deliver current scientific information. Further, computers will become an integral part of the laboratory complex, permitting research data to be entered directly into large memory banks. Thus, the total information base, composed of data received from outside secondary services and laboratory data generated by current industrial research programs, will be directly accessible with a minimum of manual manipulation. To translate our growing base of knowledge into new ideas, a new breed of information scientist will emerge. He will be highly skilled in his field and possess a unique ability to refine a large body of data and information into constructive ideas that lead to new products and new services. The information scientist will work very closely with his laboratory counterpart, who will begin to recognize the true potential of information work. There will also be a greater professional recognition of the information scientist, and the opportunities open to him.

Both scientists and managers will want and need closer interaction with the information base. Advances in computer technology will permit them to interact with current information on a conversational basis. The use of remote terminals will be commonplace.

Computers will also have their impact on management. One significant application of computers will be in the simulation of decision situations. The manager or businessman will be able to test the consequences of his decision before he proceeds to implement them. He will draw upon current information which will be continuously updated in a large memory bank. Computer technology will also permit direct interaction between the manager and his information. Further, not only will information be provided by the computer system, but it will alert the user to the need for decisions regarding current operations.

These represent but a few considerations of the future. They suggest, however, that while information operations will remain an important part of the total research and management process, their character will shift from what is more or less a service orientation to one which is directly keyed to planning and control functions and the decision-making process and, in turn, to the planning, implementation, and maintenance of even more sophisticated information systems.

LITERATURE CITED

(1) Craig, P. N., and H. M. Ebert, "Eleven Years of Structural Retrieval Using the SK&F Fragment Codes," 156th Meeting, ACS, Atlantic City, N. J., September 8-13, 1968.

(2) Gottardi, R., "A Modified Dot Bond Structural Font With Improved Stereochemical Notation Abilities," 157th Meeting, ACS, Minneapolis, Minn., April 13-18, 1969.

(3) Hayne, R. L., A. S. D'Eustachio, and A. D. Bender, "Use of a Computer-Based Information System for Processing Clinical Data," *Drug Inform. Bull.* **2**, 32-9 (1968).

(4) Bender, A. D., A. E. Strack, G. W. Ebright, and G. Von Haunalter, "Delphic Study Examines Developments in Medicine," *Futures* **1**, 289-303 (1969).

(5) Longnecker, H. C., "The Role of Science Information Department in Industrial Research and Development," *J. Chem. Educ.* **33**, 633-5 (1956).

(6) Rockwell, H. E., and H. C. Longnecker, "Information Services at Smith Kline and French," *Percolator* **35**, 32-6 (1959).

Operation of Du Pont's Central Patent Index*

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Received July 3, 1969

The Central Patent Index is one of many information centers constituting Du Pont's Information Network. The development of this index and its relationship with other centers in the network is followed by a description of its operation: input, storage, and search techniques.

A description of the operation of Du Pont's Central Patent Index is best preceded by a brief description of the corporate structure of Du Pont, since the services of this Index are provided at the corporate level.

Du Pont's Corporate Structure. Each of the twelve industrial departments of Du Pont (Figure 1) operate with considerable autonomy, but under the general policies set by the Corporate Executive Committee. These industrial departments all have research, manufacturing, and sales organizations for Du Pont products. Most of these products—e.g., synthetic fibers, molding resins—are sold to other processing companies before they reach the ultimate consumer; some others—e.g., paints—are produced directly for retail sale.

The thirteen staff departments centralize activity in fields which, as in the case of the industrial departments, are largely defined by the name of the department. While most of these functions are carried out directly by the industrial departments, each of them finds that it is to their advantage to have much of this activity performed on a centralized basis.

* Presented at the 4th Middle Atlantic Regional Meeting, ACS, Washington, D. C., February 13, 1969.

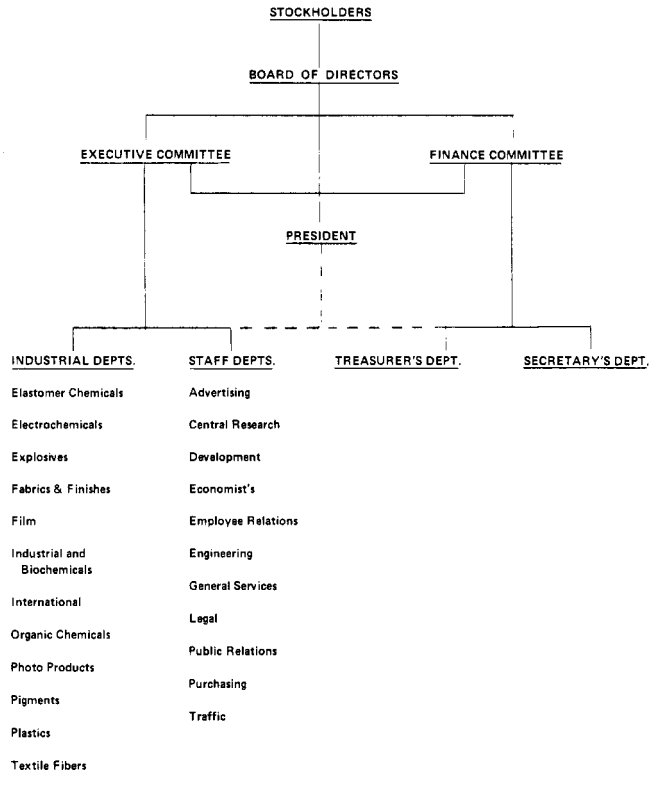


Figure 1. Organization of E. I. du Pont de Nemours & Co., Inc.

The corporate Treasurer and Secretary head departments which are responsible for maintaining the financial and nonfinancial records, respectively, of the company. The Secretary's Department serves as the secretariat for the Board of Directors and its committees, and is concerned with stockholders relations and real estate. Information activities in the Secretary's Department are carried out by the Technical Library and the Information Systems Division.

Du Pont's Information Network. The Information Systems Division is a major information center at the corporate level, which, along with other information centers, forms Du Pont's information network. These other centers range from the one-man operation serving an individual laboratory or office unit to the larger centers or libraries on a divisional or departmental level. The Lavoisier Library, for example, operated by the Central Research Department, is a library covering scientific literature and has more than 65,000 volumes, a subscription list of more than 1500 titles, and a staff of 28 people, of which 11 are professional.

The smaller and intermediate sized information centers and libraries serving specific site locations are usually specialized according to the interests of the personnel they serve. Several of these centers are administered by the Secretary's Department, or are staffed by personnel on Secretary's Department rolls. Thus, there are both decentralized departmental centers and centralized corporate information services in Du Pont's information network.

Information Systems Division. Let us now return to the organization of the Information Systems Division (Figure 2).

The Product Information Section provides a nationwide network for answering questions directed to Du Pont by its customers, potential customers, and vendors.[5]

Our Vital Records Section stores all important company records in a large subterranean vault, so that technical and personnel records or physical facilities of any unit of the company could be reconstructed in case of disaster. Most of these records are microfilmed for storage, and the microfilming services of the section assist importantly in allowing other information storage problems in the company.

The Hall of Records Section is an archival storage facility for the records, which must be kept for varying lengths of time. Some records must be maintained "forever," while others have a useful life of from 2 to 50 years. In addition to storage, all of these records must be reviewed periodically to determine need for continued storage.

The Development Section consists primarily of information consultants and information systems designers, who are responsible for advising other units of the company of new developments in the information field. They are our insurance that we are taking optimum advantage of the available equipment and new techniques. The computer programmers in the section are thoroughly familiar with information storage techniques. Keyboarding services and liaison with computer operators in our Treasurer's Department are also provided by the Development Section.

Our New Information Services Section is concerned with establishing and operating additional information centers in the company, and making use of information sources outside of Du Pont. Some of the centers now operating are concerned with commercial and business information, chemical and physical properties of materials, information on analytical test methods, and engineering design. Our On-Site Information personnel are scientists or engineers trained in information transfer techniques, and they are assigned to various offices or laboratories to provide information assistance and services to the site personnel.

Our Central Report Index Section is concerned with the indexing and retrieval of information in technical and scientific reports generated within Du Pont.[4]

CENTRAL PATENT INDEX

The Central Index is concerned with worldwide patent information. In addition to operating an information search system for the patent literature, it is also responsible for a current awareness function in the same field. Our

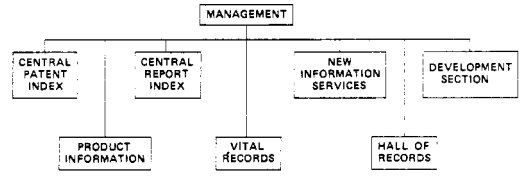


Figure 2. Organization of the Information Systems Division

primary concern is with the identification of patents relative to an inquiry. In providing this service, we supplement the legal functions of the patent personnel of the several departments concerned with the filing of applications, patent licenses, etc. The Central Patent Index is not involved directly in these legal matters.

Du Pont has been concerned with modern information handling since the early 1950's. In those days our Textile Fibers and Film Departments,[6] followed by our Central Research Department, established the first report information units based on concept coordination searching techniques. During the period 1955-1962, other departments established information centers using this concept coordination approach.

In 1964, considerable strides were made toward centralization of Du Pont information in the Information Systems Division with the formation of the Central Patent Index (CPI), the Central Report Index, and the Development Section. The primary justification for centralizing patent documentation activities was to eliminate the large amount of duplication of effort by the several departments when each was abstracting and indexing the patents relating to its own technology. The community of interests among the departments in many areas of chemistry and engineering, especially in the field of polymers, had resulted before the formation of CPI in as many as ten departments abstracting and classifying the same patent.

Since 1964 there has been continued consolidation and growth of the Information Systems Division. For example, on January 1, 1969, the patent information work which had been under the management of our Central Research Department was transferred to the Central Patent Index in the Secretary's Department. This work is concerned primarily with non-U. S. patent documentation and the publication of patent bulletins for current awareness within Du Pont. The procedures previously used for foreign patent documentation are now being revised; this paper therefore will be limited to a discussion of our U. S. patent documentation operations.

Input Operations. Each week the *Official Gazette* of the U. S. Patent Office is reviewed by personnel responsible for patent activities in the departments throughout Du Pont. They specify to the Central Patent Index which patents should be input to our system. In many cases, it has already been established that all patents issuing in some classes and sub-classes must go in. Individual patents are ordered to supplement these class orders. Our patent analysts, some of whom have become subject specialists, prepare an abstract and index the important concepts in each patent. About 20,000 U. S. patents are indexed and added to our file each year.

Links are not used in our patent indexing. Roles are used only on chemical terms.[7] Three fundamental roles are employed to designate reactant, product of a reaction, and physically processed or "just there." In addition, a set of roles is superimposed on these three fundamental roles to provide discriminating retrieval in the indexing of polymers.[2]

The abstracts are filed and can be retrieved by inventor, assignee, and number. The information on the indexing sheet is keyboarded. Chemical compounds are further fragmented, and the information is keyboarded for input and storage in computer tapes.

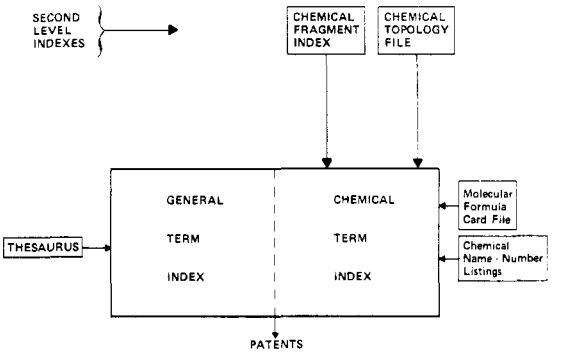


Figure 3. Schematic file organization of Central Patent Index

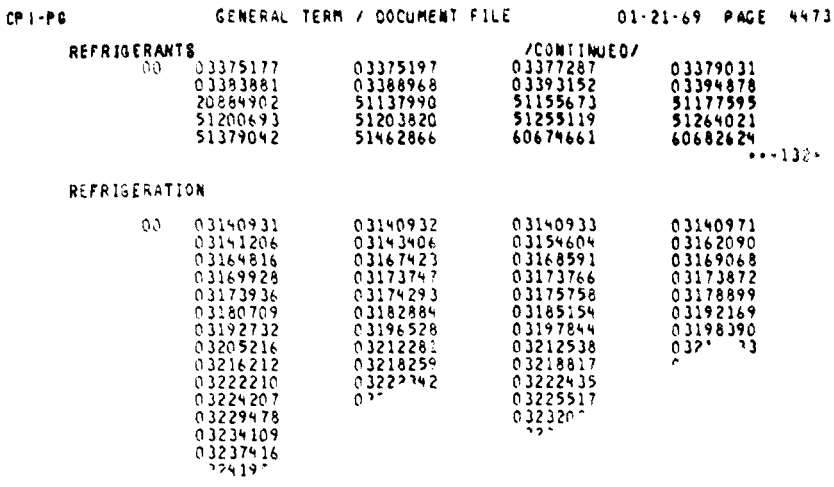
Index Structure. The computer-based index to patents utilizes essentially the same programs as the index to company reports, as described by Montague and Schirmer.[4] Major differences in procedures between the report and patent indexes include:

1. Purchase of 16-mm. microfilm of patents *vs.* our own preparation of microfiche copies of reports.
2. Use of a topological chemical structure system[9] for both input and search for reports; reliance on a chemical fragmentation system for search in the patent index, due to the largely generic nature of description of chemicals in patents. The patent index does use the topological system to register specific chemicals, i.e., to determine if the chemical has been encountered before, and assign it a registry number as unique identification.
3. Abstracts are not at present recorded in machine-readable form in the patent index.

The basic part of the patent index is represented by the large lower box in Figure 3. We make an arbitrary intellectual separation of our total file of what we call general—i.e., nonchemical—terms and chemical terms. Each of these is represented as an inverted file index to the patents. In the general term file, the patent numbers are listed under the alphabetical concepts as shown in Figure 4. Each chemical compound is assigned a C or chemical number. C-numbers are also assigned to generic families of compounds when they are described generically, e. g., by Markush Structure, in the patent. This number then becomes the chemical term to which all of the pertinent patent numbers are posted, as shown in Figure 5. This shows, for example, that Compound No. 37199 has been used as an indexing term in roles 10, 20, and 30 for the patents shown in each group. Role 30 indicates that there is information about the preparation of this compound in patent No. 3,349,073.

Chemical terms are readily identified in most cases by maintaining a chemical name–C-number list. This name-number list is presented both alphabetically (Figure 6) and numerically (Figure 7). Input may be made for any name on the list; if by the latter route, the computer will convert the name to the C-number for storage.

We do not require the use of *Chemical Abstracts* preferred nomenclature. If a chemical concept is not located readily in the alphabetical listing of unambiguous names, the patent analyst can determine the C-number for the chemi-



CPI-PC GENERAL TERM / DOCUMENT FILE 01-21-69 PAGE 4473

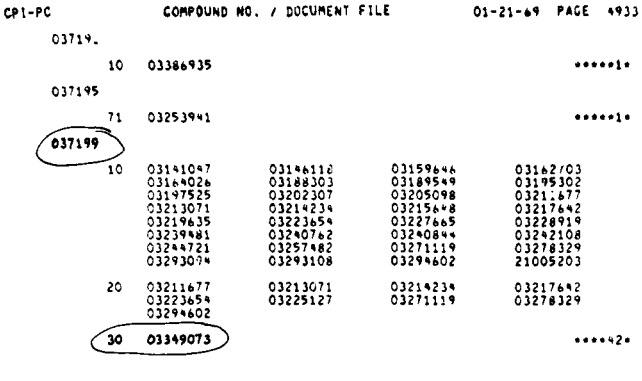
REFRIGERANTS /CONTINUED/

00 03375177 03375197 03377287 03379031
03383881 03388968 03393152 03394878
20884902 51137990 51155673 51177595
51200693 51203820 51255119 51264021
51379042 51462866 60674661 60682624

REFRIGERATION

00 03140931 03140932 03140933 03140971
03141206 03143406 03154604 03162090
03164816 03167423 03168591 03169068
03169928 03173747 03173766 03173872
03173936 03174293 03175758 03178899
03180709 03182884 03185154 03192169
03192732 03196528 03197844 03198390
03205216 03212281 03212538
03216212 03218259 03218817
03222210 03222342 03222435
03224207 03225517
03229478
03234109
03237416

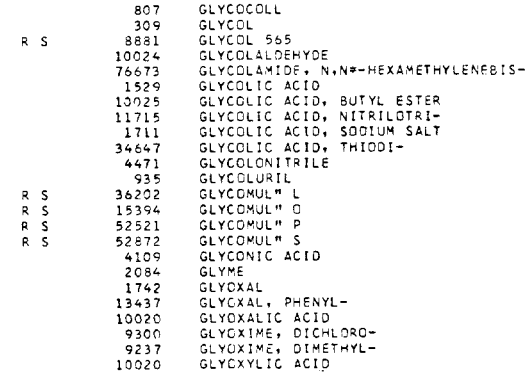
Figure 4. Inverted file—general terms



CPI-PC COMPOUND NO. / DOCUMENT FILE 01-21-69 PAGE 4933

03719.
10 03386935 *****1*
037195
71 03253941 *****1*
037199
10 03141087 03146112 03159646 03162703
03164026 03188303 03189549 03195302
03197525 03202307 03205098 03211677
03213071 03214234 03215648 03217642
03219635 03223654 03227665 03228919
03239881 03240762 03240844 03242108
03244721 03257482 03271119 03278329
03293094 03293108 03294602 21005203
20 03211677 03213071 03214234 03217642
03223654 03225127 03271119 03278329
03294602
30 03349073 *****2*

Figure 5. Inverted file—chemical terms, expressed as compound numbers



807 GLYCOCOLL
309 GLYCOL
R S 8881 GLYCOL 565
10024 GLYCOLALDEHYDE
76673 GLYCOLAMIDE, N,N'-HEXAMETHYLENEBIS-
1529 GLYCOLIC ACID
10025 GLYCOLIC ACID, BUTYL ESTER
11715 GLYCOLIC ACID, NITRILOTRI-
1711 GLYCOLIC ACID, SODIUM SALT
34647 GLYCOLIC ACID, THIODI-
4471 GLYCOLONITRILE
935 GLYCOLURIL
R S 36202 GLYCOMUL" L
R S 15394 GLYCOMUL" O
R S 52521 GLYCOMUL" P
R S 52872 GLYCOMUL" S
4109 GLYCONIC ACID
2084 GLYME
1742 GLYOXAL
13437 GLYOXAL, PHENYL-
10020 GLYOXALIC ACID
9300 GLYOXIME, DICHLORO-
9237 GLYOXIME, DIMETHYL-
10020 GLYOXYLIC ACID

Figure 6. Chemical name–number list, alphabetical order

cal, if it has been encountered before in our index, by referring to the molecular formula card file. A card (Figure 8) is prepared for each specific chemical entered into our system showing the molecular formula, C-number, structural representation, and usually an unambiguous name. These cards are filed by molecular formula.

Each of the chemical terms is indexed at a second level to chemically identifiable fragments or structural characteristics. In the file, the fragment or structural parts become the terms and the chemical compound numbers are posted to the appropriate terms. Figure 9 shows this by illustrating the chemicals posted to "Fragment" 1323 (organic quaternary amine). There are 1399 organic chemicals—those in the 500,000 series are Markush structures—which have quaternary amine groups in them. Specific chemicals are also stored at a second level by a topological system which records each atom and the bonds between atoms.[3]

All the index files are printed directly from computer to microfilm (Computer Output Microfilm-COM).[1] Instead of having to cope with a seven-foot pile of computer paper printout, we receive 12 microfilm cartridges containing our entire index files. While computer updates are made monthly, regeneration of the microfilm is done once a quarter, with two monthly supplements provided on paper in between the COM operations.

Our general term vocabulary is open-ended and strictly controlled by a thesaurus of terms illustrated in Figure 10, which shows the relationship among and between the individual term concepts. This is a standard information system thesaurus approach which utilizes "use" and "used for" references, "narrower" and "broader" term references, and "related" term references.

Each of the files shown in Figure 3, with the exception of the molecular formula card file, is maintained on magnetic tape for computer operation and control. Searches by computer can be run against any of these files, using all of the normal Boolean algebra and set-theory logic. The printout of this same information on microfilm also gives us the facility for conducting manual searches. The topological printout is not made, since it is unintelligible except to the system's design people and the specialists in chemical structure indexing.

Computer Searching. Let us assume that we are looking for patents dealing with the chlorination of *p*-aminobenzoic acid, or of any acid or ester which has a primary or

```
          11699    CETYLAMINE
          11699    HEXADECYLAMINE
          11699    PALMITYLAMINE
          11701    AZIRIDINECARBOXAMIDE/1-/, N,N*-HEXAMETHYLENEBIS-
          11701    HEXAMETHYLENEBIS-1-AZIRIDINECARBOXAMIDE/N,N*-/
          11702    DICHLORDHEXANE/1,6-/
          11702    HEXAMETHYLENE DICHLORIDE
          11702    HEXANE, 1,6-DICHLORO-
  R S     11704    HEXANENITRILE
          11704    HEXYL CYANIDE
          11705    DIPALMITOYLMELAMINE/N,N*-/
          11705    MELAMINE, N,N*-DIPALMITOYL-
P     T   11709    DIMETHYLDECABORANE/14/
          11711    DIBENZYLDIMETHYLAMMONIUM HYDROXIDE
          11715    GLYCOLIC ACID, NITRILOTRI-
          11715    NITRILOTRIGLYCOLIC ACID
          11716    ISONICOTINIC ACID, METHYL ESTER
          11716    METHYL ISONICOTINATE
          11718    PROPENESULFONIC ACID/2-/
          11719    ACETIC ACID, NITRILOTRI-
          11719    NITRILOTRIACETIC ACID
          11719    TRIGLYCINE
```

Figure 7. Chemical name–number list, numerical order

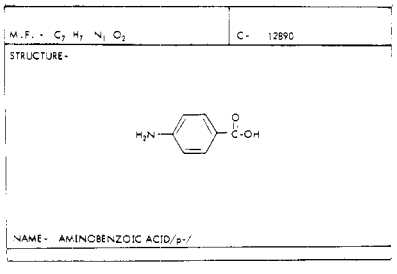


Figure 8. Molecular formula card

```
CPI-PF          FRAGMENT NO. / COMPOUND FILE          01-20-69  PAGE  3-68
 001323                                  /CONTINUED/
          517417   517418   517495   517513   517518   517519
          517649   517681   517815   517867   518065   518116
          518124   518160   518161   518162   518181   518250
          518242   518491   518533   518631   518700   518781
          518840   518850   518855   518966   519131   519346
          519559   519560   519628   519675   519684   519700
          519785   519788   519818   519880   519912   520036
          520182   520205   520311   520322   520390   520434
          520461   520530   520662   520763   520773   520799
          520843   521072   521083   521138   521192   521203
          521243   521354   521361   521361   521550   521625
          521763   521923   522042   522192   522359   522372
          522401   522408   522476   522480   522481   522489
          522512   522519   522529   522626   522639   522813
          523020   523034   523038   523079   523129   523140
          523239                                        **1399*
 CC1325
          009567   015450   054263   055918   073117   087780
          470016   470049   470102   470104   470172   470230
          470238   470253   470266   470285   470324   470328
          470330   470353   470[illegible]   470393   470398   470[illegible]
          470421   470437                     [illegible]   470522   [illegible]
          470563   470[illegible]                          470630
```

Figure 9. Second level inverted file—compound numbers posted to fragment numbers

secondary amine group. The Boolean statement would be:

> Chlorination and {*p*-aminobenzoic acid or [(*F*-acid or *F*-ester) and (*F*-primary amine or *F*-secondary amine)]}
>
> where *F*- means "chemicals containing the fragment-."

The question would be set up on a form as shown in Figure 11. The first column headed "type" directs the computer with regard to the type of answer to print out. If we desire to have a list of C-numbers of chemicals containing certain fragments, printed out from the fragment file (second-level answer), we indicate this by designating the question as type 1. If we want a fragment

```
FACSIMILE
                  USE          IMAGES

FACTICES
                  RT           ELASTOMERS
                  RT           RUBBERS

FACTOR S/ANTIBIOTICS/                    1-68 ROLES
                  USE          STAPHYLOMYCIN

FADEOMETER
                  BT           INSTRUMENTS
                  BT           MEASURING INSTRUMENTS

FADING
                  RT           DECOLORING
                  RT           DETERIORATION
                  RT           DISCOLORATION
                  RT           DISCOLORATION INHIBITION
                  RT           FADEOMETER
                  RT           WEAR

FAILURES
                  USED FOR     DUDS
                  RT           BREAKING
                  RT           BURSTING
                  RT           DEFECTS
                  RT           ERRORS
```

Figure 10. Sample of page from thesaurus of general terms

TYPE	QUESTION NO.	SEQ. NO.	FILE	TERMS	ROLES	OPERATIONS
2	001	01	PF	01285 (acid)		
2	001	02	PF	03617 (ester)		+
2	001	03	PF	06845 (1-amine)		
2	001	04	PF	12863 (2-amine)		+ * ·
8	001	05	PC	C25834 (p-NH_2 C_6H_4 COOH)	20	
8	001	06	**	2001	20	-
8	001	07	PG	CHLORINATION		*·

Figure 11. Format of question set-up for computer search

file answer to be retained in the computer memory, we designate it as a type 2 question. Similarly, if we want the patent numbers constituting an answer from the compound or general term files stored internally (first-level answer), we designate the question as type 4. A type 4 question is asked when the searcher wants to preserve (store) the results of a preliminary set of Boolean operations basic to an inquiry, and then to process these in a multiplicity of further separate operations to answer several aspects, differing in detail, of the inquiry. If we want a first-level final answer printed out, we use the type 8 designation. Our program will also print out an intermediate answer, if desired, before intersecting this answer with another term to give a final answer.

In the second column, we indicate the use of a question for identity purposes. In the third column, we use a sequence number to order the input cards. In the fourth column, we identify the file which is to be used. PF means we will look in the patent fragmentation file.

The operations will be carried out as follows:

1. (Line 2, plus sign) Unionize C-numbers posted to fragments shown in lines 1 and 2, i.e., group together in one common listing all the C-numbers filed under either of the fragment terms (acid or ester).
2. (Line 4, plus sign) Unionize C-numbers posted to fragments shown in lines 3 and 4, similar to the preceding operation. We now have two unionized listings of C-numbers.

3. (Line 4, asterisk) Intersect the two unionized listings, i.e., determine which C-numbers are common to both unions.

4. (Line 4, period) Operator indicates the end point for the type 2 question: the computer stores the result of the intersection and labels it question 2001.

Sequence card number five directs the computer to the patent chemical file (PC), where we designate patents posted to a specific chemical number in a given role. In this case, role 20 indicates that the compound we are seeking (*p*-aminobenzoic acid) is a reactant in the chemical reaction (chlorination). The two asterisks in the "file" column on sequence card number six designate the file stored temporarily in the computer memory bank. The number 2001 designates the information which was previously stored as instructed by card number four. The role indication of 20 (reactant) means this role is to be applied to all chemical numbers brought forward by this previous sub-answer.

The operations continue:

5. (Line 6, plus sign) Unionize the patents posted to role 20 under C-number shown in lines 5 and 6, i.e., group together in one common listing all the patent numbers posted to role 20 (reactant) under any of the C-numbers designated by cards 5 and 6. (Actually, this step would be unnecessary in this hypothetical, much simplified example, because C-number 25834 (for *p*-aminobenzoic acid) should be among those C-numbers resulting from the logic directed by cards 1-4).

6. (Line 7, asterisk) Intersect the patent numbers identified in the union just formed with the patent numbers posted to "chlorination" in the general term (PG) file.

7. (Line 7, period) Operator indicates the endpoint for the type 8 question, i.e., the computer is instructed to print out the patent numbers resulting from the last operation (intersection) as the final answer to the inquiry.

FUTURE PLANS

After five years of operation, our technical staff of chemists, biologists, and chemical engineers, mostly female, have developed the competence to make reliable searches for our clients. Now that our file has grown to a size (80,000 patents) which produces useful results when searched, we are begining to provide more useful search answers to our clients. This search experience provides pragmatic guidance in the continuing process of modifying our vocabularies to meet our particular needs. Families of specific terms in our general term file are being combined into the next higher generic when there have been no inquiries or few patents requiring that degree of specificity. Occasionally, a broader term will be broken into more specific terms. The set of fragments has just undergone its fourth revision to provide more discriminating retrieval of chemical information.

Our Development Section recognizes that the rapidly increasing size of our file will require new computer programs to be able to provide efficient, effective, and cost-acceptable searches several years from now. Fundamental reprogramming is now in progress.

At this writing, the interest shown in patent documentation by commercial information-supplying organizations, and in cooperative activities on an international scale by (primarily) chemical companies and patent offices, gives encouragement to those concerned with, and often frustrated by, the magnitude and diversity of patent documentation problems. The concern caused by the sheer numbers of new patent documents—i.e., including published unexamined applications—making their appearance weekly, is not lessened by the alarming predictions of even larger numbers of issuances over the next few years. A concerted effort to cope with this burgeoning volume of literature, using the most advanced techniques in information retrieval, is required on the part of all concerned with the patent literature. It makes little sense for many separate organizations to continue the duplication of this same effort.

LITERATURE CITED

(1) Anonymous, "Here Comes the C.O.M.," *Information and Records Management* **2**, 45, Oct.-Nov. (1968).

(2) Duffey, M. M., *et al.*, "Computer Indexing of Polymer Patents," J. CHEM. DOC. **8**, 85 (1968).

(3) Hoffman, W. S., "An Integrated Chemical Structure Storage and Search System Operating at Du Pont," J. CHEM. DOC. **8**, 3 (1968).

(4) Montague, B. A., and R. F. Schirmer, "Du Pont Central Report Index: System Design, Operation, and Performance," J. CHEM. DOC. **8**, 33 (1968).

(5) Rogers, M. C., and S. A. Shelley, "An Information System for Customer Telephone Inquires," J. CHEM. DOC. **5**, 180 (1965).

(6) Van Oot, J. G., "The Development of an Operating Information System," J. CHEM. DOC. **2**, 229 (1962).

(7) Van Oot, J. G., *et al.*, "Links and Roles in Coordinate Indexing and Searching. . .," J. CHEM. DOC. **6**, 95 (1966).