# Organization and Efficient Manual Searching of the Major Chemical Title and Abstract Publications

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**The main characteristics of the six most important secondary chemical source publications are presented, with special emphasis on developments during the last five years. *Science Citation Index* and several new *Chemical Abstracts'* indexes are discussed as effective tools for retrospective literature work. This is followed by a comparison of the features of *Chemischer Informationsdienst, Index Chemicus, Chemical Titles,* and *Current Contents* as the main sources of current chemical information. Relatively complete literature coverage can be achieved only by appropriate combination of all search possibilities offered.**

The primary scientific and technological literature increases at a compounded annual rate of 5 to 6 %,[1] and no slowdown of this exponential increase is expected in the foreseeable future. Thus, the question is justified whether and how long the active research scientist will be able to keep abreast of the most recent developments in his chosen field of specialization. It is certainly impossible to accomplish this task by regular reading of the entire primary literature, although about 30% of all nonpatent source documents relevant to the chemical sciences are published in "only" 250 journals.[1] Statistical studies[2] have shown that the average research chemist regularly scans only seven to eight journals, and that he keeps up-to-date on the remaining current literature by using abstract services. This conventional method of information retrieval is remarkably efficient, especially if the scientist is highly specialized; however, it does not provide complete literature coverage (100% "recall").

Since 1965 the titles, keywords, author names, and other bibliographic data of all papers covered by the major chemical title and abstract publications have been stored on magnetic tape, and these tapes are available for computer searching against personal interest profiles prepared by or for individual chemists.[3] This selective dissemination of information (SDI) by utilization of computers efficiently supplements traditional manual search methods; however, it does not replace them entirely. The use of computers for literature searching is primarily limited by the high cost, in terms of time and money, of coding all chemical structures and equations and storing them together with complete abstract texts on magnetic tape. Although author names, bibliographic data, literature citations, title words, and subjectively selected keywords may be coded and stored much more readily, this approach severely restricts the search possibilities to these very same terms. Computer methods are even less suitable for retrospective literature work since in this case the simultaneous search of each new tape against a large number of subscriber profile terms is eliminated as a major cost-saving element.

Thus, even in the computer age, traditional literature search methods are not expected to become redundant, although computerized SDI services may soon be indispensible for retrieving information from less wellknown sources. A thorough knowledge of the major chemical title and abstract publications and of the procedures for efficiently retrieving the desired information from them will therefore remain an indispensible tool of every active research chemist. The scientist can considerably increase the efficiency of his literature work, and thus gain valuable research time, by keeping up-to-date on the most recent advances in information transmission and index production. It is the aim of this paper to describe and summarize the main features (Table I) of the six major secondary chemical source publications produced in the United States and Germany: *Science Citation Index* (SCI), *Chemical Abstracts* (CA), *Chemischer Informationsdienst* (Chem-Inform, CI), *Current Abstracts of Chemistry and Index Chemicus* (IC), *Chemical Titles* (CT), and *Current Contents* (CC). Only 10 years ago, several of these services did not exist, and over the same time period, all of them have been modified and improved to such a large extent that a comparison with older issues is no longer meaningful. SCI and CA are particularly suitable for retrospective literature work while the title publications CT and CC and the more recent abstract publications CI and IC are more useful for current awareness searching.

## *SCIENCE CITATION INDEX* (SCI)

The *Science Citation Index* has been published since 1964 by the Institute for Scientific Information (ISI), Philadelphia, Pa., and is particularly suitable for retrospective literature searching for information on research topics which cannot be easily defined by keywords or chemical formulas. The most common method of retrieving data from the chemical literature consists in checking the author, formula, and subject indexes of journals, abstract publications, and handbooks. If molecular formulas or author names are not available as index entry points, the search must be started by consultation of the subject index. However, subject indexes have the characteristic of being produced by professional document analysts who select the most important keywords and phrases from each paper. The final selection represents a subjective human judgment which would probably be different if the information-seeking scientist had done this job. Owing to this different evaluation of the significant terms of a paper, the desired information is frequently not retrievable.

A citation index is a completely different kind of index

which does not depend on this subjective keyword selection.[4] It consists of an orderly list of *cited* papers or citations and gives for each citation all *citing* papers or source documents of the current year. Thus, a chemist seeking information on a specific subject does not describe his topic in terms of one or more keywords—e.g., orbital symmetry—but in terms of the bibliographic data of a relevant paper which has dealt with this topic in the past—e.g., "R. B. Woodward and R. Hoffman, *J. Amer. Chem. Soc.* **87**, 395 (1965)." The success of this approach is based on the assumption that the subject matter discussed by any recent author citing the above reference is closely related to the topic of interest, namely orbital symmetry. Woodward's theory may have been verified, applied, criticized, or rejected by the authors of more recent source documents. This example clearly shows the unique feature of a citation index: to lead the scientist from an old but very relevant target paper *forward* to the most recent publications on this subject; all other kinds of indexes lead back to less current papers. Knowledge of one specific target reference which is generally cited by most scientists working on the topic of interest is the only prerequisite for a successful literature search by this method. It is usually quite easy to locate such a target paper in textbooks, monographs, or handbooks.

SCI, the only citation index covering the natural sciences, is published quarterly and cumulated annually. Of the 2450 journals (from more than 40 nations) regularly monitored in 1972, approximately 700 were of chemical interest; 4 to 4.5 million papers were cited in approximately 400,000 source articles—i.e., 10 to 11 citations per paper. In the production of SCI, each journal is processed cover-to-cover including such items as letters to the editor, errata notices, and corrections, and the titles and bibliographic data of non-English source documents are translated into English.

Each SCI issue consists of four separate indexes. The main part is the "Citation Index," a list of all citations of the current year arranged alphabetically by author. Several citations of the same author are arranged in chronological order. The bibliographic data of all citing source articles of the current year are listed under each citation entry, as shown in the following example:

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SCHMIDT U
      68  CHEM BER  101  1381
          HUGHES AN    J HETERO CH      7   1 70
          WIEBER M     MONATSH CHEM  101 776 70
```

The paper by U. Schmidt (on phosphinidenes) published in *Chemische Berichte,* volume 101, page 1381 (1968) has been cited by A. N. Hughes and M. Wieber in the specified journals in 1970. The cited article may have been published in any year (J. v. Liebig was cited four times in 1970) while the citing source document is always a publication of the current year.

The so-called "Source Index," a complete author index of all papers published during the current year, provides further details on the citing articles—e.g.,

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HUGHES AN
  SRIVANAC.C—CHEMISTRY OF PHOSPHOLE DERIVATIVES—
    J HETERO CH  7 1 70    114 R
```

The source article by A. N. Hughes and C. Srivanac may be found in the *Journal of Heterocyclic Chemistry,* volume 7, page 1 (1970), and contains 114 literature references. The bibliography on the topic of phosphinidene chemistry identified by the above target reference by Schmidt can be easily enlarged by consulting additional papers by Schmidt, Hughes, and Wieber in all available Citation and Source Index issues and by selecting from the references cited in previously found articles a new relevant target paper as starting point of another search of the Citation Index. This "cycling" procedure leads very

Table I. Characteristic Features of the Major Chemical Abstract and Title Publications

| | *Science Citation Index* | *Chemical Abstracts* | *ChemInform* | *Index Chemicus* | *Chemical Titles* | *Current Contents* |
|---|---|---|---|---|---|---|
| Publication type (pref. search mode) | citations (retrospective) | abstracts (retrospective & current) | abstracts (current) | abstracts (current & retrospective) | titles (current) | titles (current) |
| Arrangement of entries in the main section | first cited author (alphabetical) | subject area (80 sections) | subject area (classification code) | journal title | journal Coden (alphabetical) | journal title |
| Number of issues per year | 4 | Organic and biochemistry: 26 Other fields: 26 | 52 | 52 | 26 | Phys. & Chem. 52 Life Sciences: 52 |
| Number of abstracts or titles per issue[a] | 300,000 citations 27,000 source papers | 6500 | 450–500 | 250 | 5,000 | Phys. & Chem. 1,300 Life Sciences: 800 |
| Number of journals covered[a] | 700 | 12,000 | 222 | 108 | 700–750 | 700 |
| Time delay betw. primary and secondary publication | (1–6 months) | ~3 months | 2–3 months | 1–2 months | ~1 month | 2–3 weeks |
| Type and number of indexes per year | author, subject and corporation: 4 | author, subject patent: 52; formula, and Registry Numbers: 2 | author and classification number: 52 | author, subject, and formula: 52; substructure: 12, Rotaform formula: 4 | author and subject (KWIC): 26 | first author (with address) and title word: 52 |
| Magnetic tape version of printed publication[b] | ASCA | CA-Condensates, ISF | ChemInform | ICRS, ANSA | CT | — |

[a] Only chemistry and related subjects. [b] Abbreviations used: ASCA = Automatic Subject Citation Alert, ANSA = Automatic New Substance Alert, ISF = Integrated Subject File, ICRS = Index Chemicus Registry System.

quickly to a fairly complete list of all recent publications (since 1964) on the chosen search topic.

The remaining two parts of SCI are: the "Corporate Index," a list of all papers of the current year arranged alphabetically by corporation name (e.g., university and department), and the "Permuterm Subject Index" (PSI). The latter is available since 1966 and contains the most important keywords, taken from the title, of all publications of the current year. These keywords are arranged in permuted pairs—i.e., the selection of 10 keywords results in 90 PSI entries each of which leads to the same author and, via the Source Index, to the same source document. The PSI may be used as an entry point to the current literature by locating, via subject headings, useful target references for subsequent searches of the most recent "Citation Index" volumes. The first five-year cumulative *Science Citation Index* (1965–1969) was produced in 1971.

The main advantages of SCI relative to other chemical abstract and title publications may be summarized as follows:

1. A citation index permits searches for research topics which can be identified by one or more relevant target references. Thus, the disadvantages of subjective keyword selection and continuously changing subject terminologies are avoided.
2. A citation index leads from the target reference *forward* in time to the most recent publications on the topic of interest.
3. A citation index provides answers to new types of questions—e.g.: Has any scientist recently improved or criticized the theories advanced in a relatively old reference paper? or: Are new research groups working on the project identified by the target paper? or: Does the number of primary papers published on a given topic justify the publication of a review article?
4. The multidisciplinary literature coverage provided by SCI is particularly advantageous for scientists working in borderline areas between the traditional subjects of chemistry and physics or chemistry and biology. Thus, SCI permits an efficient international as well as interdisciplinary exchange of ideas and promotes scientific progress.

## *CHEMICAL ABSTRACTS* (CA)

*Chemical Abstracts* is undoubtedly the best-known and most comprehensive chemical abstract service of the Western world. More than 12,000 journals and other source documents are monitored regularly for articles of chemical interest, and the 335,000 abstracts published in 1972 cover practically the entire chemical literature. Index volumes are issued semiannually and cumulated every five years and may be used for retrospective literature work while the weekly abstract issues are most suitable for current-awareness searching. Despite the exponential increase in the number of primary scientific papers, the CA index volumes are now produced more rapidly than in previous years owing to computerized information processing methods. So far, Chemical Abstracts Service (CAS) has issued seven cumulative indexes covering the period 1907 to 1966 (Table II). The eighth cumulative index (1967–1971) will comprise 46 volumes several of which have already been published. Since most chemists know how to use these index volumes, no explanations are needed.

Two new kinds of indexes[5] have been added in recent years to expedite efficient manual retrospective literature searches: the Index Guide (since volume 69, 1968), and the Registry Number Index (since volume 71, 1969).

The annually issued Index Guide is an alphabetical list of subject terms and compound names which are listed in the Subject Index under different, synonymous headings. Thus, it provides useful cross references—e.g., "Ketone, ethyl methyl, *see* 2-Butanone" or "Benzoic acid, methyl, *see* Toluic acid"—to facilitate the location in the Subject Index of such compounds the preferred CA name of which is not known to the reader. In addition, it contains illustrative structural diagrams of ring systems with the correct numbering sequence of all ring atoms which permits rapid verification of a compound name and of the position of various substituents as derived by use of the Index of Ring Systems. Thus, by providing access to the Subject Index, the Index Guide may be described as the most important tool to accomplish an effective and successful literature search, and it should always be consulted first by the Subject Index user. Beginning with the volume 71 Index Guide, CAS Registry Numbers (see below) are included for specific elements and chemical compounds, and beginning with volume 76 (1972), the semiannual CA Subject Indexes will be subdivided into separate Chemical Substance and General Subject Indexes.

The most recent CA innovation is the Registry Number Index the first volume of which was issued in 1971 together with the indexes to volume 71 (1969). Since 1965, CAS has numbered all compounds described in its abstracts which permits unambiguous and convenient identification of any registered compound without recourse to a nomenclature system; however, there is no correlation whatsoever between number and structure. In the Registry Number Index, the preferred CA-name of the compound and its molecular formula are listed after each number:

684-84-4 1,3-Butanediol,2-methyl, $C_5H_{12}O_2$

so that consultation of the corresponding subject or formula index both of which contain these Registry Numbers leads to abstract number and subsequently to the primary literature citation. It is also possible to start in the subject index with the known name of a compound to obtain its molecular formula via its Registry Number.

Most chemists are familiar with the methods of using the weekly CA issues for efficient current-awareness searches. The time delay between primary publication and abstract is of the order of three months; since 1967 (volume 66) the individual abstracts rather than page columns are numbered, and each issue contains a keyword, author, patent, and patent concordance index. *Chemical Abstracts* is divided into 80 sections corresponding to 80 subject areas. The odd-numbered issues contain sections 1 to 34 covering organic and biochemistry while the even-numbered issues cover the fields of macromolecular, applied, physical, and analytical chemistry as well as chemical engineering. Thus, each subject area is covered only once every two weeks. All title words, keywords, author names, bibliographic data, registry numbers, molecular formulas, chemical substance names, and general subject entries are stored on magnetic tape (CA Condensates and Integrated Subject File) and accessible for computer-searching.[3]

Table II. *Chemical Abstracts* Cumulative Indexes

| Index Number | Time Period | Index Types[a] | Number of Volumes |
|---|---|---|---|
| 1 | 1907–16 | S, A | 4 |
| 2 | 1917–26 | S, A | 5 |
| 3 | 1927–36 | S, A | 5 |
| 4 | 1937–46 | S, A | 6 |
| — | 1920–46 | F | 1 |
| 5 | 1947–56 | S, A, F, P | 19 |
| 6 | 1957–61 | S, A, F, P | 15 |
| 7 | 1962–66 | S, A, F, P, PC | 24 |
| 8 | 1967–71 | S, A, F, P, PC | 46 |

[a] S = Subject index, A = Author index, F = Formula index, P = Patent index, PC = Patent concordance

## *CHEMISCHER INFORMATIONSDIENST*

*Chemischer Informationsdienst* is an abstract service produced since 1970 by the Gesellschaft Deutscher Chemiker (German Chemical Society) and Farbenfabriken Bayer (Leverkusen, Germany), issued weekly and covering the fields of organic, organometallic, and inorganic chemistry. Rather than aiming for complete literature coverage, it reports selectively on the most significant recent developments. Delay between primary and secondary publication is two to three months. Each issue contains an author index, a list of classification numbers, and 450 to 500 abstracts which are arranged and classified according to subject area.[7] For instance, the classification number, P-0210, is used for papers on substituted acyclic ketones. Each abstract is characterized by a number consisting of letter designation, year, issue number, and abstract number—e.g., CI-1972-2-263, and contains the German title of the original paper, author names, bibliographic data, address, language, abstract text, name of the abstractor, as well as structural diagrams and/or chemical equations. The latter add considerably to the clarity of presentation and undoubtedly permit a more rapid scanning of the content than the corresponding CA abstracts published approximately one month later. However, this main advantage is counterbalanced by the absence of subject and formula indexes, publication in the German language, and, most importantly, by the incomplete literature coverage provided. Of the 222 journals regularly monitored,[7] only 33 are abstracted from cover to cover, and approximately 20 represent review journals and monographs—i.e., secondary sources.

## *CURRENT ABSTRACTS OF CHEMISTRY AND INDEX CHEMICUS* (IC)

A second abstract service featuring structural diagrams is the weekly ISI-publication *Current Abstracts of Chemistry and Index Chemicus.* It abstracts only those papers from 108 source journals which describe new chemical compounds or reactions. Owing to this specialization, the literature of organic, pharmaceutical, medicinal, and biochemistry is well-covered while the journals of physical and inorganic chemistry—e.g., *J. Phys.; Inorg. Chem.; J. Chem. Soc., Perkin Trans.,* 2; *J. Organomet. Chem.*—are excluded.

Each weekly issue contains approximately 240 abstracts describing about 3000 new organic compounds. Each abstract gives complete bibliographic data, structural diagrams, author's summary, use profile, instrumental data alert (physical methods used for compound identification), and, since January 1973, a subject, molecular formula, and author index as well as a listing of new reactions as identified by the author in his paper. To facilitate retrospective literature searching, the indexes are now cumulated quarterly (formerly monthly and semiannually) and annually and published under the name "Index Chemicus." In addition, ISI publishes a monthly "Chemical Substructure Index" (CSI) and a semiannual "Rotaform" formula index both of which are cumulated annually.

The Rotaform index which is similar to the HAIC Index published by Chemical Abstracts Service from 1966 until 1971 contains all molecular formulas (except compounds containing only carbon, hydrogen, nitrogen, and/or oxygen), in permuted alphabetical order of all constituent elements, with the order of elements based on the familiar Hill system.[6] Its organization and use are illustrated in the following example. The iridium compound $C_{12}H_{18}BF_4IrN_2$ is found under three element headings:

*B,* F4 IR C12 H18 N2
F4, B IR C12 H18 N2

and

IR, B F4 C12 H18 N2

Rewriting any of these entries in the element order corresponding to the Hill system and subsequent consultation of the formula index reveals the number of the relevant abstract which leads to the original paper where this compound has been described for the first time:

C12 H18 B F4 IR N2 ..... 172654-4

The subject and author index need no further explanation, but the so-called "Chemical Substructure Index," produced since 1967 and available in print since 1971, is unique in permitting manual searching for partial chemical structures.[8] The Wiswesser Line Notation (WLN), an unambiguous linear description of chemical structures developed by Wiswesser,[9] forms the basis of this index. The "Chemical Substructure Index" lists the WLN descriptions of all new compounds reported in the corresponding abstract issues in permuted alphabetical order of all significant structure elements thus allowing rapid retrieval of information on all substances with common functional groups. Thus, unlike the CAS Registry System, CSI lists structurally similar compounds together. A detailed knowledge of WLN coding rules is *not* required of the CSI user since a table of nearly 3000 commonly encountered substructures and their WLN codes is printed in each CSI issue. The code of any functional group or partial structure not found in this table can be derived generally from similar substructures listed and from specific examples given in the actual index, since conventional structural diagrams are drawn at the top of each new group of substructures. The same task can be accomplished by using the Ring Index and the brochure "Wiswesser Line Notations Corresponding to Ring Index Structures." For example, trichloromethyl compounds are symbolized by GXGG ..... or GGG ..... X, and the CSI-entry for the structure $CCl_3$-CHBr-O-$CH_2CH_2$Br reads as follows:

GXGGYFO2E EGOXY 175728-10

where G=Cl, X=quaternary carbon, Y=tertiary carbon, E=bromine, O=oxygen and 2=length of the saturated chain of carbon atoms. These symbols and the basic WLN coding rules are summarized on the inside cover of each issue. The main advantages of *Current Abstracts of Chemistry and Index Chemicus* as compared with other chemical abstract services are the rapidity of abstract publication, the lucid presentation of structural diagrams, and instrumental analysis method and the substructure search capabilities. The limited journal coverage may be cited as a disadvantage.

## *CHEMICAL TITLES* (CT)

Title publications provide the most rapid but also least informative description of the current chemical literature. *Chemical Titles,* a biweekly CAS publication (since 1961), contains approximately 5000 titles per issue, and the time delay between primary and secondary publication is usually not longer than one month. Actually, the titles of papers from many American journals appear in CT even before the original journal issue has been distributed. Thus, *Chemical Titles* is one of the most current chemical information sources. It is also very comprehensive in its literature coverage since the 700 to 750 journals regularly moni-

tored (and listed on the inside covers of each issue) publish nearly 50% of all chemical papers.

Each issue contains a subject (KWIC, keyword-in-context) and author index both of which give an alphameric code consisting of journal Coden and short bibliographic data. This code leads to the complete bibliographic data, including full title and names of all authors, given in the main section which is simply a list of tables of contents of the evaluated journal issues, arranged alphabetically by journal Coden. The KWIC index is a permuted list of all significant title words arranged alphabetically in the center column, with a limited number of surrounding title words also shown. To obtain additional entries for searching, the names of chemical compounds are fragmented into chemically significant component parts. The computer is programmed by a so-called "stoplist" (printed in each issue) to skip meaningless words such as "the," "of," or "study" in producing the alphabetical list for the center column. Thus, the paper "Addition of Arylsulfinic Acids to *N,N*-Dialkylquinone Dimines" by K. T. Finley, R. S. Kaiser, R. L. Reeves and G. Wernimont is entered four times in the author index and seven times in the KWIC index, namely under ADDITION, SULFINIC, ACID, ALKYL, QUINONE, and IMINES while the words or word fragments OF, TO, DI and N are prevented from indexing by the stoplist. Each of these entries leads to the same literature citation in the main section, as shown below for the subject word SULFINIC:

NE DI + ADDITION OF ARYL *SULFINIC* ACIDS TO N,N-DIALKYL QUINO . . . . . JOCEAH-0034-2083

The code in the right-hand column refers to the *Journal of Organic Chemistry*, volume 34, page 2083.

The organization of the bibliographic section of CT also permits efficient current-awareness searches by regular scanning of the tables of contents of selected chemical journals.

*Current Contents,* Physical and Chemical Sciences same purpose and is published in five editions:

*Current Contents,* Physical and Chemical Sciences

*Current Contents,* Life Sciences

*Current Contents,* Agricultural, Food and Veterinary Sciences

*Current Contents,* Engineering and Technology

*Current Contents,* Behavioral, Social and Educational Sciences

The tables of contents of chemical journals are reproduced in one or more of the first four editions. "CC, Physical and Chemical Sciences" covers about 750 journals, half of which are devoted to chemistry and closely related subject areas. More than a hundred basic chemistry journals are common to both "CC, Physical and Chemical Sciences" and "CC, Life Sciences." The latter emphasizes the fields of biology, medical sciences, and biochemistry and covers approximately 1000 journals, a third of which publish papers relevant to the chemical sciences. Including the relatively few journals of agricultural and food chemistry and chemical engineering monitored by "CC, Agricultural and Food Sciences" and "CC, Engineering and Technology," the total number of journals of chemistry and related subjects covered by *Current Contents* is estimated to be in the order of 700, approximately 550 of which are also found in *Chemical Titles.* However, this estimate must be interpreted with caution since it is difficult if not impossible to draw borderlines between the various traditional scientific disciplines. CC is extremely current in processing journals within two weeks of their publication.

Each CC issue contains an author index listing only the first author of each paper, and an address index to facilitate the ordering of reprints. A weekly subject index (WSI) was started in 1972 for "CC, Life Sciences" and is also available for "CC, Physical and Chemical Sciences" since January 1973. The multidisciplinary coverage of the scientific literature is very advantageous for scientists working in interdisciplinary subject areas. A disadvantage common to all title publications is the fact that they do not reveal details on the scientific content of a paper beyond the information given in the title.

## CONCLUSIONS

In summary, no secondary source publication can meet all the demands of all information-seeking scientists since different kinds of research problems require answers to different types of search questions. Depending on whether the research goal can be best described by keywords, compound names, element symbols, molecular formulas, substructures, or literature citations, one or the other abstract service may provide the fastest access to the desired information. A suitable combination of several types of questions by utilization of the most characteristic features of all available chemical title and abstract publications is recommended as the optimal procedure for assembling a reasonably complete bibliography on any topic of special interest. Despite the recent development of computer methods of information retrieval, efficient manual search procedures are believed to remain essential for both current awareness and retrospective literature work.

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