CONCLUSIONS

Each of these systems has its particular advantages and it is likely that all of the approaches will receive sustained emphasis and use because of the variety of needs in the chemical information retrieval field. One thing is certain—advances in computer technology will definitely play a major role in determining the relative importance and general acceptability of the three directions.

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The Singularity Sub-Link—A New Tool for Use in the Storage and Retrieval of Information*

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The singularity sub-link gives additional scope and utility to concept-coordination systems for the storage and retrieval of information. It simplifies the indexing process, reduces false retrieval, and makes it possible to locate documents in which various materials, chemicals, special agents, processes, and independent variables are compared. It does this by indicating that an indexing term or key-word is a member of a series of alternates that have been studied separately for comparison in a given context. Previous methods of doing this have required an excessive number of links since for accuracy each alternative term must be placed in a separate link in which all the nonalternative terms are repeated. Furthermore, if this proliferation of links is avoided by placing the alternative terms in one link, false retrieval of information relative to combination effects resulting from mixtures not described in the documents is an inevitable sequel. The term "COMPARISON" has been previously avoided in our concept-coordination systems of indexing because of its indefinite nature as a search term. The singularity sub-link indicates specific comparisons so that this concept becomes available by implication without ambiguity. Every reference marked by the sub-link indicates a document reporting the comparative evaluation or study of a term with other terms employed in the same context.

The functions and relations of terms are lost when they are isolated from each other in a simple inverted file. Links coordinate the terms in the respective intellectual subdivisions of the report or document. Roles preserve relationships by indicating functions, such as raw material,

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product, special agent, process, etc., in which the terms are used.

The singularity sub-link has been successfully employed in a technical report indexing system in the Electrochemicals Department of the du Pont Company. Concept-coordination systems employing links and roles are widely used in du Pont as described in papers by Costello,[1] Holm,[2] Montague,[3] and Van Oot.[4] This paper deals with the application of the singularity sub-link in systems of this type.

Use of Singularity of Sub-Link with Roles.—Examples illustrating the use of the sub-link in various roles will clarify its general utility in the indexing of technical documents. A list of roles commonly used, which are designated by number is reproduced in Table I. Links are marked by letter, A, B, C, etc. The singularity sub-link is indicated in our system by an asterisk following the link designation.

Table I[3]
Indexing Roles

Role	Function
8	Research information, Development information on, Study of, Investigation of
10	Design of, Drawing of, Design data on, Design information on
12	Patent information on (meaning claim of or disclosure of in a patent)
3	Reactants in a chemical reaction
7	Products of a chemical reaction
5	Reaction medium, atmosphere, solvent, vehicle, dispersion means, environment of, support (chemical, as for a catalyst)
4	Special agent in a reaction or operation (as a catalyst, vulcanizing agent, or color stabilizer)
6	Undesired reaction product, reaction by-product, impurity, contaminant, waste, product of a side reaction
1	Using, by means of, by
2	Independent variable studied for its effect on
9	Dependent variable studied for how it is affected
11	Receiving a physical modification (without chemical change), Passively receiving an operation (such as storage), Passive, Possessive, and Locative (such as of, in, on)
...	Adjectives, proper names, companies, persons, etc.

Role 1. Using, By Means of, By

Term	Link	Role	Link	Role
Separation	A	8	A	9
Alcohol	A	11		
Water	A	11		
Distillation	A*	1		
Extraction	A*	1		
Freezing	A*	1		
Temperature	A	2		
Pressure	A	2		

Indexing as shown above tells us that the document describes a study in which distillation, extraction, and freezing were compared as a means of separating alcohol from water, and the effect of temperature and pressure on these separations was examined. It shows that each of the items indicated by the singularity sub-link was studied one at a time and that combinations of these were not examined. Without the sub-link, this information would require three links differing only in the A*1 items.

Role 2. Independent Variable

Term	Link	Role	Link	Role
Strength	A	8	A	9
Ethylene polymers	A	11		
Films	A	11		
Vibration	A*	2		
Radiation	A*	2		
Flexing	A*	2		

In this case, it is indicated that vibration, radiation, and flexing have been separately evaluated with respect to their effect on the strength of ethylene films.

Role 3. Reactants

Term	Link	Role
Synthesis	A	8
Sodium methylate	A	7
Methanol	A	3
Sodium	A*	3
Sodium oxide	A*	3
Sodium hydroxide	A*	3
Sodium carbonate	A*	3

This indexing shows that four reagents have been tested as raw materials for sodium methylate by reaction with methanol.

Role 4. Special Agent

Term	Link	Role	Link	Role
Hydrogenation	A	8	B	8
Ethylene	A	3	B	3
Ethane	A	7,11	B	7,11
Catalysts	A	1,2	B	1,2
Chromium oxide	A*	4	B	4
Tungsten oxide	A*	4	B	4
Tungsten sulfide	A*	4	B	4
Mixtures			B	1
Yield	A	9	B	9

In this example, the sub-link is employed to index a comparative study of three hydrogenation catalysts in link A whereas link B deals with a study of the mixed catalysts. Synergistic effects resulting from mixtures of catalysts are excluded in link A.

Role 5. Reaction Medium, Solvent

Term	Link	Role	Link	Role
Synthesis	A	8		
Reaction	A	8	A	9
Sodium naphthalene	A	7		
Sodium	A	3		
Naphthalene	A	3		
Dimethyl ether	A*	5		
Diethyl ether	A*	5		
Tetrahydrofuran	A*	5		
Solvents	A	1	A	2

The effects of three solvents are compared in the addition reaction of sodium and naphthalene.

Role 7. Products with Role 3–Reactants

Term	Link	Role
Copolymerization	A	8
Ethylene	A*	3
Propylene	A*	3
Styrene	A	3
Ethylene copolymers	A*	7
Propylene copolymers	A*	7
Styrene copolymers	A	7
Physical properties	A	9
Chemical structure	A	2

This indexing shows that a separate study has been made of the synthesis of copolymers of ethylene and propylene with styrene to determine how these two alkenes differ in their effect on the physical properties of the copolymer. Only styrene copolymers have been prepared so that ethylene and propylene can be compared as comonomers. False retrievals on terpolymers and ethylene–propylene copolymers are avoided.

Role 11. Receiving Physical Modification

Term	Link	Role	Link	Role
Laundering	A	8	A	2
Cotton	A*	11		
Wool	A*	11		
Rayon	A*	11		
Silk	A*	11		
Textiles	A	11		
Durability	A	9		

The effect of laundering of four textile fabrics is compared.

In the above examples, it was noted that two roles, *viz.* 3 and 7, can be employed together with singularity sub-links. Other combinations of the singularity sub-link involving two or more roles can be employed. A case of this sort in which two textiles are drycleaned with different techniques, different solvents, and two different drycleaning detergents is shown below.

Term	Link	Role	Link	Role
Drycleaning	A	8	A	9
Cotton	A*	11		
Wool	A*	11		
Textiles	A	11		
Agitation	A*	1	A*	2
Ultrasonic vibration	A*	1	A*	2
Trichloroethylene	A*	5		
Naphtha	A*	5		
Detergent X(chemical)	A*	4		
Detergent Y(chemical)	A*	4		
Physical properties	A	9		
Detergents	A	1	A	2
Solvents	A	2		

In examples of the above type, it should be noted that the number of comparative tests indicated increases exponentially when two or more terms are used in two or more roles with singularity sub-links. At least 16 experimental tests are indexed by the example shown above. Accordingly, care must be taken to ensure against false retrieval in such circumstances. By and large, the utility of the sub-link is greatest for cases in which singularity is limited to a single role in a given link.

Collective Use of Singularity Sub-Link.—The singularity sub-link may be employed with a single term representing species or genera when members of a group have been investigated separately. In handling a document reporting the evaluation of a large number of amines, the term AMINES may be indexed as A*4. This eliminates the need for separate posting of specific amines. A report dealing with the evaluation of several hundred solvents for a material is indexed with the term SOLVENTS as A*5. Separate terms may be employed with this collective use of the sub-link to indicate individual items which have proved outstanding. This is illustrated below.

Term	Link	Role
Solubility	A	8
Hexamethylenetetramine	A	11
Solvents	A*	5
Chloroform	A*	5
Water	A*	5

The term SCOUTING may be employed in various roles to indicate a large number of studies not involving singularity. For example, SCOUTING-A5 when used in the above example indicates solubility studies involving a variety of solvents alone and in mixtures.

The term SCOUTING is used in various roles to indicate a variety of studies of processes, chemicals, materials, and independent variables which do not merit separate indexing and which do not represent the one-at-a-time testing represented by the singularity sub-link.

Patent Indexing.—In indexing patents, the singularity sub-link can be used to designate the terms in Markush claims. This convention can, for example, be adapted to the technique described by Montague[3] which involves prefixing the letter C to the link for information in claims and D for the information in the disclosure. When employed for indexing disclosed information, our singularity sub-link is employed as previously described. When employed for indexing a claim, it refers only to terms which are members of a Markush group. This is illustrated in the following example.

Term	Link	Role
Stabilization	CA	12
Formaldehyde	CA	11
Solutions	CA	11
Water	CA	5
Methanol	CA*	4
Ethanol	CA*	4
Urea	CA*	4
Melamine	CA*	4
Stabilizers	CA	1

The above indexing would represent a patent claim covering the stabilization of an aqueous formaldehyde solution with a material selected from the group consisting of methanol, ethanol, urea, and melamine.

Storage Methods.—Information indexed using the singularity sub-link may be stored by any of the techniques employed in concept–coordination systems. It is applicable to both normal and inverted files. In this connection, it may be noted that a singularity indicator can also be employed in a simple key-word index in which use it differentiates terms used in a comparative study. Singularity could be used in a sub-role if desired. However, such use would involve double posting with and without singularity for each role.

Document references for a term consist of the accession number of the document, the link designation, and the singularity sign. Thus, the reference 722A* indicates that the concept will be found in link A of the document having accession number 722 and that the term has been compared with others serving the same function.

The indexed information may be stored in normal card files, keyword card files, alphabetical term lists, etc. It may be used with computers in programmed searching or in the preparation of machine print-outs. We employ the sub-link in an alphanumerical machine print-out of terms in the form of a search dictionary in which term references are classified by roles for use in manual searching.

Searching.—In searches involving the singularity sub-link, documents covering the comparative studies of terms are located by separating references marked by the singularity indicator. Any term reference so marked deals with a comparison of terms employed in the same context in a specific document. In the system involving links and roles, references for comparative study must be for terms in the same link and role as well as in the same document.

For example, if one wished information on platinum as a hydrogenation catalyst as compared with other hydrogenation catalysts, one would search document references for platinum in role 4 (special agent) and note document accession numbers with the singularity sub-link. The terms "hydrogenation" and "catalysts" would then be searched for accession numbers with the same link and role designation. References identical in this respect would cover the desired comparative studies, and the documents would be reviewed to see what other hydrogenation catalysts had been studied. For purposes of illustration, the following indicates the term references that might be involved in the example.

Term	Role	Accession Numbers
Platinum	4	7A, 12B, 15A, *111A**, 117C, 119B
Catalysts	1	6A, 12B, 15A, 17A, *111A*, 111B, 200A, 212B, 250A, 252A, 252B, 500A
Hydrogenation	8	8A, 12B, 17A, *111A*, 120A, 121B, 300A

As will be seen from the above, document 111 should contain the desired information.

It should be noted that the absence of a sub-link in a term reference means either (1) that the specific term is not used alternatively in a comparison or (2) that it may be a constant in a link in which other related terms are compared. This is demonstrated by the use of the term "styrene copolymers" in our example on the use of the sub-link with role 7.

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