

Manual retrieval therefore will be by coordinating terms (not term-roles) and will yield document numbers (not document number-link combinations).

The usefulness of the links and roles is threefold. First, they materially help the indexer to analyze the document he is indexing, leading to more effective indexing. Second, we plan to maintain an "Accession Register" which will list all indexed documents in the order of their document numbers, together with the complete bibliographic data and all link-role-term combinations for each document. Third, the document number-link combinations (rather than document number only) will be entered on our search tape in relation to the corresponding term-role combinations.

Thus, in a manual search, terms will be coordinated to give document numbers. Location of these document numbers in the Accession Register will provide telegraphic abstracts of all the documents. In most instances this will obviate any need for reference to the original documents.

In a machine search, the read-out could give the document number-link combinations for reference to the Accession Register. Or, if the volume of tape searches warrants, it would be simple enough to have tape search results reported as print-outs of the complete information—bibliographic and telegraphic abstract—on each referenced document, from a tape master of the Accession Register.

Manual searches and the preparation of requests for machine searches will be provided by our Technical Information Section as a service to our technical staff. However, we intend to encourage use of the manual search

equipment by all who are interested in it as a quick access to specific information in past reports.

**Acknowledgments.**—The development of this index has been a group activity to which important contributions have been made by Jane A. Bennett, E. Ray Birkhimer, Joyce R. Crossley, Louise U. Matternas, and Irene H. Sachs. Donald Van H. Harrison of Atlantic's Systems and Data Processing Department provided helpful computer know-how and John C. Costello, Jr. (then of Jonker Business Machines, Inc.), invaluable instruction. Finally, without the encouragement and support of James E. Connor, Jr., the work would never have been done.

## REFERENCES

- (1) J. R. Bilhartz, "Experiences in Information System Design," presented before the Division of Chemical Literature, 145th National Meeting of the American Chemical Society, New York, N. Y., Sept. 10, 1963.
- (2) J. C. Costello, Jr., in "Information Handling: First Principles," P. W. Howerton, Ed., Spartan Books, Washington, D. C., 1963, Chapter 3.
- (3) "The Naming and Indexing of Chemical Compounds by *Chemical Abstracts*," Introduction to the Subject Index of Vol. 56, (Jan.-June, 1962) of *Chemical Abstracts*.
- (4) "The Engineers Joint Council System of Roles-Meanings-Examples-Explanations-Exclusions," Battelle Memorial Institute, Columbus, Ohio.
- (5) "Chemical Engineering Thesaurus, A Wordbook for Use with the Concept Coordination System of Information Storage and Retrieval," American Institute of Chemical Engineers, New York, N. Y., 1961.

---

## Retrieval of Analytical Research Information by a Coordinate Indexing System\*

By BARBARA A. MONTAGUE

Research and Development Division, Plastics Department,  
E. I. du Pont de Nemours and Company, Inc., Wilmington, Delaware  
Received April 3, 1964

The objective of this paper is to describe the storage and retrieval of recorded analytical research information by concept coordination using links and roles. Analytical information is retrieved by indexing the object of the analysis, the matrix in which the analysis was performed, the technique, and the reagents employed.

The results of research efforts in the field of analytical chemistry in the Plastics Department of the Du Pont Company are recorded in notebooks, correspondence, and finally in formal reports. This knowledge may comprise the main topic of an analytical report or lie buried in a report written by a scouting or product group for whom

the research was performed. The passage of time and transfer of personnel weakens the link with the past, and such recorded information becomes the prime source for the acquisition of knowledge by others. In 1959 the Plastics Department recognized a need for improved methods for retrieval of all their internal research information and initiated a program utilizing concept coordination with the expectation of obtaining faster, more selective access than was provided with shallow indexing by classification used at that time.

An information system was designed<sup>1-3</sup> using deep indexing (40 terms per document) by concept coordination with links and roles to reduce irrelevant retrieval. An example of the indexing of a technical report with links and roles is presented in Fig. 1, and the definition of the roles is given in Fig. 2. This report was indexed in one

\* Presented at the Fisher Award Symposium honoring John Mitchell, Jr., before the Division of Analytical Chemistry, 147th National Meeting of the American Chemical Society, Philadelphia, Pa., April 9, 1964.

Terms	Links	Roles
Polymerization	A	8—Research on
Ethylene	A	3—Reactant
Polyethylene	A	7—Product
Catalysts	A	1—Using
Benzoyl peroxide	A	4—Special agent
Temperature	A	2—Independent variable
Pressure	A	2—Independent variable
Molecular weight	A	9—Dependent variable
Solubility	A	9—Dependent variable
Polyethylene	A	11—Of
Benzene	A	5—Solvent

Fig. 1.—Indexing of a technical report.

1. Using
2. Cause, independent variable
3. Reactant
4. Special agent
5. Solvent
6. Impurity
7. Product
8. Research information on
9. Effect, dependent variable
10. Design of
11. Physically processed, of
00. Adjectives, proper nouns

Fig. 2.—Roles and their definitions.

link, A. Knowing the meaning of the roles, one can read back the product of the indexing as follows: there is research information reported on the polymerization of ethylene to produce polyethylene using benzoyl peroxide as a catalyst, and on the effect of temperature and pressure on the molecular weight and solubility of polyethylene in benzene. Thus, indexing with links and roles is actually an abstracting procedure which results in a mechanism for information retrieval with the added dividend of a term-role abstract which can be used for screening retrieved documents for relevance.

**Indexing Analytical Information.**—During the design period of the Plastic Department's information system, members of the Analysis Group were consulted regarding the indexing requirements for analytical information. It became apparent that the roles used for the technical reports did not provide the necessary differentiation for analytical information. For that reason a special role convention was adopted as illustrated in Fig. 3 involving a special meaning of roles 6 and 11. The analysis of cyclohexanol for adipic acid is indexed as shown with the chemical for which the analysis is performed, adipic acid, in role 11, and the matrix, cyclohexanol, in which the acid is present, is indexed in role 6. This permits differentiation

Terms	Links	Roles
Analysis	A	8—Research on
Adipic acid	A	11—Object of analysis
Cyclohexanol	A	6—Matrix
Titrimetry	A	1—Using, technique
Indicators (pH)	A	1—Using
Phenolphthalein	A	4—Special agent
Water	A	5—Solvent
Sodium hydroxide	A	3—Reactant
Adipic acid	A	3—Reactant

Fig. 3.—Analytical indexing convention.

between the object of the analysis and the matrix. If both compounds were indexed in the same role, 11 for example, false retrieval would result because the report could be retrieved for analysis of cyclohexanol as well as for adipic acid. The technique by which the analysis was performed, titrimetry, is indexed in role 1. The titration was carried out using phenolphthalein as an indicator, water as the solvent, and sodium hydroxide as the titrant.

The next example involves a report written by the Analysis Group which discusses two methods for the determination of water in nylon. The first method involves solution of the nylon in *m*-cresol followed by titration of the water with standardized Karl Fischer reagent. The alternate hot block method uses a vacuum distillation of water from the polymer followed by condensation in a cold trap and titration of the moisture with Karl Fischer reagent. The agreement between the two methods is compared along with a discussion of their application. This information is indexed as shown in Fig. 4 and reads: there is research information on the determination of water in "Zytel" nylon resin by the solution method using titration with Karl Fischer reagent in *m*-cresol solvent and using the hot block method. There is research information on the comparison of the solution method with the hot block method. The title of this report, "Chemical Development and Service Activities of the Analysis Group," which was the source for indexing by the former classification system used by the department, provides no clue to the information it contains on the analysis for water. Deep indexing with links and roles makes selective location of this report possible when information on this subject is sought.

Terms	Links	Roles
Determination	A	8—Research on
Water	A	11—Object of analysis
"Zytel" nylon resin	A	6—Matrix
Solution method	A	1—Using, technique
Titrimetry	A	1—Using, technique
Karl Fischer reagent	A	3—Reactant
<i>m</i> -Cresol	A	5—Solvent
Hot block method	A	1—Using, technique
Comparison	A	8—Research on
Solution method	A	11—Of
Hot block method	A	11—Of

Fig. 4.—Determination of water in nylon.

Another analytical report contains information on a colorimetric determination of silicon in calcium fluoride. This method involves the colorimetric measurement of "molybdenum blue," a colored complex formed with silica. It was found that fluoride from the calcium fluoride interfered with color development due to a complexing of the silicon with fluoride. This interaction is relatively strong compared with the silica-molybdate complex. The interference was eliminated by tying up the fluoride by the addition of aluminum ion. The information is indexed as shown in Fig. 5 which reads: there is research information reported on the determination of silicon in calcium fluoride using colorimetry and "molybdenum blue." There is information on the effect of fluoride ion on the analysis and recovery of silicon and on the elimination of interferences using aluminum ion as a complexing agent.

Figure 6 illustrates the indexing of the use of instrumental techniques to analyze the chemical structure of a

Terms	Links	Roles
Determination	A	8—Research on
Silicon	A	11—Object of analysis
Calcium fluoride	A	6—Matrix
Colorimetry	A	1—Using, technique
Complexing agents	A	1—Using
Molybdenum blue	A	4—Special agent
Fluoride ions	A	2—Independent variable
Analysis	A	9—Dependent variable
Recovery	A	9—Dependent variable
Elimination	A	8—Research on
Interferences	A	11—Of
Aluminum ions	A	4—Special agent

Fig. 5.—Analysis of calcium fluoride.

Terms	Links	Roles
Analysis	A	8—Research on
Chemical structure	A	11—Object of analysis
Polynorbornene	A	11—Of
Infrared spectroscopy	A	1—Using, technique

Fig. 6.—Infrared analysis of polynorbornene.

polymer. The point to be made here is that not all the detail of a report is indexed and the searcher must use his imagination to locate information. For example, if one is interested in finding information regarding the sample preparation for infrared analysis of polynorbornene,<sup>4</sup> he would ask the question to match these terms used to index the report. He must make the assumption that detailed sampling information will probably be in this report.

The type of report discussed so far has been a documentation of developmental work originating outside of the Analysis Group. An organic scouting group studied the mechanism of the reaction between a Grignard reagent, phenylmagnesium bromide, and titanium tetrachloride. As part of the study, the purity of the phenylmagnesium bromide was measured using three analytical methods: titration with Versene, determination of bromide, and reaction with iodine. Figure 7 illustrates the indexing of this information and reads as follows: there is research information on a comparison of the analysis of phenylmagnesium bromide using titration with Versene, analysis of bromide, and reaction with iodine. The analytical significance of this information lies in the observation that the theoretical molarity for phenylmagnesium bromide is obtained by both Versene titration and the bromide analysis. Comparison of these data with the molarity obtained

Terms	Links	Roles
Comparison	A	8—Research on
Analysis	A	11—Of
Grignard reagents	A	11—Object of analysis
Phenylmagnesium bromide	A	11—Object of analysis
Titrimetry	A	1—Using, technique
Phenylmagnesium bromide	A	3—Reactant
Versene	A	3—Reactant
Analysis	A	1—Using
Bromide	A	11—Object of analysis
Reaction	A	1—Using
Iodine	A	3—Reactant

Fig. 7.—Analysis of Grignard reagents.

by reaction with iodine revealed that an impurity was present as evidenced by a low iodometric molarity. The documentation significance is the ability to retrieve this valuable information which by former methods would lie buried and unsuspected in an organic scouting report.

**Retrieval of Analytical Information.**—A chemist who is interested in locating the kind of analytical information just discussed would very likely ask the following question, "Do you have any information on methods for evaluating the purity of Grignard reagents such as phenylmagnesium bromide?" The search would be performed by comparing report numbers with their link letters under three terms—comparison (role 8), analysis (role 11), and phenylmagnesium bromide (role 11)—which match the terms used to index such information as in Fig. 7 and represent the chemist's inquiry translated into system language. Simple searches such as the one just described are performed manually by means of a printed coordinate index, whereas more complex searches involving multiple terms and operations are made using an IBM 1620 computer which is equipped with disk packs for random access. The logical operations of intersections, unions, and complements which are used to frame and process searches utilize the principles of Boolean algebra. Thus, a search question is written in the form of a logical equation which is solved by means of the computer, and answers are printed out in the form of accession numbers of retrieved documents.

## REFERENCES

- (1) J. C. Costello, *Am. Doc.*, **12**, 111 (1961).
- (2) B. A. Montague, *ibid.*, **13**, 104 (1962).
- (3) B. A. Montague, *J. Chem. Doc.*, **4**, 251 (1964).
- (4) W. L. Truett, D. R. Johnson, I. M. Robinson, and B. A. Montague, *J. Am. Chem. Soc.*, **82**, 2337 (1960).