

been arable; the production of foods from oceans and inland waters; the exploitation of seaweed and plankton as significant sources of food; the fabrication of synthetic proteins from microorganisms, algae, and petrochemicals; the application of ecology, such as in the effect of air and water pollution; the application of animal and plant genetics; the production of synthetic vitamins, amino acids, carbohydrates, and the conversion of wastes into foods; the fabrication of foods acceptable to various peoples throughout the world in terms of flavor, appearance, and texture as well as religion, culture, and custom; the fabrication of nutritional foods to prevent malnutrition in areas of plenty as well as in areas of starvation and famine; the fabrication of food for the exploration of space; and the management of information in all areas of and related to agriculture and food science and technology.

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CAS as a Literature Source for Agricultural and Food Science and Technology*

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The purpose of this paper is to help users find agricultural and food chemistry information in Chemical Abstracts Service (CAS) publications and services. It is primarily a narrative catalog of the characteristics of our output, intended to help the agricultural and food chemist decide which of his information needs may be satisfied in whole or in part by a CAS publication or service.

The information needs of each and every field of science cannot be met at present. Chemical Abstracts Service (CAS) does, however, by treating comprehensively all of chemistry and chemical engineering, provide a significant amount of information to special fields, among these, agriculture and food science. The primary mission of CAS, of course, is to make chemical and chemical engineering information and its bibliographic identity more readily available, more useable, and more used.

CAS-produced sources of information about agricultural and food science include *Chemical Titles*, *Chemical Biological Activities*, *Polymer Science and Technology*, *Chemical Abstracts* Issues, Issue Indexes, Semi-Annual Volume

Indexes, Five-Year Collective Indexes, and the new *Basic Journal Abstracts* and *CA Condensates*. Soon, the Chemical Compound Registry System and the Substructure Search System for computer search of files of structural formulas will be added to CAS services now available to subscribers.

On January 1, 1968, *Chemical Abstracts (CA)* began its 62nd year of publication. The structure and format of CA have changed from the few broad, textbook-like category headings first used in 1907 to the present complex, detailed, and discipline-oriented 80 sections of chemistry and chemical engineering. This change is a fascinating and revealing reflection of the evolutionary growth and development of the sciences and technologies reported in CA. From the beginning, CA and now its parent CAS have pursued a number of objectives, including complete coverage of chemistry and chemical engineering, informative abstracting, and indexing to maximum

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specificity. As operating guides toward these objectives, the editorial staff of CAS has compiled extensive, detailed, and highly integrated sets of decisions. Frequently, these decisions affect not only CAS, but also the user of our services.

Our services lack analogy with other commodities, such as automobiles. For example, a man can become a skillful automobile operator without knowledge of the detailed design and manufacturing decisions required to produce his vehicle. Not so with a carefully structured information tool. The many reasons for selecting or rejecting an item for abstracting, the way in which the item is abstracted, where it is placed within the publication and services, how it is indexed, how the various indexes differ from each other, and so on throughout the many complexities of abstracting and indexing service production—these represent a range of decisions with direct and positive impact on the ability of the user to make optimum use of the information tools which we, and other organizations, produce.

CAS—or any information service—should be viewed as a data base that has various routes of access, each route having its own special characteristics, strengths, and weaknesses. The concept of “data base” and probably the term itself springs from the increasing impact computers are having on information service. This impact concerns producers of information services as well as users, and it helps to underscore the need to distinguish between the body of information, that is to say the data base, and the means of using it, that is, the routes of access.

THE DATA BASE

Putting information into the CAS system begins with the acquisition of journals, reports, patents, conference proceedings, and the like. CAS raw material today includes some 12,000 serial publications plus patents from 25 countries. From a first selection of 1.5 million papers and 50,000 patents, CAS will in 1968 finally select 275,000 items as fitting our definition of chemistry and chemical engineering. Of these items, about 245,000 will be abstracted and about 30,000 duplicated patents will be cross-referenced through the patent concordance to a previous abstract. The original materials and their abstracts also will be submitted to a variety of indexing processors at various times during their progress through this system.

In 1968, some 82,000 pages will be published by CAS, and large quantities of magnetic tape will be issued containing abstracts and index entries that subscribers will examine in their search for information. These tapes will also be searched on CAS computers for subscribers who wish this type of service. Much information relevant to food and agricultural science and technology is produced in magnetic tape form.

At first, any user of a reference service finds it difficult to understand the criteria that service uses to select information to cover. The information which appears in CAS services is not determined by static rules. With respect to CA itself, the rules change as the subdisciplines that constitute chemistry change. For example, basic physics research into the constitution of matter rapidly became a concern of chemists. Other fields of science, such as biology, have increasingly adopted the approaches

and techniques of chemistry, and so new interdisciplinary branches of chemistry have evolved.

CAS services other than CA have relatively simple selection criteria. Each of the special publications and services contains a printed statement of its coverage and selection criteria. To learn what sources are covered in CA, the user is best referred to the *List of Periodicals Abstracted*, with its supplements. The criteria for selection from these sources will be dealt with later in this paper.

THE IMPACT OF THE COMPUTER

CAS is in the midst of conversion to an integrated computer processing system.¹ The effect which this conversion has on users is of some interest. The conversion began in the late 1950's; it will be essentially complete in the early 1970's. This transition to computer-base also marks the transition of CAS from a publishing organization to an information service that produces publications as one form of output. Some of the many reasons for using computer support include:

(1) The computer is an extremely powerful processing device which offers hope of keeping up with the tremendous and still growing volumes of information that must be dealt with.

(2) Computer support makes it possible for CAS to eliminate redundant use of manpower, both professional and clerical. In the careful production of traditional publications redundancy is not, however, synonymous with inefficiency. With computers it is possible to maintain the intellectual input essential to a first-class scientific information service, but at the same time to conserve manpower to a remarkable extent.

(3) The manipulative power of computers gives the flexibility to design and develop special “packages” such as services intended only for one company or one laboratory. The tailor-made information services that have been the dream of science are now technically feasible. They will become administratively and economically feasible soon.

These generalizations apply not only to CAS but to other information organizations that use computers in a similar manner.

HOW TO USE CAS PUBLICATIONS AND SERVICES

CAS publications and services directly pertinent to users of food and agricultural chemical information are presented here in a somewhat chronological order. The chronology recognizes that the information user needs, first, to keep up-to-date and, second, to search the archives for answers to questions. Although computer technology is helping to bring current awareness and retrospective search capability closer together in single information tools, it seems likely that these capabilities will remain separate to function more adequately.

Chemical Titles (CT). CT was the first CAS computer-based publication, produced in early 1961 as a current awareness service. CT consists of a permuted or keyword-in-context (KWIC) index, a table of contents or bibliography section, and an author index. It covers 652 of the world's scientific and technical journals—those which contain the most papers of use for CA. Of these 652 journals, 46 are directly and completely related to food or agricultural science and technology. Another few hundred are peripherally related to these areas through their coverage of the biosciences and various applicable technological topics.

CT is published every two weeks as a printed journal, as a reel of magnetic tape for subscribers who utilize computers in their operations, or as a subscription search service performed on CAS computers. The printed version of *CT* is intended not to be read, but to be scanned—users skim the printed issues of *CT* looking for individual words that relate to their current technical interest. One can, of course, also scan rapidly for the work of particular authors or for the chemical tables of contents of particular journals. As a computer-operated service, *CT* provides the base from which to prepare selective reading lists. These lists are compiled by matching terms which describe the interests of an individual, laboratory, or a project with terms which appear in the titles of articles in currently published literature. Since it began in 1961, *CT* has dealt with some 650,000 titles. About 127,000 titles will be processed during 1968. The emphasis of *CT* is on speed and breadth of coverage; consequently, it should be one of the first places a user goes to find what of interest to him is currently being published.

Chemical-Biological Activities (CBAC). *CBAC* was the second of the computer-based publications and services of CAS. It is a highly specialized abstracting and indexing service which covers a specific, limited list of journals and treats a specific subject matter. The subject area of *CBAC* is divided into:

- (1) the effect of exogenous organic compounds on biological systems and
- (2) the metabolism of organic compounds in biological systems and in vitro reactions between compounds of biological interest.

Papers containing this subject matter are selected from 585 of the world's journals most likely to publish on those topics. As with *CT*, a significant number of these journals is directly related to food and agricultural science and technology. Fifty-six of the 585 journals have words such as food, fertilizer, agriculture, veterinary, etc. in their titles. Many more have direct or peripheral interest for workers in food and agricultural science. Each issue of *CBAC* includes, in addition to abstracts, a Subject Index, an Author Index, a Molecular Formula Index, a Registry Number Index for the compounds, all of which have been registered in the CAS Chemical Compound Registry System, and a Faceted Number Index² which helps to interrelate certain families of compounds referenced in *CBAC* and in the Registry System.

CBAC is also published biweekly as a printed journal, as a magnetic tape for searching on a subscriber's computer, or as a search service conducted on CAS computers. The information in *CBAC* has both current alerting and archival value. It is small enough in volume to permit each issue to be scanned rapidly for current papers of interest, but because of the manner in which the indexes are prepared, there is an average of 40 indexing terms for each paper abstracted. This is an indexing density of sufficient depth to support searching of the *CBAC* literature.

Polymer Science and Technology (POST). *POST* is a recent addition to the CAS family of specialized publications and services, having been in full-scale production only since November 1967. The *POST* publications cover the science and technology of plastics, films, rubber, and other elastomers.

POST appears in two separate editions, *POST-J* which deals with the journal and report literature and *POST-P* which covers the patent literature. Each appears in alternate weeks as a printed journal, on magnetic tape, or as a search service. It is estimated that during their first year of publication, *POST-J* will contain about 18,000 abstracts, and *POST-P* about 10,000.

Unlike *CT* and *CBAC*, coverage is not restricted to a core list of journals but will encompass the whole of the chemical and chemical engineering literature. Early issues of *POST-J* concentrated coverage on a core list of about 450 of the more important journals publishing in the polymer field, but coverage is being gradually expanded to include all applicable CAS sources. Wood³ has stated that 75% of the papers abstracted in *CA* originates in only 850 journals. In a specific subject area such as polymers, 450 core journals should effectively cover the subject. Extending coverage to the total list of periodicals abstracted by *CA* will ensure completeness and provide another step toward the goal of operating all CAS publications and services out of a single computerized data base.

POST-P patent coverage includes all relevant British, French, German, and United States patents. For patents from an additional 21 countries, abstracts are published only when the patents were issued to individuals or companies resident in the country where the patent was issued.

POST-J and *POST-P* cover preparation, properties, technology, and uses of synthetic and natural organic polymers, synthetic inorganic polymers, monomers, catalysts, and adjunct materials such as plasticizers, antioxidants, and fillers. In addition, coverage includes processes and equipment used directly in the manufacture of monomers and polymers, determination of the properties of monomers, polymers, and adjunct materials, and the fabrication of polymers into end products. Information on new tests and standards, as well as health and safety aspects of polymer technology rounds out the *POST* series subject coverage. Of specific interest to food and agricultural science and technology are the areas of plastics and films for use in food packaging and polymeric materials used as food additives, fertilizer ingredients, and soil amendments.

Basic Journal Abstracts and CA Condensates. During 1968, two new information services are being introduced to increase subscribers' ability to search *CA* by computer.

Basic Journal Abstracts is a magnetic-tape oriented service comprised of *CA* abstracts from 34 important chemical journals, world-wide. All of these journals have a very basic chemical nature which is almost certainly pertinent to the scientific and technical programs of organizations concerned with agricultural and food science and technology though none are specifically food or agricultural journals. During the first year of *Basic Journal Abstracts*, approximately 15,000 *CA* abstracts will be placed on tape for searching by subscribers who have computers or by CAS for subscribers who wish this type of service. Highly selective reading lists will be prepared for staff members of subscribing organizations.

CA Condensates serves a similar purpose but from a completely different approach. The *Condensates* consist basically of the headings of all of the abstracts in *CA* plus the Keyword Index entries pertinent to each abstract.

The combination of the abstract heading and its keyword subject index entries constitutes a kind of condensed abstract which can be searched by computer. Because all abstracts will be represented on tape in this condensed style, *CA Condensates* is actually the first means of computer access to all items currently abstracted in *CA*.

Developmental Services. Two services in the final development stage complete the current picture of CAS as an information source for agricultural and food science and technology. These are the CAS Chemical Compound Registry System and the Substructure Search System, described in the last section of this paper.

Chemical Abstracts (CA). The coverage described for CAS in the section of this paper on The Data Base is also the coverage for *CA*. Raw material consists principally of 12,000 primary periodical sources plus chemical patents from 25 countries. Of the 12,000 primary sources, approximately 5000 will be abstracted in a given semiannual volume of *CA* and about 7500 in two consecutive semiannual volumes.

An understanding of *CA* can be approached from two different positions, the abstracts or the indexes. To describe the content of the publication requires analysis of the abstracts; to describe how a user will, or should, seek access to that content requires analysis of the indexing. However, the science specialist confronting an information service for the first time will usually ask, "What do you cover in my field?" The various answers are indicated in the following pages which treat the issues of *CA* first and then proceed to a consideration of indexing.

Within the Biochemistry Grouping of *CA* (Sections 1-20) is a subgrouping of four adjacent sections which could be termed the "Food and Agricultural Science and Technology Subgroup." Subject areas include *Foods*, Section 17; *Plant-Growth Regulators*, Section 18; *Pesticides*, Section 19; and *Fertilizers, Soils, and Plant Nutrition*, Section 20. During 1967, these four sections contained 9430 journal article abstracts, 957 patent abstracts, and 85 new book announcements (Table 1). This represents about 15% of the Biochemistry grouping or just over 4% of the total number of abstracts published in *CA* in 1967. In a sense, coverage of the field of agriculture and food is actually greater as will be seen from the section on *Cross References*, below and Table 6.

FOODS-SECTION 17. This section covers chemical studies of foods in which the principal interest is composition and changes in composition, preparation, processing, and treatment of foods for mammalian consumption. The chemical aspects of food packaging and food preservation, including studies on ionizing radiation in preservation, are presented in this section. But studies which emphasize packaging from a mechanical standpoint, for instance, with chemistry only incidental or not applicable at all, are excluded.

Much of Section 17 deals with permissible-residue-level, tolerance limit, and safety evaluation studies of pesticides and food additives. As a regular feature, the section contains abstracts of *Federal Register* standards promulgated under the Federal Food, Drugs, and Cosmetics Act and of tolerances for permissible chemical residues that relate to foods. Studies of analytical methods specifically applicable to food analysis are found in the *Foods* section.

The arrangement of abstracts within the section is based

Table 1. Number of Abstracts Published in 1967 in the Agricultural and Food Chemistry Sections

Section		Journal Articles	Patents	Books
17	Foods	3358	433	47
18	Plant-Growth Regulators	1709	120	4
19	Pesticides	1634	235	11
20	Fertilizers, Soils, Plant Nutrition	2729	169	23
		9430	957	85
		10387		

Table 2. Abstract Arrangement

Foods-Section 17

1. Reviews
2. General
3. Food additives (Federal Register)
4. Chemical residues (Federal Register)
5. Preservation and packaging
6. Cereals
7. Flour and bakery products
8. Dairy products
9. Eggs
10. Meat and meat substitutes
11. Fish and other seafood
12. Edible fats and oils
13. Vegetables (including pickles, sauerkraut)
14. Fruits and fruit products
15. Nuts
16. Sugar and sugar products (honey)
17. Condiments and flavors
18. Chocolate
19. Beverages (excluding alcoholic beverages)
20. Animal feeds

chiefly on the food types and follows closely the order listed in Table 2. Editorial judgment regarding the subject emphasis of the paper is the final authority on abstract arrangement.

PLANT-GROWTH REGULATORS-SECTION 18. This section contains abstracts of studies concerning the biochemical effects and uses of plant-growth-regulating substances (the auxins, gibberellins, so-called plant hormones, and so on) and crop control agents (herbicides), whether on a small experimental basis or in large-scale agricultural application. Biochemical effects include metabolism and fate of the agents. Other subjects in the section are: methods of determination and analysis of herbicides (except on foods); and studies on herbicide toxicity, using the cross-reference system described below when the toxicity involves such nontarget organisms as man and livestock. Although abstracts of residues and their tolerance levels on foods appear in *Foods*-Section 17, abstracts which deal with the formulation of herbicides, for example, into fertilizer compositions are assigned to the fertilizer section.

The arrangement of abstracts within the section is relatively simple, consisting of review article abstracts, followed by growth-regulator studies, and ending with herbicide abstracts.

PESTICIDES-SECTION 19. Although the herbicides treated in Section 18 are pesticides, the pesticides of Section 19 are restricted to agricultural (plant) bactericides, fungicides, insecticides, nematocides, rodenticides, and other pest-control agents whose primary intent is non-medical. For example, whereas penicillin is a pesticide in the broadest sense of the word, abstracts concerning this antibiotic and all related drugs are found in the medically oriented sections of CA. Section 19 might be more descriptively named *Agricultural Pesticides* with the added restriction that these agents are primarily designed to control plant pests as opposed to veterinary pests.

Again, the subject emphasis is on the chemistry of the effects brought about by the use of pesticides on the target organisms. Basically, the same rules regarding metabolism, analytical procedures, and residue levels that place herbicide studies in Section 18 also place pesticide studies in Section 19. Table 3 illustrates the arrangement of abstracts within Section 19.

FERTILIZERS, SOILS, AND PLANT NUTRITION-SECTION 20. The three interrelated topics which make up the title of Section 20 are reversed in the order of their presentation within the section. After abstracts of review articles (the lead item of each CA section format), the subject of plant nutrition is covered. The plant nutrition segment contains abstracts of studies on the use of plant nutrients from the soil and the requirements of plants for these nutrients, including major, secondary, and minor elements that relate to growth, yield, and composition of the plant. As the potential overlap between Section 20 and other sections is probably greater than for almost any of the other sections of CA, extensive use of the cross-reference system is made.

Abstracts on soils are placed in this section according to the stated purpose of the author or the tone of his article.

MINERALOGICAL AND GEOLOGICAL CHEMISTRY-SECTION 53. This section also covers soil composition studies. The choice is based on the emphasis or intent (geological or agricultural) of the article. When a paper focuses on organic compounds in soil, the abstract is usually placed in Section 20; studies of inorganic soil components are usually placed in Section 53, with appropriate cross-reference.

The topic of fertilizers includes soil amendments and conditioners as well. The effects of all these substances on plant growth, yield, and quality and on soil composition are placed in Section 20.

Abstracts on the effects of compost, manure, or other natural organic fertilizer materials are included only when chemically significant, that is, if compounds are reported. Most abstracts on fertilizer and soil amendment manufacture are placed in Section 20. When the intended use or application of a given chemical cannot be determined from the abstract, the abstract is placed in the appropriate organic or inorganic synthesis section. Access to such abstracts is acquired through the Keyword Index, also to be explained later.

Methods of analysis of soils and fertilizer constituents are appropriately placed in Section 20 with cross-references to the analytical sections of CA (Sections 70 and/or 80). Table 4 outlines the positioning of abstracts within Section 20.

Table 3. Abstract Arrangement

Pesticides-Section 19

- | | |
|-----------------|------------------|
| 1. Reviews | 6. Acaricides |
| 2. General | 7. Nematocides |
| 3. Bactericides | 8. Molluscicides |
| 4. Fungicides | 9. Rodenticides |
| 5. Insecticides | 10. Other |

Table 4. Abstract Arrangement

Fertilizers, Soils, and Plant Nutrition-Section 20

1. Reviews
2. General
3. Soil composition
4. Plant Nutrition
5. Effects of fertilizers
on plant growth and quality
6. Effect of fertilizers and soil
amendments on soil composition
7. Chemistry and technology of
fertilizer and soil amendments
 - (a) Manufacture
 - (b) Analysis
 - (c) Other

CROSS-REFERENCES. It is not economically feasible to publish an abstract in more than one section of CA, even though selection criteria would sometimes allow this to be done. The answer to the problem is an effective cross-referencing system and the issue Keyword Index. A final item in each section is a segment headed "See also," which lists article titles, the section numbers in which the abstracts of the articles appear, and the abstract numbers for each of the entries. Cross-references are employed whenever an abstract could logically fit into two or more sections. They are also employed whenever the subject matter of an abstract directly extends to the interests of readers of other sections.

In addition to these specific cross-references, permanent cross-references head the "See also" entries in many sections. The purpose of permanent cross-references is to alert readers of specific sections to other sections which they should routinely consult. The interest overlap between sections having permanent cross-references is so great that it would not be practical to duplicate every title, section number, and abstract number. Therefore, the reader is alerted to the entire section. Table 5 shows the four sections of the "Food and Agricultural Science and Technology Subgrouping" and the other sections to which they are permanently cross-referred.

Table 6 illustrates the extent to which the cross-reference system is used. The data are taken from Volumes 66 and 67 (1967) and do not include the number of abstracts covered by the permanent cross-references. Note that the reader is alerted to an additional 1756 abstracts or 17% more than appear in Sections 17-20 alone.

Chemical Abstracts Indexes. It is apparent to all users of information as well as to all producers of information services that the usefulness of any body of information is greatly affected, even controlled, by the way in which it is indexed. Indexing is a major part of the total CAS production effort. For the user, optimum efficiency in

Table 5. Permanent Cross-References

Section	Permanently Cross-Referred to Section
Foods-Section 17	Animal Nutrition-Section 10
Plant-Growth Regulators- Section 18	Plant Biochemistry-Section 7
Pesticides-Section 19	(no permanent cross-reference)
Fertilizers, Soils, and Plant Nutrition ^a -Section 20	Plant Biochemistry-Section 7

^a Section 53 (Mineralogical and Geological Chemistry) readers have a permanent cross-reference to Section 20 for the soil composition studies.

Table 6. Number of Abstracts Cross-Referred to the Food and Agricultural Chemistry Sections in 1967

Section No.	Cross References
17	533
18	272
19	676
20	275
Total cross-references	1756

the use of *CA* comes only with skill in the use of the indexes. The following sections, while not an exhaustive treatise on *CA* indexes, do delineate some characteristics that are important to the user. Table 7 lists the various *CA* indexes and their frequency of publication.

Keyword Index. Each issue of *CA* is provided with a Keyword Index to the abstracts in that issue. The index is printed on colored paper and bound into the back of the issue. The Keyword Index is an interim index designed to give access to the abstracts until the Volume Subject Index is published. The Keyword Index is not a substitute for the Subject Index, however, except in that limited sense. Keywords, or more accurately key phrases, are selected by the editors during abstract editing. The phrases chosen are those that the editors feel define the subject content for the potential reader. The average number of Keyword Index entries per abstract is presently just over four.

Treatment of chemical compounds is different in the Keyword Index than in the Volume or Collective Subject Indexes. Although the Subject Indexes list each significant chemical compound described in an abstracted paper whether or not it is named in the abstract, the Keyword Index lists entries to the classes or families of compounds in the paper. For example, for a paper describing the preparation and properties of 15 different chlorinated hydrocarbons, each compound would be individually indexed in the Subject Indexes, whereas the terms "chlorinated hydrocarbons" and "hydrocarbons chlorinated" would suffice for the Keyword Index. From this point of view, the Keyword Index does not have the same in-depth coverage or sophisticated structural organization of the Volume Subject Index; this is why it is not cumulated to produce a volume index. With the CAS move toward a completely computerized information base, the best characteristics of the two types of subject indexing will be fused into an in-depth, structurally organized, yet rapidly produced, immediately available index system.⁴

Table 7. Table of Indexes to *CA*

Type of Index	Groupings of Sections	Frequency of Publication		
		Issue	Volume	Collective
1. Keyword	X ^a	X		
2. Author		X	X	X
3. Numerical Patent		X	X	X
4. Patent Concordance		X	X	X ^b
5. Formula			X	X
6. Subject			X	X

^a The Keyword Index for all sections published during a given week is printed in each of the Section Groupings issued that week. ^b Beginning with the 7th Collective Indexes (1961-1966).

Author Indexes. In addition to the Keyword Index, each issue of *CA* contains an index of names of authors and co-authors for each of the original papers abstracted in that particular issue. Author Indexes are compiled quickly and efficiently by computer. The Author Index in each issue lists single last names and initials versus the *CA* reference, and it is not cumulated into a volume index. The volume index is a different type of Author Index. It is more sophisticated than the issue indexes counterpart in that the entries consist of expanded, more complete author names, and the titles of the papers abstracted are included to help the user associate authors' names with specific fields of work.

The volume Author Index is edited carefully for correctness of spelling and transliteration, a quality control step not possible on the close schedule of the issue index. Also, the volume index lists abstract references under a given author's name to aid the user in selecting references, especially to works by authors with very common names. As are all *CA* volume indexes, the Volume Author Index is cumulated, re-edited, consolidated, and issued as a 5-year collective index. The 7th Collective Index series is now in the publication process.

Numerical Patent Indexes and Concordance. Approximately 10% of the references in the "Food and Agricultural Chemistry Subgrouping" of *CA* Sections 17 and 20 are references to the patent literature. Access to this segment of the chemical literature is given by the subject-oriented indexes and the Numerical Patent Index published in each issue and cumulated by volume as well as on the 5-year collective index basis. The Numerical Patent Index is a numerical listing of patents under each of the 25 countries granting such license which *CA* covers.⁵

Many companies seek patent protection in several countries on essentially the same chemical compounds, processes, and uses of chemical products. CAS has handled this duplication since 1963 with a type of index called the Patent Concordance published in each issue of *CA* and cumulated for the volume and collective index periods. This index is not a true concordance by the traditional definition of the word, but serves to help correlate information in duplicate patents issued in different countries. *CA* abstracts and indexes the first patent received for a given invention. Subsequent patents for the same invention issued by other countries are entered in the Patent Concordance along with the *CA* reference to the first patent. Whenever a duplicate patent of this nature is

received, the entire duplicate relationship is published. One effect of the Concordance is evident from Table 1: the 957 patents abstracted during 1967 in the food and agricultural chemistry fields is a minimum number. Coverage of the patents literature in these fields is much more thorough than this figure indicates, and additional patents to these same inventions issued by other countries can be found through the Concordance. Section-by-section figures are not available, but some idea of the coverage by the Patent Concordance can be gained from the fact that for *CA* as a whole in 1967, a total of 36,750 patents were abstracted. During this same period an additional 26,766 patents were covered through the Patent Concordance.

Formula Index. The Formula Index is used primarily to locate entries in *CA* to specific chemical compounds. It is an arrangement of empirical molecular formulas expressed in a modified Hill System format (carbon followed by hydrogen if either or both are present, followed by any other elements in alphabetic order). In addition to referring the user to the compounds in papers abstracted in a given volume of *CA*, the Formula Index gives the official *CA* indexing name which is used in the Subject Index. In this latter respect, the Formula Index is an excellent chemical nomenclature dictionary for the chemist who knows the structural formula and hence the molecular formula, but who is uncertain as to the correct chemical name.

When the name of a given compound has 10 or more references to it in a volume of *CA*, the entries in the Formula Index are replaced with cross-references to the equivalent heading in the Subject Index. The cross-references appear immediately following the molecular formula. Many of the commonly used agricultural pesticides are treated in this way.

A new supplementary index designed to be used in conjunction with the Formula Index is the Hetero-Atom-In-Context Index (HAIC Index), available for the first time as part of the Volume 66 (January-June 1967) Formula Index. The HAIC Index highlights elements other than carbon and hydrogen in compounds, thus, greatly facilitating searches for specific elements, especially the less common elements. Through computer programmed formatting techniques, the HAIC Index separates the non-carbon, nonhydrogen element symbols from the rest of the formula but keeps them in context so that the formula does not require reconstruction. Once answers to a search of the HAIC Index are found, referral to the Formula Index will provide names of compounds and references to their appearance in the literature. Food and agricultural chemists will find the HAIC Index particularly pertinent for compound searches in the pesticide and veterinary pharmacology areas.

Subject Indexes. The Volume and Collective Subject Indexes to *CA* differ markedly from the issue Keyword Indexes in that the Subject Indexes take a deeper conceptual approach to indexing than does the Keyword Index. In traditional *CA* subject indexing, a set of related terms is considered as a subject unit. Just as the abstract is written with the technically knowledgeable reader in mind, so the subject units are generated and assembled into an intellectual structure meaningful to a subject-specialist reader in the technical area concerned. Food

and agricultural chemistry abstracts are indexed at CAS by specialists with technical backgrounds, training, and experience similar to the users of those index areas. The interrelationships of the data elements in a given Subject Index entry depend upon normal grammatical construction, not upon any special coding or flagging by the indexer. For this reason, although the Subject Index is highly structured, maintenance of that structure does not depend upon rigid vocabulary control in the sense of an authority list.

The structure of the *CA* Subject Index has, of course, been designed to increase information accessibility.⁶ Two of the most useful, yet least understood or appreciated features of the Subject Indexes illustrate that fact. These features are the cross-referencing system and the use of symbols to expand some entries.

To choose the precise term(s) an index user will seek or to pinpoint the most effective index heading to describe an author's concept is difficult. These considerations and that of placing and arranging abstracts within a *CA* section are supported by the use of cross-references. Cross-references in the *CA* Subject Indexes are of two types—the "See" and the "See also" cross-references.

The "See" cross-reference is employed with commonly used terms likely to be searched for but having their references under another, more inclusive heading. Concentrating information under certain chosen headings eliminates other closely related but not mutually exclusive headings. The following examples illustrate two types of "See" cross-references:

Acaricides. See *Insecticides*
Ketchup. See *Catsup*

In these cases, no entries are made under the left-hand terms; all entries appear under the headings on the right. In an entry such as

Food, canned. See *Canned goods; Canning*

only a portion of the entries under the heading "Food" is transferred to another heading. Many references still appear at the entry "Food" and its modifications. This variation of the "See" cross-reference illustrates the basic *CA* policy of indexing to maximum specificity.

The "See also" is informational rather than organizational in character. It does not preclude the use of the heading for references but calls attention to related headings which should be consulted for possible additional information. The Subject Index heading "Fertilizers" has following it a "See also" reference to 21 additional terms which should be checked.

Three symbols commonly used throughout the Subject Index are the asterisk (*), double asterisk (**), and the dagger (†). All three are associated with the indexing of chemical compounds. An asterisk signifies that the compound name was supplied by the author and may not conform to the CAS system of nomenclature used in the index. It is used where incomplete information makes it inadvisable to apply systematic nomenclature, or where the name given by the author, differing widely from the one given by the indexer, is listed as an extra entry.

The double asterisk is placed after the *CA* reference instead of after the index heading entry; it signifies that

the entry has been made from the original journal article or patent specifications for a compound suitable for indexing but not mentioned in the abstract. This procedure illustrates the basic CAS indexing policy of indexing synthetic organic and theoretical inorganic and physical chemistry papers from the original document, not from the abstract alone. This practice allows in-depth indexing in areas having large numbers of compounds without requiring every compound of significance to appear in the abstract.

The dagger follows the name of some compounds to indicate that the entry is an extra one, that is, the name is only slightly less desirable than the first one chosen. The preferred name can be determined by reference to the Formula Index.

For a number of years, the Subject Indexes have distinguished between references to journal-article abstracts and patent abstracts by placing a letter "P" before the patent abstract reference. Recently, two additional letter designations have come into use. "PC" precedes references to entries chosen from the patent claims, and "R" precedes Subject Index references to all review articles.

CHEMICAL COMPOUND REGISTRY AND SUBSTRUCTURE SEARCH⁷

The two newest CAS services, both of which are operational but not yet available for use by the general subscribing public are the CAS Chemical Compound Registry System and the separate Substructure Search System which, however, searches Registry structure data.

The Registry System consists of computer language files, presently on magnetic tape, of structural formulas, nomenclature, and bibliographic citations for all compounds normally indexed by CA. There are now more than 800,000 different compounds represented in the Registry System by completely detailed structural formulas. More than 6000 mixtures have been registered. The nomenclature file contains more than 1,000,000 entries, and there are well over 1,500,000 bibliographic citations. The structure file of the Registry represents complete CA coverage from 1965 forward with occasional excursions into older literature such as for fluorine compounds for which the total published literature of chemistry has been screened. A number of handbooks and compendia of substances important in agricultural and food science have also provided Registry input. No attempt has been made to put the nomenclature and citation files on the same complete footing as yet. When the Registry is "full"—containing all compounds that have been published—it will contain about 4,000,000 structures. Current growth rate of the Registry is about 4000 compounds new to the file and about 9000 references per week.

Technical descriptions of the Registry System in its early stages have been published.⁸ There is no up-to-date published description of the CAS Substructure Search System which is being redesigned and programmed for current generation computer hardware. Suffice it for the chemist-user to know that all of the completely detailed structural formulas in the Registry can be searched for parts of structures, with the searchable parts not restricted to any predefined list of fragments.

Given a complete file of structures searchable by computer either for whole or parts of structures, it is possible to postulate a number of services that combine this capability with the text searching capability also present in the CAS computer-based system to obtain, for example, lists of references to particular compounds, current bibliographies for particular compounds, first references in the published literature to hypothesized structures, and so on. CAS intends to make services of this type available in the future as the demand for them is identified.

The pertinence of the Registry and Substructure Search Systems to the fields of agricultural and food science and technology are, obviously, the same as they are to any field concerned with the development and application of chemical compounds. Pilot application of these techniques outside of CAS should begin toward the end of 1968, and it is quite possible that limited subscriber use of the Substructure Search System may be made available in 1969.

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