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ABSTRACT

Part II of the Students' Chemical Information Project (SCIP), designed to spread the use of computer-based information services among research scientists and technologists, contains details of the project operations, statistics, results of questionnaires and research reports from liaison scientists (See LI 002 562 for Part I). Chapter I: Operation of the Scheme, discusses the objectives, data bases, selected population, liaison scientists and their training, general procedure, and production problems. Chapter II: Statistics, includes relevance in relation to size of output, amendments to profiles, group literature schemes, and the fate of references. Chapter III: Results from Questionnaires, covers the preliminary interview guide, follow-up interview guide, and the final questionnaire. Chapter IV: Research Reports, contains reports by the liaison scientists. The page location of the figures and tables used is listed. The appendices include: circular sent to all participants, cover letter for final questionnaire, example of a search profile, index headings used in the classification of profiles, compound index to profiles, technique and property index to profiles, and profile statistics and titles. (NH)

Report to the Office for Scientific
and Technical Information on
Project SI/21/23

June 1969

STUDENTS' CHEMICAL INFORMATION PROJECT

October 1967 - September 1968

Final Report

by

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Dr. R. Baker, Institute of Computer Science, University of London, who carried out the analysis of the final questionnaire.

Dr. A. K. Kent, Chemical Society Research Unit, whose unit was responsible for providing the fortnightly Chemical Titles service.

Dr. G. A. Somerfield, OSTI, who acted as project co-ordinator.

The report is issued in two parts:

Part I. A review of the project and the major results. This part of the report is being widely distributed to those participating in the experiment.

Part II. Details of operations, statistics, results of questionnaires and research reports from liaison scientists. One copy of this part is being sent to all university libraries and chemistry departments in the U.K. Further copies are available on request from the Office for Scientific and Technical Information, Department of Education and Science, Elizabeth House, York Road, London, S.E.1.

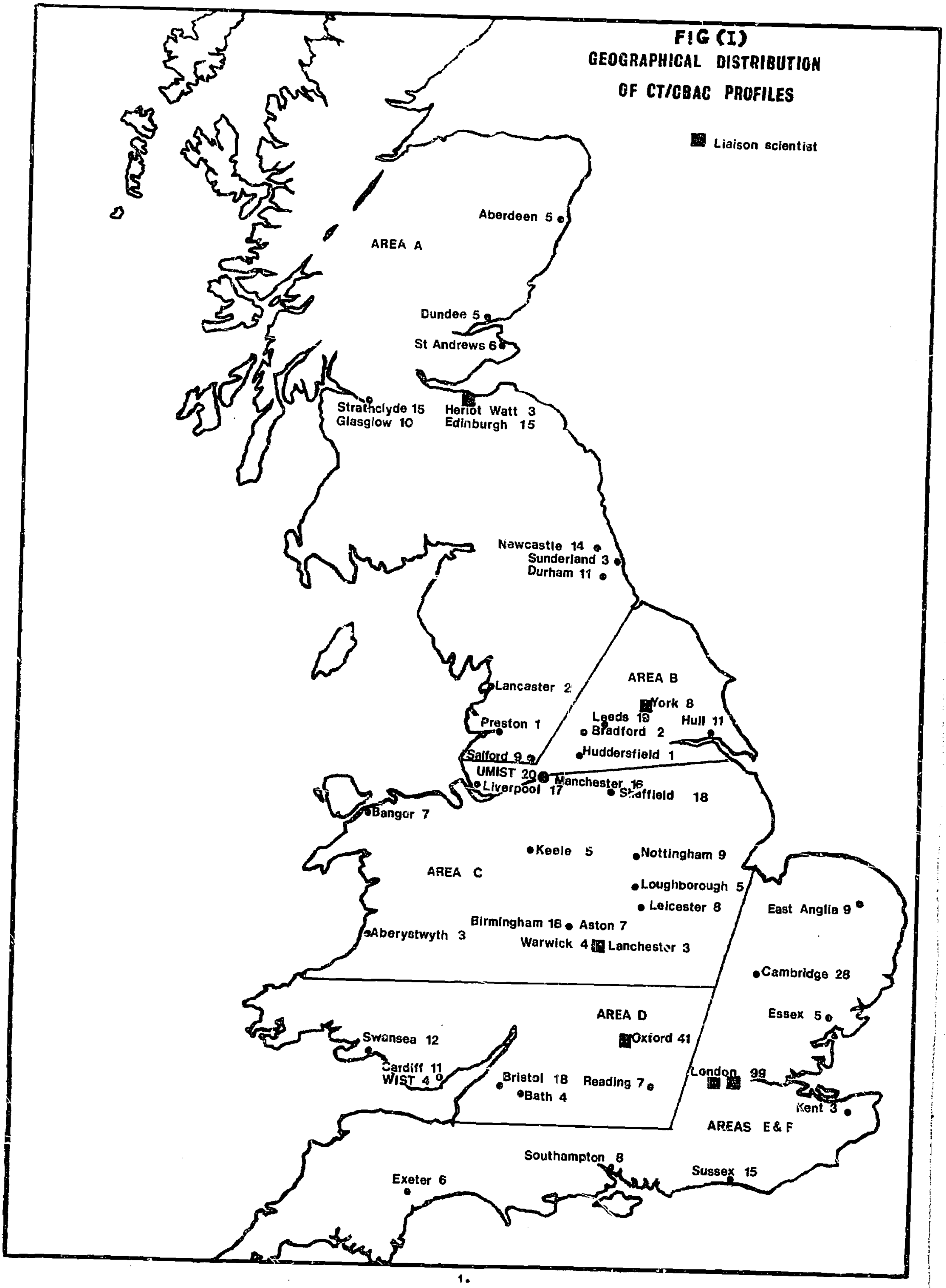

FIG (I)
GEOGRAPHICAL DISTRIBUTION
OF CT/CBAC PROFILES

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PART II

Chapter 1: Operation of Scheme

Objectives

The main objectives of the scheme were:

(a) to enable a large group of academic users to gain experience in the use of computer-based services.

(b) to improve general knowledge of all chemical information services within this group of users.

Secondary objectives were:

(1) to gain experience of the routine provision and use of computer-based services, particularly in universities.

(2) to determine whether a network of liaison scientists is a suitable way of providing these services,

(3) to determine what qualities and qualifications are required in a good liaison scientist.

(4) to determine whether pure scientists can be trained on a short course to act as liaison scientists, and if so, to determine what the duration and content of such training courses should be.

(5) to attempt to determine the value and acceptability of the services by limited user participation.

(6) to investigate the information habits of students and the effect upon these habits of the provision of a computer-based service.

Data Bases

The computer-based services Chemical Titles (CT) and Chemical-Biological Activities (CBAC) were chosen for the experiment because these two services had been provided on a routine basis by the Chemical Society Research Unit for nine months prior to the start of the experiment. Chemical Titles is available both on magnetic tape and in a printed version; it consists of a fortnightly listing of about 5,000 titles taken from approximately 700 journals in the fields of pure and applied chemistry and chemical engineering. It is possible to search for specified words contained in titles, for author names, and for particular journals. Chemical-Biological Activities, also available on tape or in printed form, consists of a fortnightly listing of about 500 titles, together with informative digests, taken from approximately 600 journals; only papers dealing with the biological activity of organic compounds are selected. It is possible to search for specified words contained in titles or digests, for author names, for compound registry numbers, for molecular formulae, and for particular journals. Other computer-based services are being developed by the Chemical Abstracts Service (CAS) and it was thought that wider use of CT/CBAC services would provide a good introduction for both user and operator to the range of services that would be available in the near future.

Selected Population

Mainly for financial reasons, the experiment had to be limited to a selected population and the group chosen consisted of all final-year Ph.D. students in Chemistry supported by the Science Research Council. This was a well-defined population, about 500 strong with good first degrees, and it provided a random sample of chemists from all British universities (except Stirling); the final geographical distribution of profiles is shown on the map (fig.1). One reason for limiting the scheme to final-year students was that they would carry their experience of computer-based services with them into a wide range of Government, academic, and industrial laboratories. At the same time, OSTI would be under no obligation to continue providing them with a free service. Furthermore, it was hoped that, at this stage of their career, students would still readily accept novel techniques and yet would have sufficient experience of chemical research to carry out a realistic assessment of CT/CBAC.

Liaison Scientists

The requirement for a number of specially-trained personnel to ensure efficient operation of the project has been discussed in Part I of this report (p. 7-8). It was thought that postdoctoral fellows, after a period of training in chemical information, would be very suitable for the liaison posts available. Six chemists were appointed, all of whom either had Ph.D.s or submitted theses during the year (see G. A. Somerfield, Chemistry in Britain, 1968, 4, 71).

Following the initial announcement of the appointments, it was suggested (R. J. Dannatt, Nature, 1967, 216, 208) that the scheme would be better operated through libraries rather than through a network of liaison scientists. However, subsequent enquiries indicated that most science librarians appeared to be too busy to undertake extensive liaison work.

Although the use of liaison scientists was a quick and precise way of transmitting information and stimulating interest in the scheme, it was also an expensive way; in future, liaison scientists may have to be used in a more limited role, with responsibility for routine profile maintenance being delegated to the user or to a staff member or librarian acting in a local liaison capacity.

Training of Liaison Scientists

To enable the liaison scientist to carry out his work, it was necessary that he should have a knowledge both of profile formulation for CT/CBAC and of general information activities and sources. Owing to the short time available, only the technicalities of profile formulation were covered in detail in the first training session and the rest of the training was spread out throughout the year. Before the first session, each liaison scientist was sent a CT/CBAC Search Manual and various introductory papers to acquaint him with the background to the project. In addition to attending the four formal training sessions held throughout the year, most liaison scientists attended a meeting of the SIC Discussion Group at Aston and a symposium on 'User Studies' at State House. These meetings are tabulated overleaf:

Table 1: Training of Liaison Scientists

Date	Place	Speaker	Topic	Time (days)
27th September -1st October 1967	Nottingham	Dr. G.A. Somerfield	The role of OSTI in the development of information services.	¼
		Mr. N. Green	Organisation of a university science library.	½
		Dr. A. K. Kent	Formulation of CT/CBAC profiles and test runs.	2½
11th October	York	Review of experience gained in formulating 10-12 'local' profiles		½
12th-13th October	National Lending Library	Dr. K.P. Barr	The literature collections and services of the NLL	½
		Dr. A.J. Harley	MEDLARS	½
		Dr. D.N. Wood	Reports and translations	½
27th November	State House	Mr. A.E. Cawkell and Information sheets from SDC, Dunfermline	ISI services	½
25th January 1968	Biodeterioration Centre, Aston	SIC Discussion Group	SICs: staffing and equipment	1
12th-13th February	Nottingham	Dr. D.C. Veal	CAS registry system	¼
		Dr. M.F. Lynch	IUPAC notation	¼
		Mr. E. Hyde	Wiswesser notation and its use in the ICI system	½
8th May	State House	Symposium	User studies	1

Over the year, the liaison scientists thus received a broad, if cursory, view of the field of chemical information.

General Procedure

Initial Contact

Initial contact with the various departments was made by Dr. G. A. Somerfield of OSTI; on July 7th 1967, he asked the heads of larger chemistry departments to advertise for liaison scientists. By September 11th, all six posts had been filled and Dr. Somerfield was able to advise all heads of department of the scope of the scheme and to give them the name of the liaison scientist appointed in their area.

In order to equalise the work load on each liaison scientist, some distribution of area boundaries was necessary; in particular Manchester was covered piecemeal by three of the liaison scientists since it had not proved possible to appoint a liaison scientist there. On 18th September, a letter and information sheet explaining the scheme were sent by OSTI to all eligible students. They were asked to divide their replies into three categories: A - would like to take part; B - would like more information; C - do not want to take part. Less than 5 per cent of students answered in the third category. About 20% did not reply and had to be contacted by the liaison scientist on his first visit, when in fact most of them took up the offer.

First Visit

When search manuals became available in quantity, they were sent out well in advance of the first visit, which was arranged for October or November 1967. A short introductory talk was offered to all members of the department interested in the scheme and many non-participants attended. The talk dealt mainly with the formulation of CT/CBAC profiles but also mentioned other chemical information services. A set of slides showing examples of profile formulation from the search manual was used to illustrate the talk. The liaison scientist then arranged a time-table to see each student individually for an hour. The student was asked to define his research interests and the profile was formulated accordingly. An example of a completed profile is given in Appendix 3. In some cases, the student brought along his card index or reprint collection and this helped in the selection of appropriate search terms. Ten minutes of the interview were spent in filling in the preliminary interview guide and the results from this are discussed in Chapter 3.

Where the head of the department had not attended the introductory talk, the scheme was outlined to him and efforts were also made to contact the science librarian and the member of staff on the library liaison committee.

By the end of November, all departments except Bangor had been visited and preliminary reports on the progress of the scheme were presented at State House on the 27th. An OSTI circular (Appendix 1) was sent out in December summarising the results from the reports and explaining the use of the terms 'relevant' and 'hit'. The purpose of the circular was to improve the consistency of feedback results as well as to keep participants informed.

Second Visit

The second visit to all participants took place early in the new year; several students felt that the second visit should have been closer to the first as profile amendments were most frequently required after receipt of the first or second printout. One student suggested that an immediate retrospective search of five CT tapes would enable the performance of the profiles to be optimised as soon as possible! At this second visit, profile amendments were discussed and a follow-up guide was completed in order to analyse the impact of the service. The results from this questionnaire are discussed in Chapter 3. In some areas, a brief third visit was arranged. Progress reports on the scheme were presented by the liaison scientists at Nottingham on February 12th.

Final Visit

March and April were 'quiet' months, in which the liaison scientist had some time available for research. However, routine analysis of profile performances and collection of useful references were still carried out. In addition, preparations were made for a final detailed questionnaire at a meeting on April 30th at State House. The final visits took place in June or July and were mostly concerned with the collection and checking of the questionnaires, which had been sent out one week in advance, together with a covering letter from OSTI (Appendix 2). Several students were absent during the final visit and they were requested by post to send in their completed questionnaires as soon as possible. A meeting was held at Warwick on August 26th and 27th to discuss the composition of the final report and small study groups were set up to prepare sections of this report.

Thesis Bibliographies

Each student was asked to send in his thesis bibliography so that recent references cited could be compared with those retrieved by the computer. Nearly 100 bibliographies have been received so far and a sample of ten contained a total of 1,759 references, of which

234 (13.8%) were dated 1967 or 1968. Of these, 190 (83%) were taken from primary journals covered by CT. The individual profiles covered varying periods and only 87 of the primary journal references were possible captures; 63 (69%) were actually retrieved. A measure of recall based on the number of items retrieved by the students is thus obtained: 69% x 83% = 57%.

A fuller report of this work will be published later.

Precision Cards

Throughout the year, postcards for each output were used to maintain contact between the user and the liaison scientist. The card contained boxes for marking the total number of titles that were relevant, irrelevant, or of undetermined relevance, and a space for noting comments or amendments. Although vacations caused some delays, the return of the precision cards was good (60-90%). No fall off in return of the cards was noticed throughout the year.

Index to Profiles (see Appendices 4-7)

An analysis of profiles according to subject category was carried out so that an index to profiles could be constructed. This will enable future liaison scientists or research workers to consult previous profiles easily to obtain an impression of the performance of the service in their field of work.

Production Problems

A number of areas of difficulty can be readily identified.

(1) Establishment of the Profiles

The nature of the population and the structure of the experiment made it inevitable that a very large number of new profiles were received as input to the scheme over a relatively short period. Approximately five hundred profiles containing an average of twenty terms each had to be keypunched in a period of six-eight weeks. Within the Chemical Society Research Unit the organisation is such that a regular low-volume intake of profiles is easily managed, but a sudden burst of this type creates severe problems. In any future exercise, therefore, it is desirable that adequate keypunching facilities be made available. It would be reasonable to expect a competent keypunch operator to process up to two thousand search terms per day.

(2) Handling of Output

At first the lack of experience of handling very large volumes of output led to considerable difficulties. The experience gained during the experiment has led to a smooth and effective organisation and there is no reason to suppose that this will create any special difficulties in the future.

The need for liaison scientists to receive copies of the output of all profiles under their control suggests that in future each liaison scientist should be allotted a continuous block of profile numbers so that all output for one liaison scientist sorts together. Each institution should be allocated a continuous block of profile numbers for the same reason. It may also be worth considering the possibility of arranging for local redistribution of output at each centre. It would reduce clerical and postal costs if all the output for one institution could be sent in one package.

(3) Profile Amendment

Profile amendments have, from time to time, been held up unreasonably at the Unit. Some consideration should be given to:-

(a) Instructing liaison scientists in the appropriate way to record profile amendments ready for the keypunch operator.

(b) Improving the format of the profile amendment form to ease the difficulties of the liaison scientists and the keypuncher.

(c) Establishing an agreed time-schedule for receipt of profile amendments and abiding by it.

(4) Type of Output

The easier type of output for the Unit to handle is cards and this would be preferred by the majority of students. This form is, however, significantly more expensive than output on single or multipart paper.

(5) Notice

In any future exercise reasonable notice must be given to the Unit of the anticipated work load so that appropriate administrative action can be taken in time. If programming changes are likely to be needed a minimum of two months notice is required even for apparently trivial changes.

Chapter 2: Statistics

Each entry in table 2 shows the number of profiles in the scheme having an average number of hits and average relevance rate within the ranges given. The distribution of relevance rate and number of hits are given in the histograms at the top of figure 2. The definition of a relevant paper was any paper satisfying the intent of the profile, i.e. the written statement of interest of the user. While some users interpreted 'relevant' to mean 'of value' others used 'of interest' as the criterion and therefore the net effect on the final figures will be small.

Also shown in figure 2 is the distribution of "hits" and "relevance" figures by area. While the dissimilarities in the histograms may reflect the individual liaison scientist's approach to profile construction and possibly his explanation of relevance to the students, there are undoubtedly wide variations between institutions, even if geographical location is of secondary importance.

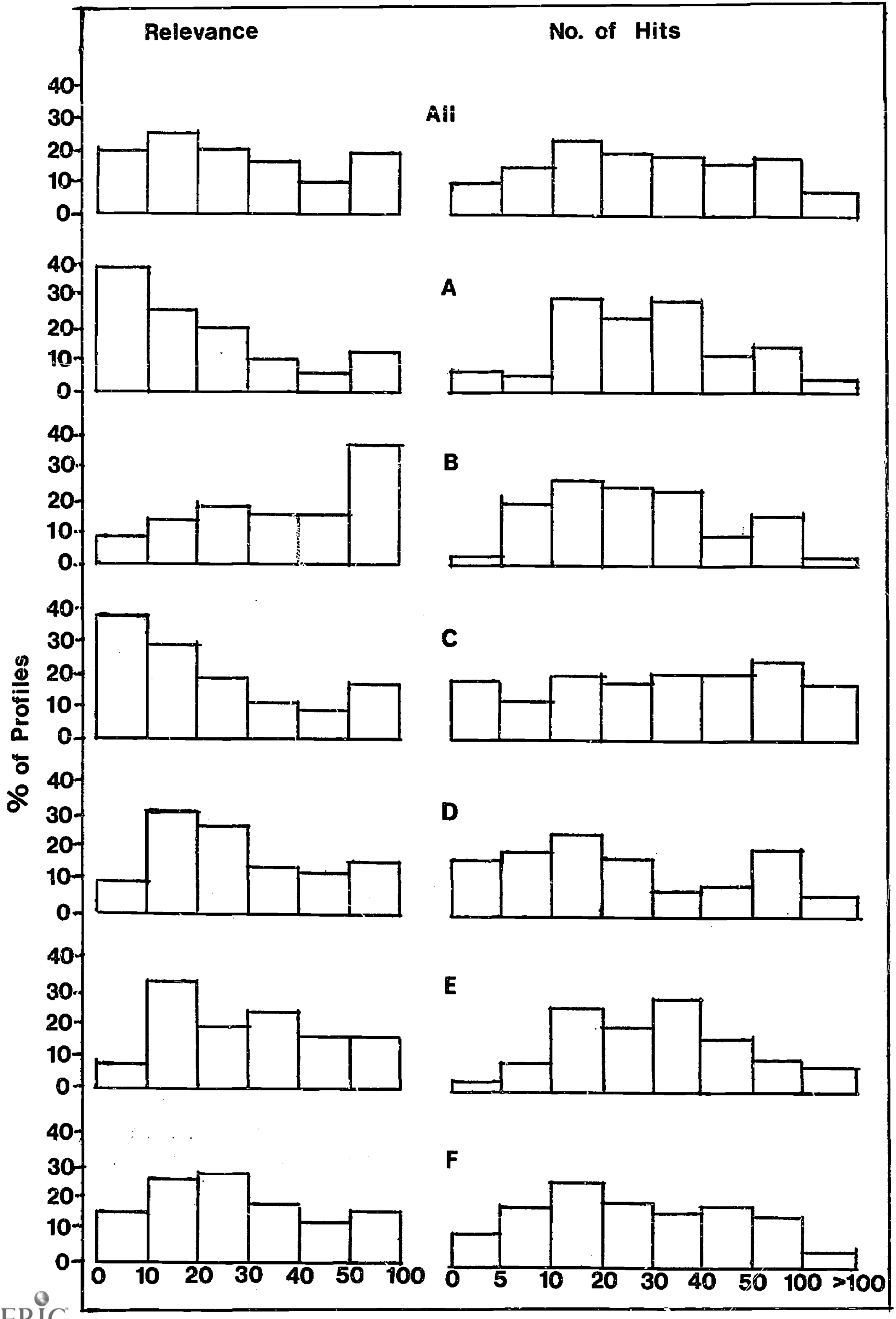
Table 2: Relevance in Relation to Size of Output

% Rel. / No. of Hits	0-10	11-20	21-30	31-40	41-50	51-100	Total
0-4	10	3	4	3	4	13	37
5-10	3	13	11	9	5	10	51
11-20	19	18	22	16	13	18	106
21-30	12	20	16	15	6	12	81
31-40	12	28	15	6	5	11	77
41-50	13	14	9	5	5	8	54
51-100	13	18	13	7	5	7	63
> 100	10	10	2	2	1	0	25
Total	92	124	92	63	44	79	494

The "average profile" produced about 30 hits/fortnight and had 30% relevance (cf. figures of 20 and 40% for the CSRU CT/CBAC experiment). A profile falling in the range 10-50 hits with 20-50% relevance was considered "well-behaved", but the number of profiles falling outside that range was large. Some 20% had less than 10 hits/fortnight; another 20% more than 50. Some 40% had a

FIG (2)

Breakdown of Relevance and Output Figures by Area



relevance rate less than 20% and 15% greater than 50%.

Examination of table 2 shows that there is a general decrease in relevance (precision) with increase in size of output. An exact inverse proportionality would obviously lead to each profile retrieving a constant number of relevant references. Whilst this was not expected, due to differences in scope and construction of profiles, it was noticeable that the variation between students of the number of relevant references was much less than that of the numbers of hits. The reasons for this are presumably:

(1) a very narrow profile will produce a high relevance rate for a small number of hits.

(2) a broad profile will produce a large amount of "trash" for relatively little increase in the number of relevant references.

Amendments to Profiles

From the five areas for which figures were obtained, 617 profile amendments were made in the first four months of the project. The majority (77%) of the profiles (377 x 1) were amended once; 20% were amended twice (95 x 2); 3% were amended thrice (14 x 3) and two profiles were amended four times. The most complete figures available are those for area A; these show that 5% of amendments gave essentially new profiles; 30% changed the profile structure in some way; 11% altered the output; 35% corrected 'avoidable errors' e.g. obvious omissions. The majority of amendments seemed to have little effect on relevance rate or number of hits.

Group Literature Schemes

It is surprising that only about 5% of the population of users take part in a formal group literature searching scheme. The numbers in these groups range from 3 to 12 and the number of journals scanned from 20 to 80 (most estimates seem to be on the optimistic side). Most of these few groups meet regularly, either weekly, fortnightly, or monthly, where abstracts are presented, or papers discussed.

About half the groups have a large central index or store of reprints. Current awareness tools used are CCP, and Current Contents, with Chemical Abstracts used as a long step and, during the past year, CT and CBAC profiles.

The Fate of References

Dr. Leggate (area A) monitored relevant references in the output of some 51 users during his second visits (January 1968) and discovered what action had been taken with respect to them on subsequent visits (June 1968). For a total of 756 references, no action had been taken for 28%. 9% had been indexed and 11% had been photocopied or a reprint sent for. Students who estimated high relevance figures tended to take no further action - although the correlation was weak. Students who used outputs for the storage of references were also likely to report 'no action'.

160 references marked as "relevance undetermined" were also noted. No action was taken for 70%.

Chapter 3: Results from Questionnaires

Preliminary Interview Guide

An attempt was made to ascertain the users' present knowledge of chemical information services and literature habits by means of a preliminary interview guide. Ten minutes were spent completing this guide in the first interview with each student. The integrated statistics for 460 users are shown in the following table:

Table 3: Integration of Statistics

Number of Student Profiles 512

Number of Universities and Colleges ... 65

Number of Interview Guides from which this table was prepared .. 460

Profiles

Important Authors Included in First Profile: 157 (Areas D and E not included)

Important Institutions Specified during Interview: 41 (Areas C, E and F not included)

Classification (Provisional)

Physical	Inorganic	Organic	Biochemical or Pharmacological	Analytical	Total
172	98	189	28	7	494

Information Habits	None	Informal Talks	1-2 Lectures	Lectures and Supervised Practical Work
Type of Training at Undergraduate Levels	257	64	48	17
Type of Training at Graduate Levels	295	48	35	2

Primary Journals mentioned by more than 30 students	No. of Students scanning journal (no figures from areas B, E and F)	Own Copy	Obtained on Loan	Look at in Library		Other
				Dept.	Univ.	
J. Chem. Soc.	133	2		41	21	A and D areas only
J. Amer. Chem. Soc.	131			53	22	
J. Chem. Phys.	61			25	11	
Trans. Farad. Soc.	47			19	7	
Chem. Comm.	46	4	1	10	4	
J. Org. Chem.	47			14	9	
Tetrahedron Letters	38			10	8	
Inorg. Chem.	34			11	7	
J. Phys. Chem.	31			15	7	
Current Awareness Publications						
CCP	347	13		161	46	
CT	170			34	28	
Current Contents Current Contents in Chemical Sciences	106	1	3	9	10	
Others						

Preferred Methods for Current Awareness

X. Scanning Primary Journals only 190

Y. Current Awareness Publications only 66

Z. Abstract Publication only 41

X and Y 69

Y and Z 6

X and Z 28

X and Y and Z 33

	Poor	Moderate	Good
Interdependence for Information with Colleagues or Supervisor	150	157	134

Participation in Group Literature Searching Schemes 43

Retrospective Searching:

Substantial Use is made of:

Chemical Abstracts	428
Physics Abstracts	4
Nuclear Science Abstracts	4
Biological Abstracts	14
Others	-

Availability of a reasonable set of Chemical Abstracts

1. University Library only	101
2. Departmental Library	
a. within same building as laboratory	299
b. elsewhere	1
3. None	1

Students' Personal Information Storage Arrangements

L. Note Book	70	
M. Card File	326	
N. Edge Notched Card	49	
P. Reprints	31	
L and M		very few instances of combined systems
L and N		
None		

The numbers in the table refer to positive replies given by students and are therefore minimum figures since there are no figures available from certain areas.

It was apparent that normally students received very little instruction in use of the chemical literature; that which was available ranged from a 'short professorial mutter' to a three day seminar including a practical exercise. Out of the 460 users, at least 200 had never received any training in use of the literature.

For current awareness, about half the students relied mainly on the scanning of 6-10 primary journals almost always obtained from the library. Almost all students were familiar with Current Chemical Papers (CCP); 34% used it regularly and 40% irregularly.

Chemical Titles (CT) and Current Contents (CC) were less popular; 6% used CT regularly and 28% irregularly whilst 6% used CC regularly and 12% irregularly. Rather surprisingly, about 15% of students used Chemical Abstracts for current awareness; this may indicate the need for more information than the title of a paper alone can give.

The section on interdependence of information between the student and his supervisor and colleagues indicated a marked lack of communication (cf. E. Rudd, New Society, 1968, 562). This was substantiated in later interviews, which showed that information from the printouts was in general disseminated inefficiently, if at all. It thus seems advisable to place more emphasis on group profiles so that more people are drawn into the scheme and perhaps to provide multiple copies of the output. One liaison scientist invited supervisors to attend his interviews with their students and this produced a 25-30% response.

For retrospective searching, 95% of students used Chemical Abstracts, a reasonable set of which was available to every student except one.

Most students used a card index for storing retrieved information; about 15% simply used a notebook and 10% used edge-notched cards.

Follow-up Interview Guide

This guide was designed to provide information for progress reports submitted by the liaison scientists in February and dealt with currency, coverage, loan requests, group literature schemes, and important references. Some of the information from this guide was not susceptible to exact interpretation and several students gave vague or incomplete answers so that the data obtained were approximate. No integrated statistics were prepared, so a sample of 89 returns from area C is quoted as an illustration:

Almost half the users thought that the printouts, in general, gave them references before the appropriate journals arrived in the library; 35% thought that the printouts arrived more or less simultaneously with the journals; only 15% said they had already seen most relevant references in the printout. References in American journals such as J. Chem. Phys. seemed to appear in the printouts as much as two months before the journal arrived and this caused some frustration. There seemed to be no doubt that students were being alerted to references of possible interest more quickly than they would have been without the CT service. However, in view of the fact that the time lag between submission of a paper for publication and its appearance in print may be over a year, advance notice of a few days does not appear to be highly significant. On average, as far as can be ascertained, about 20% of relevant references had already been seen by the user. This percentage obviously depends on how quickly the user scans the primary journals and it was noticeable that one keen student, who was writing a review on n.m.r. spectroscopy, estimated that he had already seen over 75% of the references that appeared in his printouts.

A more important advantage of the scheme seems to be that the student obtains greater coverage of the literature than he would normally do. Two-thirds of the users said that, although they would expect to pick up important papers anyway, their profiles had retrieved titles sufficiently relevant to cite in their theses but which they would not have seen without the CT service. Despite the fact that most of the users said that the service was useful in scanning 'obscure' journals, only 18 (20%) had sent in inter-library loan (ILL) requests (a total of about 75 titles) since last October. Half the users had had articles photocopied during the year and 35% had sent off for reprints. In some departments, e.g. Leicester and Keele, photocopying is restricted because of expense.

Most of the users (90% of the sample) would prefer output on 6 x 4" cards. However, the new paper format adopted by the Unit was very well received, judging from comments on the precision cards.

Final Questionnaire

The following results are based on the answers from 429 questionnaires covering 438 profiles (85% of the population). Inconsistencies among some percentages quoted are caused by no answers being given in certain cases. Information from each questionnaire was coded and transferred to punched cards for a detailed analysis.

Section A: Effect of the Service on Information Habits

Section A investigated the effect of the CT/CBAC service on the information habits of the students. The results are shown in the accompanying table. It was found that as a result of their involvement in the project, the time spent by the student in scanning current awareness publications had decreased for 52% of the users and remained the same for 41%. Time decreases were also shown for scanning abstract journals (40% of users) and primary journals 25%), while no change was reported by 54% and 68% of users for these respective classes of journals.

Effect of the Service on your Information Habits

1. How has your involvement in this project affected:

(a) The amount of time you spend	Increased	Remained the same	Decreased	No answer
(i) Scanning Primary Journals	26(6%)	294(68½%)	107(25%)	2(½%)
(ii) Scanning Current Awareness Publications	22(5%)	178(41½%)	224(52¼%)	5(1¼%)
(iii) Scanning Abstract Journals	18(4¼%)	233(54½%)	172(40%)	6(1¼%)
(iv) Reading Original Papers	189(42¼%)	238(55½%)	6(1¼%)	4(1%)
(b) The number of Primary Journals which you see regularly	66(15½%)	315(73½%)	42(9¾%)	6(1¼%)

2. Current Awareness Publications

For the three publications:		Current Chemical Papers	Chemical Titles (printed version)	Current Contents (Life, Physical, or Chemical Sciences)
(a) Since Sept. 1967, has your personal use been	Nil	106(25%)	262(61%)	324(75½%)
	Irregular	173(40¼%)	120(28%)	53(12½%)
	Regular	147(34¼%)	26(6%)	23(5¼%)
	No answer	3(½%)	21(5%)	29(6¾%)
(b) As the result of receiving regular outputs, has your personal use	Increased	12(2¾%)	23(5¼%)	15(3½%)
	Remained the same	259(60½%)	246(57½%)	314(73%)
	Decreased	148(34½%)	115(27%)	49(11½%)
	No answer	10(2¼%)	45(10¼%)	51(12%)

3. To what extent has the service replaced your own manual scanning of:

	(a) Current Awareness Publications	(b) Primary Journals
Completely	97 (22½%)	16 (3¾%)
Partially	206 (48%)	168 (39%)
Not at all	122 (28½%)	242 (56½%)
No answer	4 (1%)	3 (¾%)

The number of users spending more time reading original papers was 42% whilst 55% still spent the same time on original papers. There was no real change in the number of primary journals seen. The figures were: decrease 10%; same 73%; increase 15%. The answers to A1(a)(i) and A1(b) are linked in the following table:

Table 4: Primary Journals

Time increased for 26 users.

Numbers of journals seen	Increase	Same	Decrease
	16	9	1
Service replaced scanning	Completely	Partially	Not at all
	0	12	13

Time remained same for 294 users.

Number of journals seen	Increase	Same	Decrease
	36	248	8
Service replaced scanning	Completely	Partially	Not at all
	1	71	221

Time decreased for 107 users.

Number of journals seen	Increase	Same	Decrease
	14	57	33
Service replaced scanning	Completely	Partially	Not at all
	15	85	7

Question A2 investigated the students' use of current awareness sources and the effect on this usage of receiving regular output. Question A3 examined the extent to which the service had replaced manual scanning of current awareness publications and of primary journals. An apparent inconsistency was found in that 70% of users said that the service had partially or completely replaced their manual scanning of current awareness publications /¯A3(a)_7 whereas only 52% said that they spent less time scanning these publications /¯A1(a)(ii)_7. An attempt was made to resolve this inconsistency by examining the answers to questions A2(a), A2(b) and A3(a) in conjunction with A1(a)(ii). The detailed analysis is set out below:

Table 5: Scanning of Current Awareness Publications

(a) Time spent increased for 22 users.

		Nil	Irregular	Regular
Q2(a) Use of	CCP CT CC	2 10 16	8 9 4	12 2 1
Q2(b) Personal use of increased	CCP CT CC	0 0 0	2 7 1	5 2 2
" remained same	CCP CT CC	1 8 14	6 1 2	7 0 0
" decreased	CCP CT CC	0 0 0	0 1 0	0 0 0
		Completely	Partially	Not at all
Q3(a) Service replaced manual scanning		0	7	14

(b) Time spent remained the same for 178 users

		Nil	Irregular	Regular
Use of	CCP	38	54	80
	CT	115	43	11
	CC	135	16	15
Personal use of increased	CCP	0	3	0
	CT	0	8	1
	CC	0	2	2
remained the same	CCP	38	36	75
	CT	97	34	9
	CC	118	12	13
decreased	CCP	1	14	6
	CT	5	11	1
	CC	4	1	0
		Completely	Partially	Not At All
Service replaced manual scanning		22	58	96

(c) Time spent decreased for 224 users

		Nil	Irregular	Regular
Use of	CCP	62	110	52
	CT	134	68	12
	CC	169	34	6
Personal use of increased	CCP	0	1	0
	CT	0	3	1
	CC	0	0	0
remained the same	CCP	33	28	33
	CT	88	16	0
	CC	132	14	4
decreased	CCP	27	80	19
	CT	37	49	11
	CC	23	19	2
		Completely	Partially	Not At All
Service replaced manual scanning		75	140	9

From this table the following points emerge:

(a) More time was spent scanning current awareness publications by 22 users, although for 7 of these users the service had partially replaced manual searching of current awareness publications. The reason for this seems to be that the partial replacement of, say CT, was offset by increased use of CCP and CC.

(b) The most obvious anomaly is the case of 22 users for whom the service completely replaced manual scanning of current awareness publications and yet who still spend the same amount of time scanning these publications manually. No explanation is available for this anomaly and it is necessary to discount this relatively small number of answers; it is possible that the 22 users did not understand the phrase 'current awareness publications'.

The same anomaly occurs for the 58 users for whom the service partially replaced manual scanning of current awareness publications and still spend the same amount of time scanning these publications. It could, however, be said as before that the users had spent less time on CT and more on CCP and CC so that the time spent on overall manual scanning had remained constant.

The most important point that this part of the questionnaire was intended to establish was whether the time spent on scanning current awareness publications had in fact decreased as a result of the service. For an answer to this question, it seems better to take the percentage from A1(a)(ii), i.e. 52% of users spent less time, rather than the doubtful figure of 70% given in A3(a). This is substantiated by the figures in the last part of the table:

(c) Less time was spent scanning current awareness publications by 224 users (52%) and the service partially or completely replaced manual scanning in all but 9 cases. In agreement with this, there was a substantial decrease in the personal use of CCP, CT, or CC shown in 2(b) for these users.

Section B: Use of Library Services

This section examined the use of library services by the students. It was intended to cover any library or information service normally used, irrespective of whether it was from a university, departmental, college, or public library.

In only 7% of cases were journals used which were not available at some time in the library. Some of the larger libraries seemed to have excellent coverage of journals cited in CT. In nearly half the cases where journals were not available, they were obtained by inter-library loan. The library staff were rarely asked for help in finding references apart from routine loan requests; only 2½% of users frequently asked the advice of the library staff and 52% never asked.

67% of users were informed of interesting titles in languages they could not read; of these, less than half took any further action. The majority of students (87%) stated that they had never used an index to translations or tried to have a paper translated other than by a colleague (question 9 below). The most frequent language causing difficulty was Russian (71% of readers) followed by German (37%) and Japanese (23%).

Use of Library Services

Summary of Replies

	Frequently	Occasionally	Rarely	Never	No Answer
1. How often has a required journal not been available in the library?					
(a) immediately	115(26¾%)	214(50%)	89(20¾%)	7(1½%)	4(1%)
(b) later	30 (7%)	107(25%)	158(37%)	109(25%)	25(6%)
2. How often has the required journal been obtained from another library?	70(16½%)	135(31½%)	123(28½%)	90(21%)	11(2½%)
3. Apart from initiating a loan request, how often have you asked a member of the library staff for help in finding references?	11 (2½%)	58(13½%)	135(31½%)	224(52½%)	1 (0%)

4. Have you been notified of interesting titles of papers in languages which you cannot read yourself?

YES: 288 (67%) NO: 140 (33%) N. ANSWER: 1 (0%)

If yes, please answer questions 5-9.

5. Which languages occurred most frequently?

Russian	204 (71%)	East European	16 (5½%)
German	106 (37%)	Italian	12 (4%)
Japanese	67 (23%)	Scandanavian	4 (1½%)
French	21 (7%)	Spanish	4 (1½%)
		Chinese	2 (½%)

	Always	Often	Sometimes	Never	No Answer
6. How frequently have you taken further action	43(15%)	75(26%)	36(47%)	24(8½%)	11(3½%)
7. How frequently have you attempted to find (a) an abstract in English?	92(32%)	55(19%)	83(29%)	40(14%)	19(6%)
(b) a regular cover-to-cover translation?	22(7½%)	43(15%)	84(29%)	119(41½%)	21(7%)
(c) a colleague who can read the language?	19(6½%)	38(13%)	97(33½%)	115(40%)	20(7%)
8. Have you ever used an index to translations?	0(0%)	3(1%)	14(4%)	250(87%)	22(8%)

9. Have you attempted to have a paper translated other than by a colleague?

YES: 32 (11%) NO: 250 (87%) NO ANSWER: 7 (2%)

If yes (a) by whom and in which language?

(b) how often were you successful?

The answers to 9(a) and (b) are summarised in the following table:

Table 6: Translations

Methods	Language	Success
Professional Translator	Russian	No - too expensive
	Russian	Once only
University Staff	Russian	Once only
	German	Each time
	Russian	Always
Translation Service	(Russian	Each time
Library T.S.	(Japanese	Too expensive
Computer	Russian	Successful
ASLIB T.S.	Japanese	Too expensive
DSIR	Russian	Always
Libraries: NLL	Russian	No
	Chinese	Unspecified
Chem. Soc. Lib.	German	Unsuccessful
Science Lib.	French) German)	Unspecified
Library Staff	Polish	Successful
	Czech	"
Industry ICI	Japanese	Once - successful
	Japanese	
Pharmaceutical	German) French)	Always
Language Centres	Unspecified	Usually
	Russian) Slovak)	Occasionally
Students/Friends	Hungarian) Japanese) Italian)	Generally

+ 4 unspecified methods

In the following sections summaries are given for those answers which could not be coded for the punched card analysis. A complete list of summarised comments is available together with the profile number to identify them. These will be of use if a more detailed analysis is required.

Section C: User's Impression of Scheme

1. What have been the useful feature(s) of the service? More than one item may be marked or alternatively, none.

Provides a more comprehensive search of the literature than previous methods	220 (49%)
Convenience - "makes life easier"	203 (47½%)
Provision of background material	142 (33%)
Alerting to the appearance of new journals	46 (10½%)
Other useful features (listed below)	30 (7%)

2. What are the disadvantages (if any) of the service?

3. What improvements would you like to see in the scheme?

4. How do you think the service compares with conventional secondary sources of information?

5. Do you consider that the scheme could have been operated without liaison scientists?

   YES: 42 (10%) NO: 376 (88%) NO ANSWER: 11 (2%)

6. After experience of the present scheme, do you consider that
   (a) you could formulate an acceptable profile for a new research project?

   YES: 383 (89%) NO: 41 (9½%) NO ANSWER: 5 (1½%)

   (b) instruct other research workers how to formulate profiles?

   YES: 295 (69%) NO: 119 (28%) NO ANSWER: 15 (3%)

7. Do you know more about methods of obtaining information now than you did before the project started?

   YES: 290 (67½%) NO: 136 (31½%) NO ANSWER: 3 (1%)

   If yes, (a) do you consider that the scheme is mainly responsible?

   YES: 274 (94½%) NO: 10 (3½%) NO ANSWER: 6 (2%)

   (b) what have you learnt from the scheme?

C1: Other Useful Features Listed

(a) Coverage of foreign journals or of other journals that the user was unaware of or did not have available.

(b) Prior notice of useful references.

(c) Provided a useful printed list that could be used retrospectively.

(d) Provided an insurance policy i.e. a check on the user's own search methods.

Amost everyone had remarks to make on the disadvantages of the service and/or improvements they would like. It is possible to classify only broadly the various answers to questions C2 and C3. These are given in order of frequency of appearance. The items marked with an asterisk are really criticisms of the CT data base and the items marked with a cross are also unfair comments on the actual project.

C2: Disadvantages

* 1. The titles of papers are not very good guides to the full contents, which leads in turn to points 2 and 4.

2. General profiles provide a large amount of irrelevant references. Narrower profiles may well miss references.

* 3. The range of journals covered is limited.

4. Difficulty in constructing a profile to cover a research interest that is wide or constantly changing.

5. Print-out of references arrives before the journals are available in the library (however, see point 7).

6. Service could make the user lazy in that he neglects to read outside the scope of Chemical Titles.

7. Journals arrive in the library before the print-out arrives and so most references have already been found.

+ 8. References cannot be filed easily because of paper print-out.

* 9. No facility for retrospective searching.

*10. No patent coverage by the service.

C3: Improvements

* 1. Scan abstracts as well as titles. Cover Chemical Abstracts.

* 2. A method to carry out a retrospective search.

* 3. Card output for more convenient filing.

* 4. Titles of papers should include a set of keywords and/or reflect the contents of the paper. Standardise titles.

* 5. Extend the range of journals covered.

6. More opportunity to change profile and more time spent on planning the profile.

* 7. Classify titles.

* 8. Provision of abstract with print-out, and author addresses.

9. Supply journal list including the abbreviation and code or print-out full title.

10. Make the service available to other students in other years.

11. Extend to group profiles.

*12. Some method of formulae and/or structure search.

The answers given to question C4 shows that more users consider the service just as good if not better than other secondary sources of information than consider the service inferior. (259 better or as good; 3 not as good; 27 not as comprehensive as manual search). 50 users commented that the service was quick.

Over 80% though that liaison scientists were necessary for the scheme to operate. About 10% gave methods which could eliminate the need for liaison scientists. Of those users who think that the scheme could run without liaison scientists, about half suggest providing a detailed instruction manual and another quarter suggest using a member of staff in the department who is competent to construct profiles. Others think that the liaison scientist is only required at the beginning when profile construction and introduction to the scheme is taking place. It is noteworthy that only 10% of users think liaison scientists are not necessary especially when 90% think they could construct their own profiles for a new research topic for themselves and 70% could for other research workers.

At the end of the project, 89% of users felt confident that they could formulate a profile for a new project and 69% felt that they could instruct others. The accuracy of these statements will be checked during the present exercise (1968-70) for those students who have moved to new projects in universities in the United Kingdom. The majority (67%) of users said that they now knew more about information methods than before the project started and practically all of these (94%) considered that the scheme was mainly responsible.

Section D: Future Occupation

421 questionnaires were analysed to determine the future of the students participating in the scheme.

32 users had already completed their theses when they completed the questionnaire and a further 295 hoped to have finished their theses by October 31st 1968.

301 had definite posts to go to while a further 109 were uncertain about the future.

A break-down of the 301 definite posts is given below:

Temporary research abroad e.g. postdoctoral fellowship	99
Permanent research in industry in U.K.	80
Temporary research in other universities in U.K.	26
Temporary research in same university in U.K.	19
Teaching in U.K. universities	16
Teaching in U.K. schools	7
Other posts in industry in U.K.	14
Industry and Government abroad (permanent research)	14
" " " " (temporary ")	7

Of those who did not have definite posts to go to the principal choices of career are given below:

1st choice:	Postdoctoral fellowship abroad	31
1st choice:	Industrial research U.K.	17
1st choice:	Postdoctoral fellowship U.K. universities	15
1st choice:	U.K. university teaching	12
2nd choice:	Postdoctoral fellowship U.K. universities	15
2nd choice:	U.K. industrial research	14
2nd choice:	Postdoctoral fellowship abroad	9

As can be seen from the figures 130 of the 421 students will be going, or would like to go abroad for temporary university research posts while 97 chose industrial research in the United Kingdom.

Section E: Vital references

A 'vital' reference was defined as one that had a definite impact on the user's research work. Students were asked to list all such references that had appeared since September 1967.

Section E of the questionnaire was not fully understood by some users and so the liaison scientist had to carefully check the answers and, where appropriate, ask for further information at the final interview. Some students were not available for the final interview and sent in their completed questionnaires by post; in these cases only those answers which appeared to be self-consistent have been used.

Vital References

Area	A	B	C	D	E	F			Total
No. of refs. first seen in print-out	97	86	106	62	30	140			521
No. of refs. first seen elsewhere	76	28	69	46	35	64			318
No. of refs. found only by service	18	24	29	21	14	28			134
No. of refs. found by conventional methods (inc. service)	155	90	146	87	51	176			705
No. of questionnaires data taken from	50	37	55	31	23	47			243
									Total refs.: 839

62% of all references listed as useful were first seen in the print-out and of the total number of all references an average of 16% would have been missed had the service not been used.

Most papers referred to by the service and listed as useful were available within one week of notification. Those which were not were often papers in foreign languages for which translations were needed.

General Comments

The section on "general comments" in the questionnaire was often used to reiterate points made previously in answer to specific questions. It is therefore permissible to treat these comments as underlining the more important advantages and disadvantages listed by the users. A selection of comments is given below:

Profiles should be made more selective by using negative weighted keywords.

Profile takes time to perfect and so it would be better to start the project in the second year.

If the author name is made a keyword in the profile it is possible to retrieve work of that author.

The longer the profile runs the more useful the service becomes.

Profile can produce an extremely wide selection of references and gives a vital check against missing important references.

Profile should give more individual output.

Difficult to get an exact profile. Should have regular revision and change of profile as research topic develops.

User resorted to manual search because topic changed but profile still covered basic project.

Is enough time spent on planning the search profile?

Would like a method of adding to the profiles more quickly.

Difficult to define general interests and so difficult to formulate a profile to cover these.

Profile to cover reviews would produce too much irrelevant information.

Important references can be missed because of improper design of profiles.

Profile setting up and polishing is quick enough now. If abstracts were added the output would be too large.

Profile needs to be more precisely defined to cut irrelevance.

It is important to define the question precisely before constructing the profile.

Profiles containing common reagent names are not particularly useful because title would not cover these.

It would be better to have 'combination-words' before recording a 'hit'.

A lecture given two weeks before formulation of the profile would give students time to draw up a list of keywords.

User thinks he could do search just as quickly as his very broad profile.

User would like to construct a profile to cover general interests but to give not too much output.

It took a long time to change profiles from CBAC to CT.

A really successful profile can only be constructed after studying titles of important references because "you can say the same thing several ways".

Profile amendment increased relevance without decreasing output.

The scheme is very useful provided you can put a research topic into a profile.

A profile with narrow limits proved successful since relevance was high when a reference was recorded as a "hit".

Profiles should be constructed more carefully.

It is better to have too wide a profile than too narrow.

User would like closer contact with the liaison scientist so that more rapid amendments to the profile can be made as the topic changes.

Profile is only as useful as titles allow.

User would not rely solely on scheme because of inadequacies in the profile. These are: (1) it selects only from titles (2) interest changes with experience.

User had difficulty in formulating a profile which gave specific references rather than general background references.

Profiles do not always contain the right keywords.

It is better to alter the profile as research interest changes.

The scheme is good provided the profiles are kept up to date.

More involvement of the student in formulating the profile and greater explanation by the liaison scientist.

Only one comment does not mention the word "profile" and this one is still concerned with words. By far the most frequent comment concerned the need to amend the profile as the research work changes: several users would have liked "more opportunity to alter the profiles". Clearly, some users were unaware that it was their responsibility to instigate an amendment (cf. Interview Sheet Q3).

It was apparent that some users had a research topic that was not suitable to be covered by a titles-only search and this seemed particularly true for organic chemists engaged in synthetic work and physical chemists interested in particular techniques.

Perhaps the whole scheme can be summed up by the following comment: "the scheme is very useful providing your research topic can be expressed in terms of keywords and providing the profile is kept up to date".

Interview Sheet

A supplementary sheet to the final questionnaire was filled in by the liaison scientist on his final visit to each user. As can be seen from the combined statistics from 438 profiles for 429 users, most students were satisfied that 3 or 4 visits per year were sufficient. A noteworthy point is that even students with large outputs spent only about 15 minutes per fortnight scanning their lists of titles. The high percentage of users who thought that the scheme was worthwhile offers encouragement for future work.

Interview Sheet: Combined Statistics

Question	No. of Students	Notes
1. Number of interviews with each student: 1	1	Total of 1339 visits No answer given : 25
2	26	
3	225	
4	149	
5	3	
2. Student would like: More	46	No answer : 59
Same	290	
Less	34	
interviews		
3. Profile modifications:		Total : 617 No answer : 58
(a) at interviews	354	
(b) at other times	263	
4. Average number of references per issue: 0-10	70	No answer : 58
11-20	104	
21-30	82	
31-50	96	
750	54	
5. Time taken per fortnight to scan printout: 15 min	267	No answer : 61
15-30	65	
30-45	5	
45-60	24	
60-90	2	
90-120	3	
120	2	

Interview Sheet: Combined Statistics (continued)

Question	No. of Students	Notes
6. Fate of printout:		
Throw away *	112	* Includes those who keep useful references by making notes or cutting up the printout.
Keep	110	
Pass on	133	
Unspecified	83	
7. SRC student on same topic next year:		No answer : 77
Yes	144	
No	108	
Don't know	44	
Probably	21	
Unlikely	19	
Possibly	16	
8. Students attitude:		No answer : 39
Enthusiastic	142	
Worthwhile	216	
Apathetic	27	
Waste of time	5	

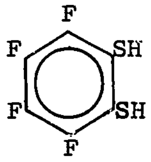
Chapter 4: Research Reports

The liaison scientists would like to thank OSTI for financial support and their respective Heads of Department for the use of departmental facilities.

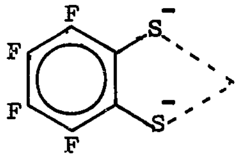
A. Callaghan: Chelating Properties of Tetrafluorobenzene 1, 2 - dithiol

Introduction

Research was carried out during the year in the field of organometallic chemistry and was concerned with the chelating properties of a potentially powerful new ligand, tetrafluorobenzene 1, 2-dithiol

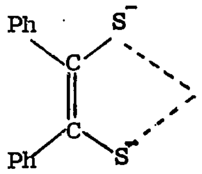


tetrafluorobenzene dithiol

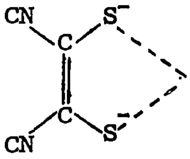


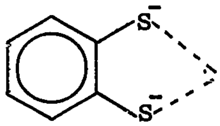
tfbt

This ligand can be considered as one of a class of 1,2-dithiols, some members of which have been previously investigated. Typical examples of these are:-



sdt





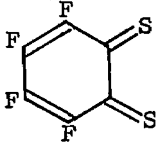
Studies of the transition metal complexes of these ligands have been rewarding in the past due to the discovery of a number of unusual features. Firstly, square planar geometries of bis complexes are stabilised over a large range of metals including Fe, Co, Rh, Ni, Pd, Pt, Cu, Ag and Au. Secondly, more than one oxidation state of a bis complex may be stable, e.g. $[\mathrm{Ni(sdt)_2}]^{0}$, $[\mathrm{Ni(sdt)_2}]^{-1}$ and $[\mathrm{Ni(sdt)_2}]^{-2}$ are all known. Thirdly, some of the neutral six-coordinate tris complexes, e.g. $\mathrm{Re(sdt)_3}$, have been shown to have trigonal prismatic stereochemistry rather than the more normal octahedral one. Very few molecular complexes have trigonal prismatic stereochemistry, and some unusual physical properties, e.g. magnetic, result.

The position of the present ligand in the range of 1,2-dithiols is an extreme one. The fully fluorinated benzene ring promotes strong acid behaviour and one might reasonably expect to find pseudo-halogen activity, giving an interesting series of new compounds. There were two main problems in working with the ligand. Firstly, it was expensive and difficult to produce, and only a small sample was available (initially 5 ml., later supplemented by a further 2 ml.). This meant that considerable care had to be taken to minimise waste, and work with small quantities. Secondly, the 5 ml. of ligand which was originally available was only ~ 75% pure. This resulted in difficulties in the purification and re-crystallisation of some products.

Experimental and Results

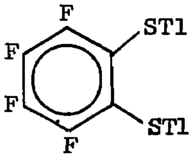
It is not intended here to present a rigorous research report; a brief outline of the principle points of interest seems more suitable.

It was immediately apparent that the ligand was a powerful complexing agent. In transferring small quantities with a syringe, the dithiol dissolved away part of the metal in the syringe to form a strongly coloured complex. The dissolved metal was shown to be copper, and subsequent experiments proved that the ligand had no difficulty in dissolving this metal at room temperature. (Hopes of a breakthrough in precious metal chemistry were not realised, however, when it was found that Ag, Au and Pt were unaffected.) Isolation of the copper complex produced a black powder of variable composition with the most likely ligand-to-metal ratio being 2 to 1. A second compound was isolated from the reaction between copper and the ligand. This crystallised as pale yellow needles and proved to be an oxidation product of the ligand, tetrafluorobenzene dithione.



Tetrafluorobenzene dithione

The ligand reacted easily with transition metal ions in a variety of oxidation states to form complexes. Due to impurities, however, the end product tended to be an oil, from which it was difficult in many cases to isolate a pure complex. This problem could be overcome by using the dithallium salt of the dithiol as starting material. This compound was



prepared from the reaction between thallium acetate and tetrafluorobenzene dithiol in methanol, followed by centrifugation of the product. By this means not only were soluble impurities washed away in methanol, but small amounts of mono-thiol impurity were isolated, this being much lighter than the dithiol compound, and was consequently found on the surface after centrifugation. In using this salt for the preparation of complexes a chloro compound of the transition metal under investigation was normally used as co-reactant, whereupon thallium chloride would be precipitated. After filtration, this left a solution of the pure complex for further study.

Products prepared to date are of two types, neutral complexes of first transition series metals, e.g. $Ni(tfbt)_2$, and charged complexes of second row metals, e.g. $[Et_4N]^+_2$ $[Mo(tfbt)_3]^{--}$. Charged complexes of first row transition metals have also been identified, but seem to be stable only with very large cations of the type $[Ø\ As]^+$. With the tetraethyl ammonium cation a variety of products are produced. Unfortunately the analysis of arsenic in the presence of fluorine and sulphur is causing problems, and so new large cations are being investigated with which to precipitate the first row metal charged species. At the present time data is most complete for the molybdenum compound mentioned above. This will therefore be presented now in some detail as an example of the line of approach used, and will conclude this section.

The starting material for this product was Mo II acetate. (This had to be prepared independently from molybdenum hexacarbonyl and glacial acetic acid.) Mo II acetate was dissolved in acetone and tetrafluorobenzene dithiol was added. A dark green solution resulted, from which it was impossible to isolate anything except a viscous oil. On addition of tetraethyl ammonium chloride, however, the colour changed to deep blue, and a blue crystalline product could be forced out of solution with benzene. The analysis of this product was as follows (%):

C: 41.4 H: 4.1 N: 3.1 F: 22.8 S: 19.1

The calculated analysis for a compound of composition $[C_2H_5)_4N]_2$ $[Mo(C_6F_4S_2)_3]$ is:

C: 41.1 H: 4.0 N: 2.8 F: 23.0 S: 19.3

This is a very good agreement.

As a 2:1 electrolyte the compound would be expected to have a molar conductivity of approximately 150 mhos. Experimentally the value found was 159 mhos, again in good agreement.

The formal oxidation state of the molybdenum is IV, giving a d^2 system. With octahedral stereochemistry this should result in a magnetic moment of ~2.83 B.M. Instead, the compound was found to be diamagnetic at both room and liquid nitrogen temperatures. The measured diamagnetism was $\chi_M = -500 \pm 50 \times 10^{-6}$ cgs, compared with a theoretical value of $\chi_M = \sim -527 \times 10^{-6}$ cgs, and so there was no underlying paramagnetic component. This result is consistent with trigonal prismatic stereochemistry, as it is possible in this configuration for both d electrons to be paired in a low-lying dz^2 orbital, resulting in diamagnetism.

Optical spectra were taken on a Unicam SP 800 from 325 mu to 700 mu. There were two broad absorption bands, one at ~17,000 $cm.^{-1}$ and one at ~29,000 $cm.^{-1}$, both with high extinction coefficients of the order of 10^4. This result should be compared with the spectra of the $Re(sdt)_3$ neutral complex mentioned earlier. In the Re case there were also two broad bands with high extinction coefficients, but these were at 14,000 $cm.^{-1}$ and 24,000 $cm.^{-1}$. In the case of the charged species therefore there has been an appreciable shift to shorter wavelengths.

Conclusions

The initial objective of the research - to demonstrate the potential of a new ligand - has been achieved. Further work is open-ended in the number of new compounds which may be prepared, any one of which could have interesting properties.

T. H. Cannon: Ph.D. Thesis

Total time doing active research was about a month, most of it wasted. Even simple preparations take time, and machines may take days to get working in the way one wants. There can be few practical projects that can be carried out concurrently with a job that requires some time every day and which may take one away unexpectedly at short notice.

The completion of the thesis has been long delayed, and probably not given full attention for periods longer than a day or two. Some writing was possible in the periods late February/early March, mid-May and July/August. One chapter has been written (and a few confirmatory experiments done), one rewritten, and the rest edited and transcribed since October.

Also, a chemistry part II student was started on his project and advised periodically, although this did not cause undue strain.

Summary of Ph.D. Thesis

This work describes some aspects of dynamic nuclear polarisation (the Overhauser Effect) and its application to various chemical problems.

Chapter one gives a general introduction to dynamic polarisation, showing how, when the electron paramagnetic resonance absorption of a free radical in solution is partially or totally saturated, the solvent nuclear resonances are drastically modified, being either enhanced or inverted. The theory of the effect, based on a treatment by Solomon of a two spin system, is given. A short discussion of spectral densities and correlation times, and their importance in the interpretation of Overhauser effect experiments, follows. The various models for modulation of nuclear-electron coupling and experiments to distinguish between them are described. A summary of Natusch's theory of the three-spin effect is given and the final section deals with a novel phenomenon, chemically induced dynamic nuclear polarisation.

Chapter two deals briefly with the apparatus used in Overhauser effect experiments and especially with aids in detecting weak signals. The possibility of stimulated emission in Overhauser effect experiments is investigated and concluded to be a very small correction for most measurements.

Chapter three deals with the dependence of dynamic enhancements on the nature of the free radical used. It starts with a review of the properties, reactions, detection and identification of stable free radicals and includes a list of radicals used in these experiments. Dynamic enhancements of solvent resonances are tabulated for the various radicals (a) in benzene, the protons of which are dipolar coupled to the unpaired electron, and molecular parameters may be calculated, (b) in hexafluorobenzene, where the fluorine muclei show mixed dipolar and scalar (contact) coupling to the electron, so that complete evaluation of results is not possible but a qualitative comparison of radicals can be made; and the applicability of equations based on various models is discussed. Less strictly quantitative measurements on ^{31}P and ^{13}C, using various radicals, are also briefly mentioned.

Chapter four investigates the differences in dynamic enhancement between different protons within the same molecule. Consistent differences of the order of 10% are found between aliphatic and aromatic protons. Geometrical considerations show that this may be accounted for by variation in distance of closest approach between proton and radical electron.

Chapter five deals with the application of the Overhauser effect to observe natural abundance (1%) ^{13}C spectra. Surprisingly the ^{13}C nucleus in simple organic molecules shows a considerable degree of scalar coupling to the free radical electron, especially in halogenated aliphatic compounds. The mechanism of scalar coupling is explained in terms of "spin-conducting" and "spin-insulating" atoms and groups in the structure of the molecules. ^{13}C spectra are ideal for observation of "three-spin" effects, where the proton polarisation affects the ^{13}C polarisation. This is especially noticeable at low concentrations of radical. Finally, the observation of an isotope shift in ^{13}C spectra, between benzene and perdeuterobenzene, is observed and explained.

E. J. Herbert: Photocyclisation of Anilinopyrimidines

Chemical mutagenesis arising from the action of various aminoacridines on bacteriophages has been extensively studied. It has been proposed that the mechanism of action involves intercalation of the planar acridine molecule between successive base pairs in the DNA structure, with increase in the spacing of the latter from 3.4 Å to approximately 7 Å. This increase in spacing gives rise to a misreading of the genetic code, one consequence of which can be recognised as mutation.

Convincing evidence of intercalation has been provided by studies of viscosity and small angle X-ray diffraction. Clearly the intercalated base might be more effective if specific hydrogen-bonding could occur with a purine or pyrimidine base in the complementary nucleic acid chain. All naturally occurring nucleotides contain hydrogen-bond donor and acceptor sites in a 1:3 relationship, and in consequence it is of interest to generate such systems involving acridine and related nuclei. Since donor as well as acceptor capacity is required, attention was paid to aza-substituted carbazoles, e.g. carbolines, pyrrolodipyridines, and pyrimido-indoles.

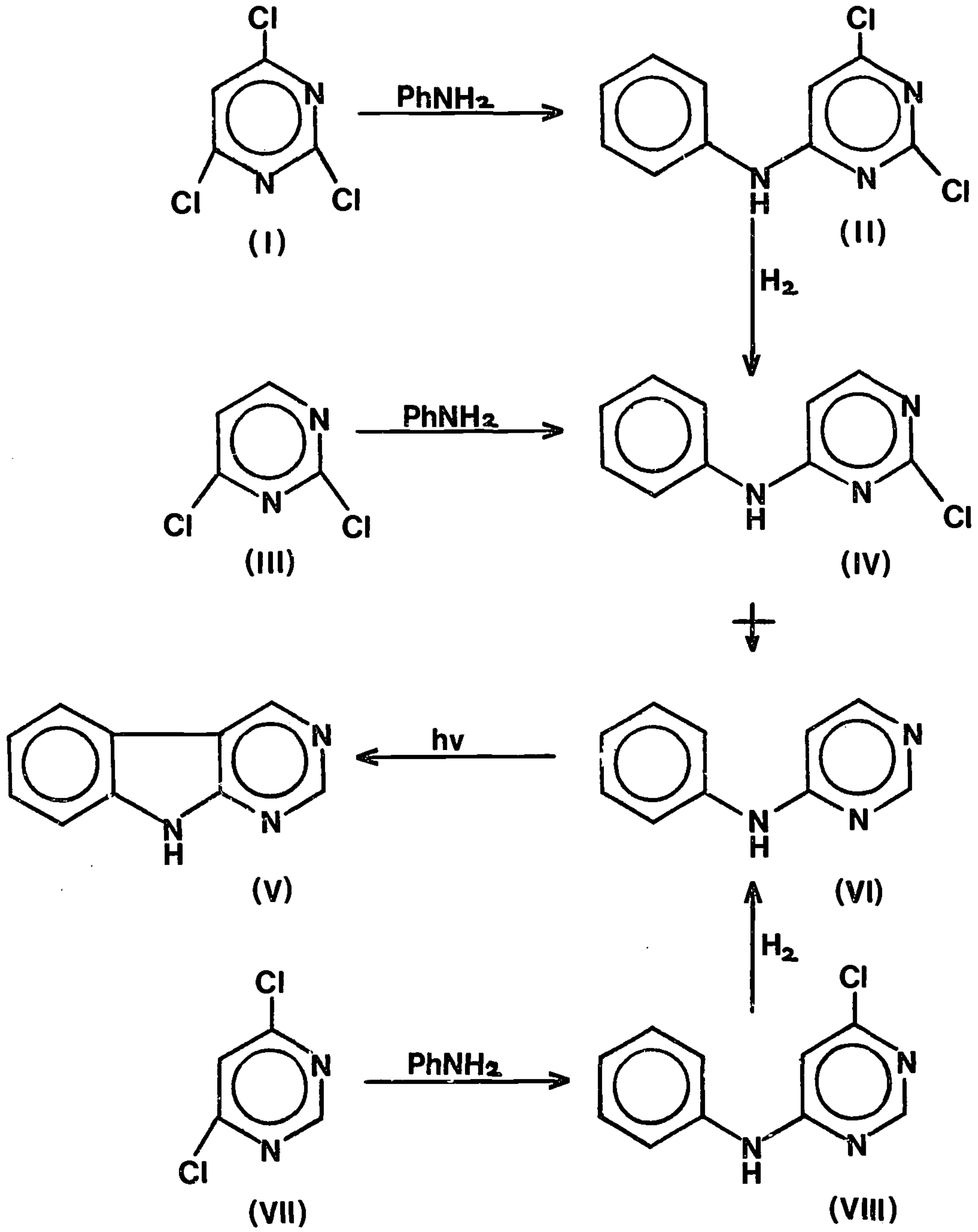
On irradiation in a variety of solvents, diphenylamine undergoes oxidative photocyclisation to carbazole. By analogy, anilino-pyridines should yield carbolines, dipyridylamines should yield pyrrolodipyridines, and anilinopyrimidines should yield pyrimido-indoles. Last year's work provided examples of the first two cases and the third is illustrated by the present work, in which 4-anilinopyrimidine (IV, Fig.3) is photoconverted to 9H-pyrimido-(4, 5-b) indole (V).

The anilinopyrimidine was prepared by catalytic dehalohydrogenation of 4-anilino-6-chlorophyrimidine (VIII). Hydrogenation of 4-anilino-2, 6-dichloropyrimidine (II) was less successful as a mixture of 4-anilinopyrimidine (VI) and 4-anilino-2-chlorophyrimidine (IV) was obtained. Irradiation of the anilinopyrimidine for 48 hours gave the required ring system in 80% yield.

In order to determine if cyclisation involving a ring nitrogen atom could be effected, 2-anilinopyrimidine was irradiated for 36 hours in tetrahydrofuran. The main chromophore was gradually destroyed but no new peaks appeared in the u.v. spectrum of the reaction solution. Irradiation in the presence of iodine also

FIG (3)

Preparation of 4-anilinopyrimidine and photocyclisation to the pyrimidoindole (V)



failed to bring about cyclisation.

A proposed cyclisation involving the formation of a six-membered ring is now being investigated with 9-anilinofluorene, prepared from 9-chlorofluorene.

REFERENCE

V. M. Clark, A. Cox and E. J. Herbert, *J.Chem.Soc*. (C), 1968, 831.

P. Leggate: Further Information Work

Time allocated for research work was used for the preparation of various standard parameters and on an extra project involving the follow up of marked references. (See section in Chapter 2 on fate of references).

C. M. Lee: Inventory of Secondary Information Sources*

In essence, ALL time was spent on information work with a few hours a week spent discussing research problems with postgraduate students. The major part of time (between visits) in 1968 has been the preparation of "An Inventory of Some Secondary Services in Science and Technology". The Inventory covers over 100 different secondary services (see list) and attempts to provide a convenient synthesis of information on information. An example of the layout for the inventory is also included (on MEDLARS). A paper entitled 'The Jigsaw Puzzle' has also been written trying to examine the differences between scientific and artistic creativity and presenting some of the recent trends in Information Science.

An Inventory of Some English Language Secondary Services in Science and Technology

Introduction

This Inventory was designed to keep me aware of all the variety of secondary services available to the scientist and technologist. Believing in the heuristic approach, I know that the best way to learn is to teach and I have tried to present a survey of some of the multitudinous ways one can search for information in Science and Technology.

Method

Perhaps a word is in order on the method of data compilation for this Inventory. In the great majority of cases I was able to examine the printed version of the service in detail along with descriptive literature and references. At this stage a "work-sheet" on the service(s) was prepared and sent to the Service for their comment and correction. In most cases this cooperation was forthcoming and the revisions incorporated in the final copy; however, any and all errors remain my responsibility. Because of budgetary and other considerations the layout is not as attractive, in some cases, as I would have liked; furthermore certain errors have managed to pass my 'sparrow-like' scrutiny. I would greatly appreciate being informed of any errors of commission or omission as well as errors of stupidity in the event another edition is published.

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* Updated and reproduced by OECD, March 1969.

Indexes

I have included a number of indexes so we can look at the raw information from many different viewpoints. The Subject Index (by colour) is based on different disciplines and I have included some services (e.g. law) that are not strictly science and technology. The Source Index, divided into governmental and non-governmental (societies and commercial) includes organizations that have been helpful to me even though no 'products' appear in the Fact Sheets (e.g. SATCOM, OSIS). The Functional Index classifies the different approaches to Information Retrieval and the Alphabetical Index provides a complete listing of ALL Publications and Services mentioned in the Fact Sheets and Source Indexes.

Features

Some special features of this Inventory might be noted. The Fact Sheet format has the following features: unbound pages, two services on a sheet, and colour subject indexing. The unbound sheet, besides being more convenient production-wise allows easy additions and one can make side-by-side comparisons of similar services in different subject areas (e.g. the three Current Contents, Current Chemical Papers and Current Papers in Physics). One can also compare all the services in one area at one time. I have tried to place similar services of the same subject on the same sheet so that direct comparisons may be made (e.g. DMS and Sadtler IR Spectra Services). Finally the Colour Coding makes all of the comparisons easy and also looks attractive.

Coverage

A few facts about the coverage of Secondary Services are shown in the table appended to the end of this Introduction. They show that a very low percentage of the journals scanned are required to provide 90% coverage. The first 15% of Chemical Abstracts coverage is contributed by only 18 journals while the last 15% requires scanning of over 8000 journals (1). The number of journals scanned is not necessarily a reflection of the comprehensiveness of coverage. Chemical Abstracts scans about 12,000 publications a year but only 6000 different serials are cited in each half-yearly volume. Whether it is necessary to cover the last 10% of journals at great expense and time (because they are usually obscure foreign journals) is debatable.

The ICSU-Abstracting Board (whose members are the services shown on the attached table) has listed 107 'Major' journals in Physics, 220 'Major' journals in Biology and 259 'Major' journals in Chemistry; coverage of only these journals would yield most of the important papers in their respective areas (2).

I have tried to indicate whenever possible how comprehensive the coverage is e.g. 'Journals completely abstracted'. Science Citation Index (SCI) is probably unique in its comprehensive coverage with twelve different categories indicated: original articles, papers or reports; abstracts; book reviews; corrections; discussions; editorials; awards etc.; letters; meetings; notes; patents; and reviews. Another interesting feature of SCI is that it is a calendar year index, i.e. the 1967 SCI covers all issues of a journal published in 1967 be it one or fifty-two issues.

It is my hope that my effort will help not only scientists and technologists but management and administration to be aware of the wealth of access points to the pieces of the jigsaw puzzle available today. I hope you also have fun using it!

Acknowledgements:

I wish to thank those mentioned in the Source Indexes for their cooperations (especially those who took time out to see me on my last US trip in January 1968). This work was supported by OSTI, Chelsea College, Apple Corps., and myself.

References:

1) "Chemical Literature Expands" by Dale B. Baker in Chemical & Engineering News, 44, 84-86, 88 (June 6, 1966).

2) See ICSU-AB in the Source Index: Governmental & International.

Bibliography:

1) F. Joachim Weyl et al, "Secondary Services in the Private Sector", SATCOM working paper (not for publication) 1967, 66 pp. A very valuable and comprehensive paper.

2) J. Richards, "Guide to the Abstracting and Indexing Services Available in the College Library", Chelsea College, 1967, 29 pp.

3) J. C. Troutman, "An Inventory of Available Data Bases", Institute of Library Research, UCLA (Dec 15, 1967) 57 pp.

4) Leonard Cohen, ed., "Directory of Computerized Information In Science and Technology" Science Associates, New York City, 1968, $175.

5) OECD Group for Scientific and Technical Information Policy "Information Activities of Some Major International Organizationa", August 8, 1967, 95 pp.

AN INVENTORY OF SOME ENGLISH LANGUAGE SECONDARY SERVICES IN SCIENCE AND TECHNOLOGY

CHEMICAL SCIENCES

Chemical Abstracts / Chemical Abstracts Basic Journal Abstracts
Chemical Titles (CT) / Chemical Abstracts Condensates
Current Contents Chemical Sciences / Current Chemical Papers (CCP)
Polymer Science and Technology - Journals/Patents (POST-J/P)
Index Chemicus (IC) / Analytical Abstracts

CHEMICAL/BIOLOGICAL CODES

Chemical Abstracts Registry System / Auxilliary Chemical Module
Index Chemicus Registry Service / Derwent Ring Chemical-Biological Code
de Haen Chemical-Biological Code / DMS Chemical Code

BIOLOGICAL SCIENCES

Chemical Biological Activities (CBAC) / International Pharmaceutical Abstracts
RINGDOC / VETDOC / PESTDOC
MEDLARS (Medical Literature Analysis and Retrieval System) Tape / Printed
Research Grants Index (PHS) / WHO Biomedical Information Centre
Excerpta Medica Abstracts / Excerpta Medica Information Retrieval System
Unlisted Drugs / de Haen Pharmaceutical Information Services

PHYSICAL SCIENCES

Physics Abstracts / Computer-based Physics Abstracts
Americal Institute of Physics (AIP) Information Project / Technical Infor. Proj.
Current Contents Physical Sciences / Current Papers In Physics (CPP)
Nuclear Science Abstracts (NSA) / EURATOM Nuclear Documentation System (ENDS)

SPECTRAL SERVICES

Preston NMR Abstracts / DMS NMR Literature Lists
Preston GLC Abstracts / DMS Infrared Literature Lists
Sadtler Infrared Spectra / DMS Infrared Spectra
Sadtler NMR Spectra / Sadtler Ultraviolet Spectra
Mass Spectrometry Bulletin / Sources of Mass Spectrometry Information

MULTIDISCIPLINARY AND SOCIAL SCIENCES

Science Citation Index (SCI) : Source Index / Citation Index
SCI: Permuterm Indes / ASCA III (Automatic Subject Citation Alert)
DATRIX (Direct Access to Reference Information: Xerox) / Dissertation Abs.
Science Information Exchange (SIE) / National Referral Centre
PANDEX / Educational Resources Information Centre (ERIC)

PATENTS, REPORTS AND DATA

Derwent World Patents Abstracts / World Chemical Patents Index
FARMDOC / AGDOC AND PLASDOC
US Govt. R and D Reports / US Govt. R and D Reports Index
Uniterm Index to US Chemical Patents / Other Sources of Patent Information
Bureau of Census Data Files / 1970 US Census of Housing and Population
Materials Data / Technical Data
INDATA

TECHNOLOGY AND OTHER AREAS

Engineering Index / Current Awareness and Document Retrieval (CADRE)
LITE (Legal Information Thru Electronics) / Sources of Legal Information
Electrical and Electronics Abstracts / Control Abstracts
Solid State, Electronics, Information Processing Abstracts / Sources Computer Prog.
International Aerospace Abstracts (IAA) / Scientific and Technical Aerospace Rept.
SYMBIOSIS (System for Medical and Biological Science Information Searching) SUNY
MARC II (Machine Readable Cataloguing) / Sources of Library Information
Current Research Information System (CRIS) Agriculture
American Petroleum Institute Refining Abstracts in Literature / Patents

A sample sheet from the Inventory is reproduced overleaf.

Biomedical Sciences
MEDLARS (Medical Literature Analysis & Retrieval System)
Free Demand Retrospective & SDI Searches

Comprehensive Coverage of *2300 Biomedical Journals (45% foreign, 40 languages) plus monograph & serial titles

*250 Primary Journals with Median Currency of 56 days

Jan 1964 : Store of * 700,000 Citations from mid 1963 & 30,700 cataloged citations since 1966 from monographs & serial titles
1967: * 180,000 citations & 18,000 titles added

For Printed Services see Right

SEARCH BY:

1) FIXED TEXT TERMS (MeSH, Medical Subject Headings) * 7500 terms. Average 6.7, with 10 from 'depth' journals 5 non depth journals

2) JOURNALS

May be limited by language, time, location journal etc.

Different Forms of output & arrangement e.g. cards or paper author, journal title, language year of publication, subject headings

Three Levels of Searching
AND/ OR/ NOT Logic
MeSH headings printed with citation

Time of Search in US (11-30 days)

Other Centres (US: UCLA, Colorado, Alabama, Michigan, Harvard, Ohio State), UK: Newcastle, Sweden: Karolinska Institute

One 12 inch tape = 30,000 Citations
(File = 23 tapes)
Usually batch 25-30 searches a time

PRINTED MEDLARS SERVICES

A) INDEX MEDICUS (same data base as MEDLARS) Monthly 3 Print Index Terms

B) CUMULATED INDEX MEDICUS: 1 author 3 subject volumes (IM subscribers * 7000)

C) Medical Subject Headings (MeSH)

D) List of Journals Indexed In Index Medicus

E) Bibliography of Medical Reviews

F) NLM CURRENT CATALOGUE: Biweekly quarterly & annual cumulations

G) RECURRING BIBLIOGRAPHIES
  1) Bibliograhy on Medical Education (monthly)
  2) Cerebrovascular Bibliography (quarterly)
  3) Fibrinolysis, Thrombolysis, and Blood Clotting (monthly)
  4) Index of Rheumatology (monthly)
  5) Index To Dental Literature (quarterly)
  6) International Nursing Index (quarterly)
  7) Artificial Kidney Bibliography (quarterly)

H) DEMAND BIBLIOGRAPHIES:
Some 100 e.g Dimethly Sulfoxide
List available from Assistant to the Director
NLM, 8600 Rockville Pike, Bethesda, Md
20014, USA

OTHER COMPUTER-BASED PHOTOCOMPOSITION

a) PHOTON ZIP 901 (800 characters/ sec)

b) LINOTRON 1010 (CBS-Mergenthaler) * 1100 characters /sec, used by GPO

c) RCA VIDEOCOMP (Spectra 70)

d) IBM 2680 (Produced by Alphanumeric)

NLM: Honeywell H-800, H-200 with printing by GRACE (Graphic Arts Composing Equiptment, Photon 900 : 226 characters, speed *300 characters/sec) 7 magnetic tape drives
Other computers: English Electric KDF 9, IBM 360, 7094, 7040, 7090

NLM
STAFF: * 175
US Tape Searches * 8500/year
UK Tape searches *1900
Cost 1,000,000 $ + a year

MEDLARS II:
New hardware in 1970, Abstracts on file
On-line Acces and time -sharing facilities

M. Poustie: Reactions of Lead Tetracarboxylates

Three reactions of lead tetracarboxylates have been studied, viz, the reaction in acetic acid of lead tetra-acetate with iodine; the reactions in trifluoroacetic acid of lead tetra-acetate and lead tetrapropionate with tetramethylsilane; the reactions in dimethylformamide and acetic acid of lead tetra-acetate with the acids Ph-$(CH_2)_n$-COOH for n = 1-4.

The Reaction of Acetic Acid of Lead Tetra-acetate with Iodine

It had previously been found that lead tetra-acetate and iodine in acetic acid react at room temperature (to give iodine acetate?) and that this second-order reaction is catalyzed by the presence of sodium acetate.

It has now been discovered that with an excess of lead tetra-acetate reaction continues to give a precipitate which has the following properties:

(i) it is insoluble in all organic solvents

(ii) it dissolves in c.HCl with liberation of chlorine

(iii) in other aqueous solvents it reacts to give iodine, lead diacetate and lead iodate.

Gravimetric determinations of the lead content coupled with iodometric titrations suggest the precipitate to be composed of a 1 : 1 molar mixed crystal of lead diacetate and lead iodate (94%) and lead iodide (6%).

The Reaction in Trifluoroacetic Acid of Lead Tetra-acetate and Lead Tetrapropionate with Tetramethylsilane

Previous results had shown that it was not possible to use tetra-methylsilane as an internal reference for NMR spectra of lead tetra-carboxylates in trifluoro-acetic acid, as the tetramethylsilane reacted with the lead salts. The products of this reaction have now been identified as follows:

for lead tetra-acetate - Methyl acetate and methyl trifluoroacetate - by vapour phase chromatography (VPC) and NMR spectra.

Trimethylsilyl acetate - by treatment of a reacted solution with excess ethereal diazomethane, removal of the low-boiling esters so-formed and of ether, hydrolysis of the liq. organic residue and analysis of VPC and mass spectrometry of the products of this hydrolysis, acetic acid and hexamethyldisiloxane ($Me_3SiOSiMe_3$). (Trimethylsilyl acetate on hydrolysis would yield acetic acid and trimethylsilanol, the latter readily dehydrates in acid solution to give hexamethyldisiloxane).

for lead tetrapropionate - Methyl propionate replaced methyl acetate.

(Trimethylsilyl propionate presumably replaces the acetate, but has not been looked for).

If the reaction takes place in mixed pyridine-trifluoracetic acid the yield of methyl trifluoroacetate increases and that of methyl acetate (or propionate) falls to almost nothing.

The Reactions in Dimethylformamide and Acetic Acid of Lead Tetra-Acetate with Carboxylic Acids ($Ph-(CH_2)_n-COOH$)

Reaction between lead tetra-acetate and w-phenyl-acetic, propionic, butyric and valeric acids has been found to give products as shown below:

$$Ph - CH_2 - COOH \xrightarrow[\substack{DMF \\ O_2, H_2O}]{LTA} Ph - CHO \qquad LTA = Pb(OAc)_4$$

$$Ph - CH_2 - COOH \xrightarrow[AcOH, O_2]{LTA, NaOAc} Ph - CHO$$

$$Ph - CH_2 - COOH \xrightarrow[AcOH, N_2]{LTA, NaOAc} Ph - CH_2 - OAc$$

$$Ph - (CH_2)_2 - COOH \xrightarrow[DMF]{LTA} Ph - Et$$

$$Ph - (CH_2)_3 - COOH \xrightarrow[DMF]{LTA} Ph - {}^nPr$$

$$Ph - (CH_2)_4 - COOH \xrightarrow[DMF]{LTA} Ph - {}^nBu + \text{1,2-3,4 tetrahydronaphthalene}$$

The formation of these products can be accounted for by a free radical reaction as follows:

$$Pb(OAc)_4 + Ph(CH_2)_nCOOH \rightleftharpoons Pb(OAc)_3(OCO(CH_2)_nPh) + AcOH$$

$$Ph(OAc)_3(OCO(CH_2)_nPh) \longrightarrow Pb(OAc)_3 + CO_2 + Ph(CH_2)_n\cdot$$

with subsequent reaction of the so-formed $Ph(CH_2)_n^{\cdot}$ radical.

Appendix 1: Circular sent to all Participants

DEPARTMENT OF EDUCATION AND SCIENCE

OFFICE FOR
SCIENTIFIC AND TECHNICAL INFORMATION
State House, High Holborn, LONDON W.C.1
Telephone: CHAncery 1262

Our ref: SI/21/23 A

Christmas, 1967.

Students' Chemical Information Project

The aim of this circular letter is to inform all participants about the overall progress of this experimental project. Both OSTI and the liaison scientists welcome any comments you may have on the scheme or the content of this letter.

The first series of interviews between students and liaison scientists was completed in October and early November, and most participants will have received at least one output before the end of the first week in December. If there are no delays in the supply of magnetic tapes from Chemical Abstracts Service, outputs will now arrive by post at fortnightly intervals. We hope that the lists of references will prove useful in your research work, but do not hesitate to contact your liaison scientist if you think your output might be improved in any way.

We are keen to provide an acceptable service during this experiment but can only do so if there is close contact between yourself and the liaison scientist. The postcards supplied by the liaison scientist are one means of doing this and we hope that you will complete and return these within a few days of receiving your computer print-out. The following definitions may help you to complete these cards:

Total hits - the number of references included in the print-out. This is given at the end of the list.

Relevant - those references satisfying the short description of your research interests which you gave to the liaison scientist.

These cards provide a good indication of your profile's selectivity and accuracy and the results will help us to decide whether the experiment should be continued in future years. Furthermore, the cards provide an easy way for you to express your satisfaction or other feelings about the scheme: constructive comments are most welcome.

About 450 interviews have been held and the liaison scientists have learned much about your present literature habits. Many students were not familiar with the "current awareness" type of publication, designed to give a quick appraisal of new literature, or the mechanised version of the service which they are now receiving. However, Current Chemical Papers is used regularly by about one-third of the students and is more widely known than any other current awareness publication. A surprising number rely upon Chemical Abstracts to keep up-to-date but the majority of students scan about 10 primary journals. Chemical Abstracts is used almost universally for retrospective searches.

/Inadequate

Inadequate knowledge of information tools and services may be due to the lack of training. Nearly half the students interviewed said that they had received no training (or by the time of the interview had forgotten completely about it) and of the remainder only about 10% had received formal training which included practical work. The most usual form of training seems to be a short lecture or a short chat with the student's supervisor.

The project has been received enthusiastically in most chemistry departments. The outputs have been seen by many colleagues and keen interest has been shown by supervisors, some of whom sat in during the initial interviews. Already questions are being asked about the future developments of the project, but a decision on its extension for a further year cannot be reached until March, 1968, at the earliest. Many students consider that the time spent with the liaison scientists has been most valuable as a means of learning about present and future information handling techniques. The liaison scientists have enjoyed the work so far: however, this method of operation, while necessary in the first place, is expensive and changes may be necessary if the scheme is to continue and perhaps expand in the future. If liaison scientists are retained, it may be necessary to charge some of the costs to the users or their departments or to an alternative source of support. On the other hand, it may be possible for departments to perform the liaison scientist's functions, with the help of experience gained in the present exercise and after some training for staff members or senior research workers, thereby making liaison scientist redundant. The experimental approach of this year's study will provide a basis for such decisions.

Developments in the mechanised services themselves are also planned and perhaps the most interesting of these is the addition of selected key-words to the titles of the articles, which will permit the retrieval of topics not included in the titles. Such a system is planned by Chemical Abstracts Service for all articles appearing in Chemical Abstracts.

May we repeat once again that your comments and suggestions for improving the scheme are most welcome.

G. A. Somerfield.	
A. Callaghan.	University College, London.
T. H. Cannon.	University of Oxford.
E. T. Herbert.	University of Warwick.
C. M. Lee.	Chelsea C.S.T., London.
P. Leggate.	University of Edinburgh.
M. Poustie.	University of York.

Appendix 2: Covering Letter sent out with Final Questionnaire

DEPARTMENT OF EDUCATION AND SCIENCE

OFFICE FOR
SCIENTIFIC AND TECHNICAL INFORMATION
State House, High Holborn, LONDON W.C.1
Telephone: CHAncery 1262

Our ref: SI/21/23

May, 1968.

To all participants in

STUDENTS CHEMICAL INFORMATION PROJECT

The main purpose of this project has been to improve knowledge about methods of finding chemical information and in particular to extend experience of mechanized chemical information services. From the results so far both OSTI and the liaison scientists have formed the impression that the project has been well received in chemical departments throughout the country and that it has been successful - in particular that the service of references has assisted research work.

The preliminary results of the project have clearly established that there is a need for further education and training in the use of chemical information for all research workers. Accordingly, OSTI has decided to develop a new project which, whilst similar to the present scheme, will place greater emphasis on education and training. It is hoped to increase both the number of participants in the scheme and the range of services available, but in return more detailed evaluation of the services will be required from participants. The project will last for two years and staff are being recruited at present, but the exact details will be determined only when the final results of the present scheme are available.

Your liaison scientist will wish to make his final visit in the near future and will be seeking to find out whether our impression of the success of the scheme is correct. To help this assessment the liaison scientists and OSTI have prepared the enclosed questionnaire and we hope that you will complete it to help evaluate the project. Many questions can be answered simply by ticking the appropriate answer. Others seek an opinion and the liaison scientists will discuss any answers which are not clear during the final interview. They will make their own arrangements with you to ensure that the completed questionnaire is returned to them either before or at the interview. The results of the questionnaires and interviews will be analysed when all visits have been completed and in due course a report will be available.

I hope that you personally have found the project beneficial and that the experience gained will be of value to you in your future career. Please do not hesitate to put your comments and suggestions frankly at the interview or if you prefer, send them direct to me.

Yours sincerely,

(G. A. Somerfield)

Appendix 3: Example of a Search Profile

Parameter Number	Term Type	Logic	Term Weight	
1	T	Or		HEAT*
1	T	Or		ENERG*
1	T	Or		ENTROP*
1	T	Or		ENTHALP*
2	T	Or		REACTION*
2	T	Or		COMBUSTION
2	T	Or		FORMATION
3	T	Or		*SULF*
3	T	Or		*THIO*
3	T	Or		*THIA*
3	T	Or		*MERCAPT*
3	T	Or		*CYST*
4	T	Not		THEORET*
4	T	Not		CALCUL*
4	T	Not		ESTIMAT*

Appendix 4: Index Headings used in the Classification of Profiles

The "general" headings, which are marked with an asterisk, are provided for use where no specific heading is considered to be suitable.

Compound Index

Atoms	All phases
Ions	All phases
*Simple molecules	All phases
Non-metals	
Fluorinated compounds	
Non-transition metals	Or not specified
Transition metals	Not complexes or organometallics
Complexes	All metals
Organometallics	All metals
*Organic	General
Aliphatic	
Alicyclic	
Aromatic	
Heterocyclic	
Dyes and paints	
Alkaloids	
Steriods and terpenes	
*Natural products other than above	
Synthetic polymers	
Organic macromolecules	Peptides, nucleir acids, polysacchorides
Radicals	Gas or liquid phase, organic or inorganic
Molecular complexes	Charge transfer

Technique and Property Index

Biosynthesis	
Synthesis	
Structure determination	Degradative and unspecified methods
Stereochemistry	Conformation, configuration
Mechanism	Action or reaction
Thermochemistry	Thermodynamics, thermophysics, pyrolysis
Kinetics	Including rates of physical growth and relaxation
Physical properties	

Electrochemistry	Including polarography and electophoresis
Catalysis	Homo - and heterogeneous, and surface chemistry
Photochemistry	Including fluorescence and phosphorescence
Diffraction methods	X-ray, electron, neutron
Scattering, light or particle	Including molecular beams
Radiation chemistry	Radiolysis and tracer techniques
Ultraviolet and visible spectroscopy	Also X-ray spectra
Infrared spectroscopy	
Raman spectroscopy	
Microwave spectroscopy	
E.p.r.	
N.m.r./n.q.r.	
Mössbauer	
Mass spectroscopy	
*General spectroscopy	Unspecified
Optical rotatory dispersion	
Chromatography	All types including ion exchange
Miscellaneous techniques	
Theoretical chemistry	

Appendix 5: Compound Index to Profiles

ORGANOMETALLIC All Metals

B32 B36 B48 F12 F16 F22 F24 F26 F36 F64 H16 J44
K08 K36 M10 M14 M18 M36 M48 M58 M72 M96 M98 P08
P16 P32 P40 Q52 Q64 R28 R32 T06 T14 T16 T22 T32
W02 W10 W46 W92 X78

*** ORGANIC** General, not in categories below

B44 B72 C04 C56 C76 C96 D84 D94 E32 E40 E44 E72
F42 F46 F54 H28 H44 H68 L64 M08 M34 M62 M82 M88
M92 M96 P24 P28 P32 P64 P76 Q58 R66 S72 T10 T40
W14 W26 W28 X00 X04 X08 X32 X36 X56

ALIPHATIC

C08 C36 C92 D94 F28 F30 F42 H12 H24 H48 H68 H92
J48 L16 M88 P04 P20 P32 P44 P64 P84 R74 R78 S32
S52 W94 W96 X16 X32 X72 X76 Y08

ALICYCLIC

B64 B80 B92 D86 E20 E36 F28 F60 F68 H64 H68 L04
M88 P84 Q16 Q20 Q44 S68 V00

AROMATIC

B76 D16 D78 E04 E36 F18 F20 F44 F46 H20 H28 H48
H56 J40 L16 L80 M98 P60 Q04 Q24 Q44 Q48 Q52 R50
R74 S16 S40 S44 S48 S52 W00 W08 W16 W64 W76 X00
X20 X52 X99 Y16

HETERO CYCLIC

B72 C24 C48 D50 D84 E36 E56 E60 E84 E96 F52 H08
J32 J60 J80 L20 L28 P52 P68 P72 Q16 S36 S88 T32
V20 W72 X68 X76 Y32

DYES, PAINTS

B02 B14 B08 B12

ALKALOIDS

E16 E60 E84 H32 H36 H56 J24 J52 M64 M70 R54 W60
W72 W80 W82

STEROIDS and terpenes

D66 E08 F14 H32 H36 H48 H64 L92 M30 Q28 R70 W60
W68 X98 X99 Y28

ORGANIC MACROMOLECULES

B04 B16 C20 C28 C48 D54 D72 E48 H60 J72 J76 J90
K20 K40 K52 L48 L76 M68 Q62 Q64 S88 X00 X84 X90
Y32

* NATURAL PRODUCTS other than above

B92 C60 D50 D70 D82 D96 E24 E80 F62 H60 J08 J32
J72 J84 J88 K52 L08 L12 L88 M58 Q24 Q52 R90 S60
W04 W86 W88 W90 X00 X16 X28 X30 X44 X52 X76 Y00
Y24

POLYMERS synthetic

B84 B88 H80 H84 H88 H92 J28 J36 J56 K70 K72 V16
W78 W96 W98

MOLECULAR COMPLEXES

D08 F18 F20 K44

Appendix 6: Technique and Property Index to Profiles

BIOSYNTHESIS

F14 H36 H56 L88 M26 M28 M70 Q24 R70 X52 Y36

SYNTHESIS

B80 B92 D84 D90 E48 E60 H60 H64 J40 J84 K08 L12
L72 Q56 T26 W64 X16

STRUCTURE determination, degradative and unspecified methods

B04 C28 F18 F34 K04 L48 L96 M24 M32 M40 Q36 Q60
T08 T14 T22 V24 X68

STEREOCHEMISTRY Conformation, Configuration etc.

E20 L36 L52 Q16 Q28 S52 V12 X56

MECHANISM of action or reaction

(i) Splitting, Reactions, -Lysis, decomposition

B92 E32 F48 H24 H52 H92 L80 M62 P04 Q92 R74 S72
X32 X60

(ii) Addition reactions

E00 F12 F28 F58 P32 P36 R24 S44 X08

(iii) Oxidation or reduction

C92 H56 H68 M64 P04 S16 S88 V04 Y16 Y32

(iv) Methatheses or displacement reactions

D94 F44 F46 F56 H28 H32 L20 L28 M96 P44 R50 W94
Y08

(v) Other, including physical interactions

C48 D54 D82 E50 H64 J36 J40 J44 K08 K72 L48 L92
M16 M90 P28 Q24 R66 S28 S36 S48 S68 T26 X90 X98
Y00 Y04 Y28

THERMOCHEMISTRY Thermodynamics, Thermophysics, High Temperature work, Pyrolysis etc.

B16 B48 D12 H04 H16 J04 P92 R20 R82 S68 S72 T10
T40 V08 W98 X04 X36 X60 X68

KINETICS including rates of physical growth and relaxation

(i) Gas

E92 H68 M12 W26 W62 X04 X32 X36 X60

(ii) Solution

D24 D36 D72 S76 T30 T34 T50 W84

(iii) Phase unspecified

E28 F38 F64 F72 M48 M80 Q92 Q96 Q98 V04 Y40

*** PHYSICAL PROPERTIES**

B84 C60 C80 C86 D20 E28 F02 H00 L32 L52 M56 M72
P56 R20 R66 R94 S04 S64 T02 T08 T14 T16 V12 X60
X94

ELECTROCHEMISTRY Polarography, Electrophoresis

B44 D16 D24 H96 J28 Q20 S24 T50 W84 X24

CATALYSIS AND SURFACE CHEMISTRY

B16 E32 F50 H20 H72 K56 K84 M42 M44 M50 M52 P48
P56 P92 R08 R12 R16 S64 T18

PHOTOCHEMISTRY Fluorescence, Phosphorescence

C00 C44 D16 D62 F40 H88 J16 K48 K74 L40 L92 M12
M70 M86 M92 Q56 Q58 T04 T26 W92 X32

DIFFRACTION X-Ray, electron, neutron

F22 Q32

SCATTERING Light or particles; molecular beams

K12 K32 K48

RADIATION CHEMISTRY Radiolysis, Tracer techniques

F14 F40 H88 J12 K48 W12 X12 X64

UV, VISIBLE OR X-RAY spectra

D32 E68 E88 H88 K80 M46

IR, RAMAN OR MICROWAVE spectra

B40 E92 J26 J80 J92 J96 K00 K28 M02 M20 R04 W14
W36 W62

E.P.R.

B52 D00 D08 D78 H96 K16 M22 M94 Q04 Q08 Q80 V16
W14 W32 X20

N.M.R., N.Q.R.

C84 C88 D00 D08 D12 D44 E64 H96 J84 K20 K74 L24
L36 L68 M84 P52 R36 W82 X84

MÖSSBAUER

K12 M04 M32 M42

MASS SPECTRA

E96 J48 K48 L00 M16 P52 R78 X12 X80

O.R.D., C.D.

E08 L44 S80 X52

SPECTRA General and unspecified

C36 C64 E88 F66 H48 K62 L16 M34 P92 S64 W44 X56

CHROMATOGRAPHY including ion-exchange

F32 M52 R78 T12 X36 X72

* MISCELLANEOUS techniques

THEORETICAL

C84 H96 K62 L32 L68 M06 M66 Q72 Q80 R20 S00 S04 S20

Appendix 7: Profile Statistics and Titles

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
A12	10	298	31		
A14	10	278	9		
A18	10	282	21		
A20	10	389	3		
A22	10	482	1		
A24	10	339	3		
A26	10	426	5		
A28	10	563	8		
A30	10	445	40		
A32	10	240	12		
A34	10	1283	12		
A50	10	69	3		
A52	10	238	8		
A54	10	177	2		
A60	10	358	10		
A62	10	138	19		
A64	10	481	68		
A66	10	360	22		
A68	10	159	52		
A70	10	726	6		
A72	10	360	36		
A74	10	306	76		
A76	10	135	2		
A78	10	300	12		
*B00	10	57	4	PHARMACY	Pseudomonas
B02	10	52	2	PHARMACY	Antibiotics or Pigments and Pseudomonas Aeruginosa
B04	10	242	5	ORGANIC	Degradation of Proteins and Dyestuffs, Acids or Bases
B08	6	113	38	ORGANIC	(Photo or Semi Conductivities and Organic Dyes) or Light Fastness
B12	10	256	33	ORGANIC	Pigments and Particle Size or Colour

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
B16	10	194	23	PHYSICAL	(Thermodynamics and Dyeing) or (Absorption and Azo Dyes, Water or Organic Vapours and Cellulose)
B20	10	167	4	PHYSICAL	Aerosols: or Small Particles, Drops etc.
B24	5	195	14	INORGANIC	Di (or Poly) Nuclear Cobalt or Chromium Complexes: Oxygen - 18 and Nitrite or Sulphite
B28	10	455	66	"	(Carbonyl, Phosphine, Arsine, Amine) and Nickel or other Transition metals
B32	10	401	54	"	(Alkyl, Aryl, Acyl, Sulphonyl, Azide) and Group VIII (or other Transition) Metals
B36	10	269	97	"	Complexes of Poly Amino Carbonylic Acids
B40	10	376	17	"	Ligands of Group 5B or 6B elements and Silver or infrared
B44	10	295	74	PHYSICAL	Polarography (especially for Aluminium): Uptake of Organics at Dropping Mercury Electrode
B48	10	230	39	INORGANIC	Thermodynamics and Organo Metallics
B60	10	1187	27	PHYSICAL	Radiation (not Infrared)
B64	7	255	15	ORGANIC	Small Ring Systems
B72	10	161	70	"	Phenazine, Chemistry or Nitroso compounds or Nitrenes or Reductions and Nitro Compounds
B76	10	67	28	"	Peri Naphthenones or Peri Naphthanones or Related Syntheses
B80	10	120	12	"	Synthesis or Related Reactions and Cyclo Hexane - Lactonic Acids
B84	10	266	36	PHYSICAL	Osmometric, Phase or Thermodynamic Studies and some Polymers
B88	8	83	26	"	Co Polymers or Styrene or Methyl Meth Acrylate
C00	10	31	32	PHYSICAL	Mercury Photo Sensitization and Chlorinated Compounds
C04	10	445	15	ORGANIC	Organo Fluorine Chemistry
C08	10	85	38	"	Carbanions
C12	10	108	43	"	Carbohydrates

Profile No.	No. of Issues	Total Hits	% Relevant		Index Times
C16	10	191	22	ANALYTICAL	Analytical Determination and Alkali Metals
C24	10	131	36	ORGANIC	Organo Sulphur Compounds, particularly Asymmetric 1, 4 - Oxo Thianes
C28	10	161	32	"	Structural Studies and Poly Saccharides
C32	10	856	9	"	Carbohydrates
C36	10	65	100	"	Spectroscopic Studies and Acetylenic Systems
C40	10	143	11	INORGANIC	Ceric, Manganic and Cobaltic Halides
C44	10	318	39	PHYSICAL	Flash Photolysis and Halides or Nitroso Compounds
C48	10	198	33	ORGANIC	Reversible Interaction and Bio Macro Molecules
C52	10	59	21	"	Nitrogen Bridged Bi Cyclic Ring Systems
C56	5	60	13	"	Organo Silicon Compounds
C60	10	147	33	PHYSICAL	Humic Acids and Soil Chemistry (Physico Chemical Studies)
C64	5	121	30	"	Spectroscopic Studies and N^{14}, N^{15}, C^{13}, O^{17}, B^{11} Isotopes
C68	5	296	1	ORGANIC	Nucleic Acids or their derivatives
C76	10	62	100	"	E.S.R. and Organo Sulphur Radicals
C80	10	405	19	PHYSICAL	Electron Affinity of Negative Ions and Structure
C84	10	166	5	"	Calculation and N.M.R. Chemical Shifts
C86	5	41	48	INORGANIC	Sub Stoichiometry
C88	10	116	13	PHYSICAL	N.M.R. and Solvent Shifts
C92	10	350	25	"	Anti Oxidants or Stabilisers and Hydrocarbons
C96	5	55	4	ORGANIC	Organo Silicon Compounds
E00	5	19	40	INORGANIC	Donor Properties and Sulfur
E04	11	14	50	ORGANIC	Sesqui Fulvalenes or N Analogues
E08	16	14	28	"	Lano sterol or ORD Studies

Profile No.	No. of Issues	Total Hits	% Relevant	Index Terms	
E12	5	35	45	INORGANIC	Complexes of Tin (II)
E16	15	26	52	ANALYTICAL	Analytical Det. and Barbiturates or Amines
E20	16	7	32	ORGANIC	Conformational Analysis and Cyclo Hexane series
E24	9	17	11	"	Sclerotin Series
E28	16	16	6	PHYSICAL	Evaporation of Liquids and Particulate Beds
E32	10	20	15	"	Intra molecular Catalysis and Ester Hydolysis
E36	16	50	31	ORGANIC	Unsaturated Cyclic compounds
E40	5	18	45	"	Diazo Compounds
E44	8	14	26	"	Carbene Chemistry
E48	6	12	39	"	Oligo ribo nucleotide Synthesis
E50	16	38	19	"	Meta phosphates as Reaction Intermediates
E56	13	25	70	"	Hetarynes
E60	10	36	29	"	Synthetic Alkaloids
E64	14	48	59	PHYSICAL	Solvent Effects and NMR
E68	16	17	61	"	Lasers
E72	14	35	10	ORGANIC	Diazo Compounds
E76	16	47	48	PHYSICAL	Hydrogen Atoms and SO_2
E80	14	46	5	ORGANIC	Aphid Pigments
E84	16	21	47	"	Indole Alkaloids
E88	12	24	4	ANALYTICAL	Analytical Aspects and Precision Spectrophometry
E92	15	13	33	PHYSICAL	Relaxational Vibrations
E96	13	16	79	ORGANIC	Mass Spectroscopy and Hetero Cyclic Compounds
F02	10	435	35	INORGANIC	Magnetic Properties and Transition Metal Compounds
F12	10	201	23	"	Organo Metallic and (Cyano Complexes or Insertion Reactions)
F14	6	57	13	ORGANIC	Biosynthesis and (Mono Terpenes or Radio Tracers)
F16	10	83	54	INORGANIC	Organo Metallic and (Sigma bonds or mercury or chromium)

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
F18	10	80	38	ORGANIC	Anthrone or disorder in molecular crystals
F20	10	471	5	"	Phenazine or mixed organic crystals
F22	6	178	6	INORGANIC	Tri Alkyl metal complexes or X-ray diffraction techniques
F28	6	90	37	ORGANIC	Cyclo Addition and conjugated dienes or Bi cyclic compounds
F30	10	478	12	"	Dienes
F32	5	159	26	"	Halogenation or Gas Chromatography
F34	7	80	44	"	Olefinic Arsines or /Structure and (Arsine or Phosphine)/
F36	10	166	61	INORGANIC	Organo Metallic and (Carbonyls or Sigma Bonds)
F38	8	70	47	"	Organo Metallic and Kinetics
F40	10	323	16	PHYSICAL	Aqueous Solutions and (Radiolysis)
F42	10	686	17	ORGANIC	Allenes or Acetylenes or Activated Esters
F44	10	105	19	"	Free Radicals Aromatic Substitution
F46	10	234	22	"	Organic Per Oxides or Organic Nitr Oxides or Arylation
F48	10	387	15	"	Elimination reactions or Carbon Hydrogen Acidity
F52	10	318	17	"	Aromatic Hetero Cyclics or Ace Pleiadylene
F56	10	277	47	"	Acylation or (Association and Non ionic Solvents)
F60	10	114	11	INORGANIC	Antimony Halides or (Halides and Ring Systems)
F62	10	242	29	ORGANIC	Chemistry of Penicillin
F64	10	140	31	INORGANIC	Organo Metallic and Kinetics
F66	10	78	37	"	Spectra and (Phosphorus or Amines or Aziridines)
F68	10	192	52	ORGANIC	Bridged Poly Cyclic Olefins
G00	10	141	34		
G04	10	170	6		
G06	10	370	64		
G08	10	434	14		
G10	10	762	16		

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
G12	10	742	42		
G14	10	102	8		
G18	10	143	49		
G20	10	145	7		
G40	10	459	25		
G42	10	199	10		
G44	10	149	5		
G46	10	164	91		
G48	10	289	37		
G62	10	46	39		
G64	10	369	22		
G66	10	234	26		
G68	10	317	2		
G80	10	197	25		
G82	10	91	8		
G84	10	118	4		
G86	10	184	15		
G88	10	165	23		
*H00	10	334	60	INORGANIC	Magnetic Properties and Bi or Poly Nuclear Transition Metal Complexes
H04	10	429	37	PHYSICAL	Thermodynamic and Fluid Systems
H08	10	142	44	ORGANIC	Thiophenes or Sulphur Hetero Cycles
H12	10	422	21	PHYSICAL	Gas Phase Oxidations and Hydrogen, Hydrocarbons or Simple Derivatives
H16	10	375	33	INORGANIC	(Thermochemistry and Organo Metallic Compounds or Transition Metal Oxides) or Metallocenes
H20	10	568	21	"	Gold Palladium Alloy or Hydrogenation or Deuteratior and Alkyl Benzenes and Metallic Catalysis)
H24	10	328	19	PHYSICAL	Pyrolysis or De Hydro Halogenation and Halo Hydrocarbons

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
H28	10	202	8	ORGANIC	(Alkoxide Ion and Nitro Compounds or Di Nitro Benzenes Anilines Reactions
H32	10	326	13	"	(Some) Alkaloids or Terpenes or Formylation Reactions
H36	10	702	71	"	Biosynthesis and Alkaloids or Terpenes
H40	10	210	84	"	Some Natural Products (Porphyrin, Hemin, Chlorophyll, Bile Pigment etc.)
H44	10	54	98	"	Organic Sulphur Chemistry
H28	10	188	42	"	(Conformation and Hydrocarbons) or (Spectral Studies and Fluorinated Aromatics, Terpenes, Pinanes or Pinenes)
H52	10	143	71	"	De Hydro Halogenation, especially in Non Aqueous Solvents
H56	10	668	100	"	Biosynthesis or Some Alkaloids or (Oxidation or Coupling and Phenols)
H60	10	405	65	"	Gastrins or (Synthesis or Conformations and Peptides)
H62	10	67	27	PHARMACY	Antigens and Gastrin
H64	10	371	54	ORGANIC	Some Terpenes or (Synthesis or Reactions and Cyclic Systems)
H68	10	54	52	PHYSICAL	Cool-Flames or (Gas-Phase Oxidations and Ethanol, Propanes, Propenes or Cyclo Hex*)
H72	8	23	52	"	Gaseous (especially Nitrogen) Adsorption and Transition Metal (Filaments)
H80	10	135	58	"	Dielectric, Visco Elastic or Physical Investigation or Properties and Polymers
H84	8	308	43	"	
H88	8	168	57	"	Poly Methyl Methacrylate or (UV or Radiation, Phosphorescence, etc., and Carbonyl containing Compounds)
H92	10	95	57	"	Stable Carbonium Ions or (Solvolyses and Non-Aqueous Solvents) or Poly Ethers
H96	10	523	99	"	Calculation or Computation or Redox Reactions or Magnetic Resonance

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
J04	10	143	10	PHYSICAL	Thermodynamics and the Glassy State
J08	5	75	31	PHARMACY	Metabolism and Tryptophan in Ergot Species
J12	10	191	50	PHYSICAL	Radiation Chemistry and Water, Aqueous systems, Organic Solvents
J16	10	550	30	ORGANIC	Photo Chemistry and Organic Compounds
J20	10	121	37	PHYSICAL	O, CH or OH Radicals in the Gas Phase not Photo Chlorination
J24	10	320	53	ORGANIC	Alkaloids, particularly Indoles, Tryptamines or Pyridines
J26	5	144	75	INORGANIC	Vibrational Studies and (Inorganic Complexes with) Metal-to-Metal Bonds
J28	10	17	93	PHYSICAL	A conducting Polymer incorporating Tetra Cyano Quino Di Methane
J32	10	101	74	ORGANIC	Benzo Furans or (Breakdown and naturally occurring Phenyl Alanine)
J36	10	24	50	INORGANIC	Polymerisation and Phospho Nitrilic Compounds
J40	10	138	41	ORGANIC	Synthesis or Reactions and Peri-fused Aromatic Ring Systems
J44	10	78	40	INORGANIC	Organo Functional Groups and Metal Amines or Metal Oxygen Bonds
J48	10	548	36	PHYSICAL	Rearrangement Processes and Mass Spectrometry, or Hydrocarbons
J52	10	118	32	ORGANIC	Indole Alkaloids
J56	10	116	34	PHYSICAL	Polymerisation and Propylene Sulphide or Propylene Oxide
J60	10	12	25	ORGANIC	Halo or Nitro Indoles or Pyrroles
J72	5	42	57	"	Bacterial Enzymes which degrade Galactoses
J76	5	56	34	"	Sulfatases
J80	5	50	33	PHYSICAL	Microwave Spectroscopy and Imidazole
J84	5	44	39	ORGANIC	(NMR and Carbohydrates) or (Synthesis and some di Sulphates of Galactose)
J88	5	92	21	INORGANIC	Complexes of Metals and Carbohydrates
J92	5	73	32	PHYSICAL	Microwave Spectroscopy (High Sensitivity Techniques)

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
J96	5	157	17	PHYSICAL	Double Radiation Microwave Spectroscopy
L00	15	25	48	ORGANIC	Organic Mass Spectrometry
L04	12	3	95	"	Medium Ring Chemistry
L08	16	8	28	"	Insect Hormones
L12	16	20	8	"	Tetra Cycline Synthesis
L20	13	30	48	"	Spectroscopic Properties and Conjugated Molecules
L24	16	59	14	PHYSICAL	High Resolution NMR Spectroscopy
L28	16	41	19	ORGANIC	Electrophilic Substitution and Amino Pyridines
L32	12	25	32	PHYSICAL	Dispersion Forces or Pfeiffer Effect
L36	16	36	64	"	NMR and Conformational Analysis
L40	7	30	24	"	Asymmetric Photo chemistry
L44	16	64	29	INORGANIC	CD and Transition Metal Complexes
L48	15	34	20	ORGANIC	Binding of Molecules and Poly peptides or Polynucleotides
L52	9	24	32	"	Dipole Moments and Conformational Analysis
L56	16	29	20	PHYSICAL	Photo excited States
L60	10	5	24	INORGANIC	Inorganic Compounds of Silicon
L64	12	51	58	ORGANIC	Organo germanium compounds
L68	5	13	80	PHYSICAL	Nuclear Spin Spin Coupling Constants
L72	14	93	23	INORGANIC	Boron Halides and Inorganic Synthesis
L76	16	1	100	ORGANIC	Alpha Chymo Trypsin
L80	12	31	36	"	De Tritiation Reactions in Phenanthrene Systems
L84	12	14	38	INORGANIC	Phospine Complexes and Osmium, Iridium and Platinum
L88	5	5	60	ORGANIC	Chemistry or Biosynthesis and some Mould Metabolites
L92	16	52	25	"	Studies in Photo Chemistry and Steriods or Radical Reactions
M02	10	163	46	PHYSICAL	Symmetric top molecules or laser raman spectroscopy
M04	10	376	59	"	Mossbauer effect

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
M06	10	305	22	PHYSICAL	Theory of Chemical bonding
M08	10	387	18	ORGANIC	Organo silicon or germanium compounds
M10	10	387	28	INORGANIC	Organo metallic carbonyl complexes
M12	10	1083	15	PHYSICAL	Flash photolysis or (Kinetics and gas)
M14	10	118	28	INORGANIC	Organo metallic and (cyclo penta dienyl or carbonyl)
M16	10	409	28	PHYSICAL	Atomic reactions or mass spectrometry
M18	10	311	61	INORGANIC	Organo metallic carbonyls or cluster complexes
M20	10	210	66	PHYSICAL	Raman Spectroscopy
M22	10	48	25	PHYSICAL	Electron Para magnetic resonance and gas phase
M24	10	2341	37	"	Metal oxidation or electronic properties of defect solid state
M30	10	398	19	ORGANIC	Absolute configuration or terpenes
M32	10	382	22	PHYSICAL	(Structure and iron complexes) or Mossbauer
M34	10	71	20	ORGANIC	Spectra and Organo halides
M36	10	348	17	INORGANIC	Organo metallic and nitrogen
M40	10	261	16	"	Electronic properties and mixed oxides
M42	10	213	63	PHYSICAL	Mossbauer or adsorption on iron oxides
M44	10	153	55	"	Field ion microscopy or metal surfaces
M46	10	283	36	"	Atomic absorption or flame spectroscopy
M48	10	383	34	INORGANIC	Reaction kinetics and carbonyls or (Palladium and platinum complexes)
M50	10	395	18	PHYSICAL	Hetero geneous catalysis in solution
M52	10	110	72	"	Zeolites or ion-exchange
M56	10	257	16	"	Viscosity or Alcohol water mixtures
M62	10	131	15	ORGANIC	Hydrolysis and (esters or amides or carbamates)
M64	10	136	41	"	Oxidative coupling, especially in alkaloids
M66	10	312	33	PHYSICAL	Quantum theory
M68	10	416	32	ORGANIC	Peptides or Poly amino acids

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
M70	10	207	20	ORGANIC	(Biosynthesis and alkaloids) or Photo oxidation
M72	5	87	41	INORGANIC	Organo metallic and electronic properties
M80	10	123	16	PHYSICAL	Kinetics and free radicals
M82	10	260	4	ORGANIC	Thio ketones or amino ketones
M84	10	454	36	PHYSICAL	Nuclear magnetic resonance
M86	10	287	13	"	Chemi luminescence
M88	10	442	23	ORGANIC	Cyclic hydrocarbons or azo ketones
M90	10	390	25	"	Reaction mechanisms and organic
M92	10	102	17	"	Photo chemistry and (esters or amines)
M94	10	76	42	PHYSICAL	Electron spin resonance and gaseous species
M96	8	263	21	ORGANIC	Grignard reagents or silicon compounds
N02	10	352	12		
N06	10	465	16		
N08	10	568	21		
N10	10	208	6		
N12	10	392	20		
N16	10	128	27		
N34	10	323	26		
N36	10	339	12		
N42	10	168	5		
N44	10	260	5		
N48	10	258	64		
N50	10	180	7		
N52	10	339	11		
N54	10	514	21		
N56	10	549	10		
N58	10	352	10		
N60	10	254	19		
N76	10	220	18		
N80	10	332	45		

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
N82	10	170	14		
N84	10	305	22		
N86	10	610	24		
N88	10	267	15		
N90	10	206	30		
N92	10	404	67		
N98	10	475	9		
*P00	10	213	30	ORGANIC	Metal (especially lead) carboxylates
P04	10	258	27	INORGANIC	Amines and Metal (Copper, Manganese, Cobalt or Iron) Salts or Oxides or Oxidation or De Alkylation
P08	10	685	67	"	Complexes (metallocenes, Carbonyls, Alkyl, Olefin) and Transition metals
P12	10	230	19	"	Oxygen and Transition Metal Ions or Complexes
P16	10	268	27	"	Cobalt, Nickel or Other Transition Metal Alkyls or Complexes and Macro Cyclic or Multi Dentate Ligands
P20	10	62	45	ORGANIC	(Peroxides and Oxides of Nitrogen) or Alkyls or Alkonyl Radicals
P24	10	114	39	"	Nitrenes, Azenes or Axides
P28	10	204	37	INORGANIC	Palladium Hydride, Chloride, Acetate or (Reactions, on Group VIII Metals and Olefins, Aldehydes or Ketones)
P32	10	394	19	ORGANIC	Organo Silicon Compounds or (Halo Methyl Compounds and Transition or Group IVB or VB Metals) or Addition Reactions to Double Bonds
P36	10	99	78	"	Hydrazides or Hydrazines or Cyclo Addition
P40	10	148	88	"	Organo Tin Chemistry or Tin Nitrogen Compounds
P44	10	334	27	"	Halogeno Mono Enes, Di Enes or Acetylenes, especially Per Fluoro Compounds or (Rearrangements and Fluoro Olefins)
P48	10	651	46	INORGANIC	Transition Metal Carbonyls or Hydro Formylation or (Hydrogenation and Rhodium or Indium

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
P52	10	72	66	ORGANIC	Poly Halogenated Pyrimidines or (Mass Spectra or Fluorine NMR and Hetero Cycles)
P56	10	297	63	PHYSICAL	Physical Properties or Activity and Metal Oxides and Hydrogenation or Hydrogen Deuterium Exchange Reactions
P60	10	134	44	ORGANIC	Per Fluoro Silanes or (Silyl Radicals and Poly Fluoro Aromatics)
P64	10	138	53	"	Unsaturated Fluoro Compounds and Azides
P68	10	282	38	"	Poly Halo Hetero Cycles
P72	10	80	87	"	Diaza Thia Naphthenes or Related Hetero Cycles
P80	10	295	22	INORGANIC	Bases (Amines, Carbanions) and Phosphides
P84	10	192	39	ORGANIC	Eight Co-ordinate Complexes or Cyanide or Iso Cyanide Complexes (especially of Molybdenum or Tungsten)
P92	10	418	15	PHYSICAL	Cyclo Propanes or Carbenes or Tri Fluoro Methyl Compounds Spectra or Thermodynamics and Wetting or Adsorption and Inorganic oxides
Q04	10	347	93	ORGANIC	E.S.R. and Aromatic Free Radicals
Q08	10	438	36	"	E.S.R. Spectra and Free Radicals formed in Crystals by γ-irradiation
Q16	10	918	4	"	Conformational Analysis and Cyclo Hexane or Piperidine Derivatives
Q20	10	296	17	"	Electrolysis and Organic Compounds containing Cyclo Propane Rings
Q24	10	279	17	"	(Biosyntheses and natural Phenolic Acids) or Shikimic Acid pathway
Q28	10	267	49	"	Conformational effects and Steroids
Q32	10	184	51	INORGANIC	X-ray Crystallography and Transition Metal Complexes
Q36	10	230	67	"	Crystal Structures and non transition metal compounds
Q44	10	112	51	ORGANIC	A Cyclo Hepta Fluorene
Q48	10	198	16	"	Natural Phenolic Compounds
Q52	10	484	94	"	Natural Phenolic Compounds
Q56	10	166	31	"	Production of Free Radicals and Mercury Photo Sensitization

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
Q58	10	79	25	ORGANIC	Photolysis and Ketones, Aldehydes, or Azo Compounds
Q60	10	796	45	INORGANIC	Molecular or Crystal Structures and Actinide Elements
Q62	5	25	67	"	Ferredoxin
Q72	10	197	42	PHYSICAL	Ferredoxin
Q80	10	79	65	"	Molecular Orbital Calculations
Q92	10	57	34	"	E.S.R. and Molecular Orbital Calculations
Q96	5	131	20	PHARMACY	Uni Molecular Decomposition processes and Chemically activated Systems
Q64	10	42	54	"	Growth of Protozoa
Q98	10	537	17	"	Growth of Protozoa
S00	12	12	24	PHYSICAL	Vibration Calculations and Helium or Lithium States
S04	15	26	25	"	Theory of Inter Molecular Forces
S08	8	42	6	"	
S12	10	19	27		
S16	9	5	30	ORGANIC	Oxidative Coupling and Phenols
S20	7	11	24	PHYSICAL	Configuration Interaction or Bonding and TM Complexes
S24	13	22	30	"	Dispersion of Conductance and electrolyte solns.
S28	13	16	44	INORGANIC	Nitrous Oxide (Gas Phase) Reactions
S32	15	42	8	ORGANIC	Aliphatic and Electrophilic Substitution (Sat. Carbon)
S36	14	14	41	"	Substituent Effects and Carbazoles
S40	16	29	10	"	Poly Fluoro Bi Phenyls
S44	9	7	20	"	Diels Alder Reactions and o - Benzo Quinones
S48	16	23	18	"	Benzyne Mechanism and Poly Fluoro Aromatic Compounds
S52	11	10	21	"	Stereochemical Studies and Polyenes
S56	6	150	10	INORGANIC	Nitrogen Halogen Radicals
S60	14	65	34	ORGANIC	Carotenoids or Related Polyenes
S64	11	65	31	PHYSICAL	Spectra or Work Function Changes and Absorbed Gases/Metals

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
S68	16	34	35	INORGANIC	Conformation Equilibria and Cyclic Esters of Inorganic Acids
S72	16	84	16	ORGANIC	Thermal De Carboxylation
S76	9	25	24	PHYSICAL	Proton Transfer Reactions and Solution
S80	16	53	57	INORGANIC	Optical Activity and Metal Complexes
S84	5	31	27		
S88	5	20	0	ORGANIC	Meso Oxidation and Porphyrins, Mechanistic
T02	10	236	33	PHYSICAL	Viscosity and glass transition
T04	10	130	36	"	Photo chemistry or atomic oxygen
T06	10	1519	42	INORGANIC	Organo metallic copper complexes
T08	10	152	53	"	(Electronic properties or structure) and copper compounds
T10	10	1125	19	ORGANIC	Thermo dynamic properties and organic compounds
T12	10	722	8	PHYSICAL	Solvent extraction or ion-exchange or concentrated halide systems
T14	10	1363	13	INORGANIC	Organo metallic and (structures or molecular weights)
T16	10	1433	10	"	Organo metallic and electronic properties
T18	10	631	57	PHYSICAL	Oxides and Catalysis
T22	10	319	11	INORGANIC	Organo metallic and (nickel or bonding)
T26	10	441	46	PHYSICAL	Energy transfer mechanisms and photosynthesis
T30	10	277	32	"	Fast reactions in solution or iron salts
T32	10	632	14	INORGANIC	Organo metallic and Titanium or thorium or 8 - hydroxy quinoline)
T34	10	991	33	PHYSICAL	Fast reactions in solution
T40	10	318	19	"	Calorimetry or Boron compounds or carboxylic acids
T50	10	444	12	"	Electro chemical reaction kinetics
T52	5	8	88		

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
*V00	8	98	46	ORGANIC	Cubane or Penta Cyclo Nonanes or Decanes
V04	10	696	24	PHYSICAL	Kinetics or Mechanisms and Oxidation Reduction Reactions
V12	7	233	45	INORGANIC	(Shapes or Chromatography and Polymers) or Silanones or Silicones
V16	10	534	35	PHYSICAL	Electron Spin Resonance
V24	7	225	20	ORGANIC	Solvent or Structure and Reactivity of Organic Compounds
W00	5	45	96	PHARMACY	The mould "Penicillium Wortmannii" or any Bi Anthra Quinones
W02	10	82	42	INORGANIC	Ferrocene or other Metal Cyclo Penta Di Enyls
W04	10	154	94	ORGANIC	Tropical Natural Products (of commerical importance)
W06	5	78	9	INORGANIC	Alkali and Alkaline Earth Metals and Carbon or Nitrogen
W08	10	235	7	ORGANIC	Quinone Methides
W10	10	346	91	INORGANIC	Nitrates or Carbonyl Compounds and Rhenium
W12	10	578	34	PHYSICAL	Effect of Radiation and Crystalline, Glassy, Plastic or Liquid Solvents or Solutions
W14	10	63	42	"	E.S.R. and I.R. and the Chromium Tri Oxide / Silica / Ethylenic System
W16	10	100	25	ORGANIC	Quinone Methides
W28	10	424	21	INORGANIC	Simple Organic Molecules and Transition metal complexes
W32	10	562	7	PHYSICAL	E.S.R. and Nitrogen containing compounds
W36	10	311	14	"	I.R. and Raman Spectra and Complex Halides
W40	10	420	56	INORGANIC	Complexes and transition metals
W46	10	142	25	INORGANIC	Organo Arsenic Chemistry or Arsonium Ylids
W48	10	691	13	"	Metal Fluorides
W60	10	27	22	ORGANIC	Mono Terpene Alkaloids
W62	10	49	31	PHYSICAL	Vibrational Relaxation or Vibration Energy Transfer
W64	10	39	3	ORGANIC	Synthesis and Poly Cyclic Aromatics

Profile No.	No. of Issues	Total Hits	% Relevant		Index Terms
W68	10	14	46	ORGANIC	Aza Steroids
W72	10	77	23	"	Alkaloids, Indolizines, Pyrrocolines, Indoles or Pyrroles
W76	10	195	53	"	Benzynes
W78	5	6	100	PHYSICAL	Butadiene Styrene Block Co Polymers
W80	10	68	28	ORGANIC	Amaryllidaceous Alkaloids
W82	10	62	72	"	(Hydrogen Bond Effects and N.M.R.) or Morphine Chemistry
W84	10	37	45	PHYSICAL	Faradaic Impedance or (Kinetics and Electrode Reactions)
W86	10	23	100	ORGANIC	Afla Toxins
W88	10	42	33	PHARMACY	Neuro Chemistry and Histamine, Spermine or Spermidine
W90	10	6	100	"	Afla Toxins
W92	10	251	7	INORGANIC	Phthalo Cyanines or Photo Conductivity
W94	10	77	37	ORGANIC	Friedel Crafts Acylation and Aliphatic Compounds
W96	10	587	3	PHYSICAL	Anionic Polymerisation and Alkenyl Ketones
W98	10	145	25	"	Heats and Mixing, Dilution or Solution and Stereo Regular Polymers
Y00	8	52	15	PHARMACY	Urinary Excretion or (Metabolism and Amphet Amines)
Y04	5	53	48	"	Metabolism Studies
Y08	5	34	40	"	Alkylating Agents or Neo Plastic Tissues
Y12	9	3	60	"	Antagonists and Analgesics
Y16	11	5	12	ORGANIC	Oxidative Coupling and Phenols
Y20	15	2	0	PHARMACY	Bactericides, Chemicals
Y24	15	12	0	ORGANIC	Sclerotin Series
Y36	16	62	27	PHARMACY	Biosynthesis
Y40	16	65	10	PHYSICAL	Growth or Form and Bacterial Colonies
Y44	6	100	11		

% Relevance: This is 100 x $\frac{\text{No. of Relevant Hits}}{\text{Total no. of hits}}$ in no. of issues stated

except profiles B, H, P, V (*) where % relevance is

$$\frac{100 \text{ x No. of Relevant Hits}}{\text{No. of Hits where relevance is determined}}$$

No combined figures are available for profiles D, K, R and X.