atom, its bonding, and the number of hydrogens attached to it. Although other atoms are also designated, the system is oriented to notations for organic carbon compounds. Chemical structures are represented in the notation system essentially in an atom-by-atom correspondence with the way chemists draw organic structures and number the atoms.[8,10-12,14]

A notation system for computer-assisted chemical research design must do more than yield a unique and unambiguous

Table I. Comparison of Two Notation Systems for Computation of Molecular Weights

Formula	WLN Notation	WLN Notation units: Symbol	WLN Notation units: MW contribution	Skolnik Notation	Skolnik Notation units: Symbol	Skolnik Notation units: MW contribution
1. CH_4	1	1	16	AH	A	15
					H	1
2. CH_3CH_3	2	2	30	A2	A	15
3. $CH_3CH_2COCH_3$	2V1	1	15	ACKA	A	15
		2	29		C	14
		V	28		K	28
4. $ClCH_2COOH$	QV1G	1	14	LCKQH	C	14
		G	35.5		H	1
		Q	17		K	28
		V	28		L	35.5
					Q	16
5. $CH_3C{\equiv}CH$	2U1	1	13	AVU	A	15
		2	27		U	12
		U	0		V	13

notation for each chemical structure. It must facilitate the storage and retrieval of chemical structural information both generically and specifically, i.e., by class of chemical, by functionality, and by chemical fragment; it must have a high degree of recognizability, i.e., the notations should describe chemical structures similarly to the way chemists prefer to draw them; and among other things, it must have characteristics that enable a programmer to manipulate the notations easily, effectively, and economically in a computer.

If a notation system is compatible with computer processing, the degree of compatibility may be measured by the complexity of the program by which we compute the molecular weight of chemical compounds by the notations assigned to them. Table I compares the WLN and the Skolnik notation systems in terms of notations assigned to five chemical structures and the ease of specifying the contribution of each symbol in the notations to the molecular weight of each molecular structure.

Because each symbol in the Skolnik system has a fixed molecular weight contribution, e.g., A = 15, C = 14, K = 28, etc., the program for calculating molecular weights of compounds is straightforward and simple, involving a small look-up table. Symbols in WLN, however, do not have a fixed molecular weight contribution, e.g., 1 = 16, 15, 14, or 13 and 2 = 30, 29, or 27 in the examples, and consequently the program to calculate molecular weights must be relatively complex, involving many conditional statements, and thus relatively time-consuming of the CPU. Considerably more unfavorable examples for WLN could have been selected, such as molecules that employ WLN symbols X, Y, R, and position symbols (A, B, C, etc.) in ring structures, that reveal various complexities that the programmer needs to solve in computing molecular weights.

A notation system that designates the bonding and the number of hydrogens associated with carbon in particular and with other atoms in general, as in the Skolnik system, yields a notation symbol formula index that discriminates among all possible isomers of compounds having the same stoichiometric formula index. For example, there are 15 compounds which can be listed under C_4H_8O. By treating the different symbols of a notation in the same way as we do the different and number of atoms in a structural formula, we obtain a notation symbol index in which none of the 15 compounds is duplicated by any of the other 14, as shown in part in Table II.[11]

Table II. Notation Symbol Index for C_4H_8O Compounds

Formula	Notation	Symbol index
1. $CH_3CH_2OCH{=}CH_2$	ACQBE	A/C/Q/B/E//
2. $CH_3OCH_2CH{=}CH_2$	AQCBE	A/Q/C/B/E//
3. $CH_3CH{=}CHCH_2OH$	AB2CQH	A/B2/C/QH//
4. $CH_3(CH_2)_2CHO$	AC2KH	A/C2/KH//
5. $CH_3CH{=}CHOCH_3$	AB2QA	A,2/B2/Q//
6. $CH_3CH_2COCH_3$	ACKA	A,2/C/K//
7. $CH_2{=}CHCH_2CH_2OH$	EBC2QH	E/B/C2/QH//

COMPUTER-ASSISTED CORRELATIONS WITH A NOTATION SYSTEM

Reactivities, reactions, physical properties, and uses of chemicals are correlatable through functional and moiety relationships. Functionalities and moieties can be designated easily, clearly, and economically by a notation system that is sufficiently flexible to do what a correlation requires. For example, **1**, isoamyl methyl ketone, is composed of the fragments:

$$\overset{\overset{O}{\|}}{-C-},\ -CH_2-,\ -CH_2CH_2-,\ CH_3-,\ >CH-,\ \text{and}\ (CH_3)_2CH-$$

$(CH_3)_2CHCH_2CH_2COCH_3$

1

A2YC2KA

2

Each of these fragments is designated in notation **2**. For certain correlation studies, such as the effect of groups α, β, or γ to the carbonyl group, the notational fragments can be written as **3**:

A2/Y/C2/K/A//

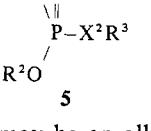
3

or as **4** if the isopropyl group should be considered to be an important factor:

A2Y/C2/K/A//

4

In the case of organic synthesis work for pesticidal activity, it is important to correlate parts of the chemical structure with given toxophoric fragments. For example, many thousands of organic phosphorus compounds have been tested as pesticides. Much of this research has been of an intuitive nature or Edisonian. Many permutations are possible for structures such as **5**:



5

where R^1, R^2, and R^3 may be an alkyl, alkaryl, cyclic, or heterocyclic moiety and X^1 and X^2 may be sulfur or oxygen. Table III illustrates one format for input of notations for computer processing of phosphorus-containing compounds to show the effect of chemical modifications. When this input is combined with test results on pests, plants, and animals, we have a means for correlation and for planning how to further

Table III. Computer Input for Phosphorus-Containing Pesticides

Structure	Notation	Computer input
1. $(CH_3CH_2O)_2PSCH_2SCH_3$	ACQ,2P(S)SCSA	ACQ,2/P(S)S/CSA//
2. $(CH_3CH_2O)_2PSCH_2SCH_2CH_3$	ACQ,2P(S)SCSCA	ACQ,2/P(S)S/CSCA//
3. $(CH_3CH_2O)_2PSCH_2CH_2SCH_3$	ACQ,2P(S)SC2SA	ACQ,2/P(S)S/C2SA//
4. $(CH_3CH_2O)_2PSCH_2CH_2SCH_2CH_3$	ACQ,2P(S)SC2SCA	ACQ,2/P(S)S/C2SCA//
5. $(CH_3CH_2O)_2PSCH_2C_6H_5$	ACQ,2P(S)SC.DB5.	ACQ,2/P(S)S/C.DB5.//
6. $(CH_3CH_2O)_2PSCH_2SC_6H_5$	ACQ,2P(S)SCS.DB5.	ACQ,2/P(S)S/CS.DB5.//
7. $(CH_3CH_2O)_2PSCH_2CNHCH_3$	ACQ,2P(S)SCKMA	ACQ,2/P(S)S/CKMA//
8. $(CH_3CH_2O)_2PSCH_2CN(CH_3)_2$	ACQ,2P(S)SCKNA2	ACQ,2/P(S)S/CKNA2//

modify the phosphorus-containing chemicals more effectively.

The Skolnik notation system yields a meaningful correlative index of NMR chemical shift data[14] in which basic proton and environmental groups are related, as illustrated below for propyl alcohol:

$$\underset{6}{CH_3CH_2CH_2OH}$$

$$\underset{7}{ACCQH}$$

The notation in units of proton groups with their chemical shift data may be expressed in the following form for computer input:

A / C / C / QH// 8a
0.92/1.57/3.58/2.28//

which, by a wrap-around program, results in the additional inputs:

C / C / QH// A / 8b
1.57/3.58/2.28//0.92/

C / QH// A / C / 8c
3.58/2.28//0.92/1.57/

QH// A / C / C / 8d
2.28//0.92/1.57/3.58/

Thus, every proton group is an index entry with its chemical shift or vice versa a chemical shift index with its proton group as affected by environmental groups. By computer processing, tables are produced which bring together all structurally similar compounds in correlation with chemical shift data.

ON-LINE DATABASES

Until the 1960s, the information industry consisted of two basic segments: producers of primary and producers of secondary publications. Both segments strove to produce high-quality products, and the secondary producers, especially, devoted considerable effort and thought in the design and maintenance of effective indexes for retrieval. Many of the advances in classification and indexing philosophies, logic, and systems resulted from this effort and thought. Faced with mounting literature, increasing labor costs, and inflationary printing, paper, and mailing costs, producers of publications turned to the computer during the 1960s. Thus was created a rapidly growing new kind of information industry consisting of the database producer and the database broker for on-line users. The database industry, as it evolved over the past decade, was made possible for the most part by government grants for the development of database production and service centers and for the improvement of database systems and products. At the same time, the government itself became involved in the development of databases for on-line retrieval, such as the National Library of Medicine's TOXLINE.

We now have more information products and services than ever before, but not necessarily greater access to desired information, nor are the many database products and services cost effective for the users. In the development of many databases, most of the effort was directed to having the computer do what people do better. The basic problems of information storage and retrieval essentially were ignored. Database producers have been relatively successful, however, in reducing clerical operations and in developing the concept of keyword indexes and chemical registry systems.

As pointed out earlier in this paper, keyword indexes based on titles, or even on author abstracts, are poor surrogates for intellectually produced subject indexes. Keyword indexing via computer is cost-effective for the database producer, but the user also must be a part of the cost-effective equation. Chemistry is not concerned with references per se, but with data and information in the references, with the relationship between facts, the dependence of facts upon other facts, the underlying principles that govern relationships among facts, and the systematic arrangement of information. These goals remain for the future, a future in which chemical information science with the computer as a tool will play a major role.

REFERENCES AND NOTES

(1) G. Birkhoff, "Mathematics and Computer Science", *Am. Sci.*, **63**, 83–91 (1975).
(2) P. E. Blower, Jr., and H. W. Whitlock, Jr., "An Application of Artificial Intelligence to Organic Synthesis", *J. Am. Chem. Soc.*, **98**, 1499–1510 (1976).
(3) M. H. Dilke, "Can Computers Help with Polymer Information?", *Br. Polym. J.*, **3**, 291–292 (1971).
(4) P. J. Hayes, "Computer Programming as a Cognitive Paradigm", *Nature (London)*, **254**, 563–566 (1975).
(5) K. Hensler, "Programmed Organic Synthesis", *Science*, **189**, 609–613 (1975).
(6) P. Kent and T. Gäumann, "Considerations on the Interpretation of Mass Spectra via Learning Machines", *Helv. Chim. Acta*, **58**, 787–794 (1975).
(7) D. E. Knuth, "Computer Science and Its Relation to Mathematics", *Comput. People*, 8–11 (Sept 1974).
(8) H. Skolnik, "A New Linear Notation System Based on Combinations of Carbon and Hydrogen", *J. Heterocycl. Chem.*, **6**, 689–695 (1969).
(9) H. Skolnik, "The Multiterm Index: A New Concept in Information Storage and Retrieval", *J. Chem. Doc.*, **10**, 81–84 (1970).
(10) H. Skolnik and J. T. Hays, "A New Notation System for Indexing

Polymers", *J. Chem. Doc.*, **10**, 243–247 (1970).
(11) H. Skolnik, "A Notation Symbol Index for Chemical Compounds", *J. Chem. Doc.*, **11**, 120–124 (1971).
(12) H. Skolnik, "A Chemical Fragment Notation Index", *J. Chem. Doc.*, **11**, 142–147 (1971).
(13) H. Skolnik, "The What and How of Computers for Chemical Information Systems", *J. Chem. Doc.*, **11**, 185–189 (1971).
(14) H. Skolnik, "A Computerized System for Storing, Retrieving, and Correlating NMR Data", *Appl. Spectrosc.*, **26**, 173–182 (1972).
(15) H. Skolnik and J. C. Snyder, "Input/Output Considerations for Large Data Bases", *J. Chem. Inf. Comput. Sci.*, **15**, 28–31 (1975).
(16) H. Skolnik, "Milestones in Chemical Information Science", *J. Chem. Inf. Comput. Sci.*, **16**, 187–193 (1976).
(17) E. G. Smith, "The Wiswesser Line-Formula Chemical Notation", McGraw-Hill, New York, N.Y., 1968.
(18) J. R. Ullmann, "The Credibility of Machine Intelligence", *Nature (London)*, **257**, 547–549 (1975).
(19) W. S. Woodward and T. L. Isenhour, "Computer Controlled Television Scan System for Direct Coding of Chemical Structure Models", *Anal. Chem.*, **46**, 422–426 (1974).

Computer Control of Data Acquisition, Reduction, and Display in Rapid Scanning Liquid Chromatography†

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An outline of the on-line computer system and supporting software used in a preliminary study on utilizing a rapid scanning spectrometer as a liquid chromatography (RSS/LC) detector is given. Refinements of this system in data acquisition, reduction, and display that were made out of convenience or necessity are then described in more detail. The present system allows computer control of the RSS, variable CATing, automatic absorbance calibration, rapid plotting of absorbance (A) vs. wavelength vs. time (3D chromatograms) and A vs. time (conventional chromatograms), and, finally, an automated integration routine for quantitative measurements.

INTRODUCTION

In a preliminary paper, the feasibility and advantages of an oscillating mirror rapid scanning ultraviolet–visible spectrometer as a detector for liquid chromatography were demonstrated.[1] It was felt that the optimum spectrometric detector for liquid chromatography (LC) would monitor the entire UV–visible region throughout a chromatogram, thereby facilitating qualitative and quantitative measurements. The coupling of an oscillating mirror rapid scanning spectrometer (OMRSS) with a high-performance liquid chromatograph has proven quite successful in moving toward meeting this objective. The emphasis of this paper was on the actual experimental techniques used, the RSS/LC system, and the resulting chromatograms from a standpoint of hardware capability. This paper describes the computer system and supporting software required for practical application of this spectrometer as a routine detector.

The marriage of rapid scanning spectrometry and liquid chromatography led by necessity to computer interaction for two reasons: first of all, for on-line experimental control and storage of the massive amounts of data generated, and, secondly, for post-run data analysis and display. A description of the minimum capabilities needed for computer interaction in RSS/LC will be made, followed by an outline of what was added or refined out of necessity and convenience.

PRELIMINARY STUDY

Experimental. A Raytheon 704 minicomputer with 16K memory and 16 bit word length was used for all RSS/LC studies. The peripheral devices include the following: two direct memory access (DMA) Raytheon magnetic tape drive units, a cartridge disc unit for all driver routines and LC programs, a high-speed paper tape reader, a teletype or Tektronix T-4002 graphic computer terminal, a Tektronix 601 memory oscilloscope, an 8 channel multiplexed ADC and 4 channel DAC, and X–Y recorder display units for plotting three-dimensional (3D) chromatograms.

A second generation Harrick rapid scan spectrometer (RSSB) was used for all of the preliminary studies. This instrument and the chromatographic system used were described previously.[1]

Data Acquisition. In the original system, the Raytheon 704 triggered a scan of the RSSB galvanometer mirror (GM) each second (while not the upper limit of repetition rate, this is more than sufficient for most LC applications). The computer merely caused a transistor to short the trigger input of the Harrick RSS signal processing module to ground using a +10-V pulse. Control of GM during the scan itself, however, was done by the Harrick processing module. The absorbance signal from this same module was then amplified 5× by standard circuitry and inputed to the ADC by the Raytheon. Initially a separate baseline spectrum was taken prior to each chromatogram. This greatly increases the number of runs necessary, and, to avoid this, the first 20–100 scans of a chromatogram (solvent background) were averaged and used as a baseline. This will obviously not work if the retention time of any compound is very small. The software routines were, therefore, altered so that an averaged baseline spectrum is taken only once for a particular solvent system and is then automatically subtracted from each spectrum. More will be said along these lines in later sections.

Data Reduction. The original software for data manipulation and display has been described previously.[2,3] The software for data reduction was limited to routines for averaging baseline spectra and subsequent subtraction before plotting spectra on a X–Y recorder.

Data Display. Examples of the first 3D liquid chromatograms can be found in Figures 2–5 of ref 1. Each of the 3D plots represent 3–5 h of work with the initial software. The procedure involved the use of two mag-tapes and several teletype commands. One mag-tape held the stored data while the averaged baseline was written on the second tape. This baseline was then subtracted from the data and stored in core ready for plotting. Usually 1000–1500 spectra were taken each run, and this procedure had to be repeated for each spectrum that was to be plotted.

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