

## Access to Polymer Information in *Chemical Abstracts*<sup>†</sup>

ELIZABETH M. LANGSTAFF and G. KENNETH OSTRUM\*

Chemical Abstracts Service, Columbus, Ohio 43210

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Abstracts of the world's polymer chemistry literature, including patents, are found in the Macromolecular Sections (Sections 35–46) of the weekly issues of *Chemical Abstracts* (CA), with a few specialized topics appearing in other sections. In these weekly abstract issues, abstracts about a given topic can be located by use of the natural-language Keyword Indexes. Semiannual volume indexes provide in-depth indexing of the complete original documents. For specific, chemically defined polymers, access is provided by CA Index Names in the Chemical Substance Index and molecular formulas in the Formula Index, both of which also contain CAS Registry Numbers. Additional information about polymers is found at a series of controlled vocabulary headings for classes of substances, properties, processes, reactions, uses, etc., in the General Subject Index. The Index Guide is an invaluable tool for identifying pertinent index headings related to a given information need.

### INTRODUCTION

The slogan, "Key to the World's Chemical Literature", appears on the cover of the weekly abstract issues and the semiannual indexes published by Chemical Abstracts Service (CAS). Previous papers by CAS staff have described how the weekly abstract issues and the semiannual indexes are prepared in a timely manner, and how computer support is used to maintain and improve their quality.<sup>1–4</sup> A paper specifically on the indexing of polymers in *Chemical Abstracts* (CA) and stressing polymer nomenclature and some general indexing policies has even appeared,<sup>5</sup> but the emphasis of this paper, as indeed of all the others, was on the way printed CA was assembled and produced. What has been lacking is an examination focusing on how the individual scientist can use printed CA and its indexes to find specific information on polymers and polymer-related topics, a "how-to" approach informing the user community precisely what access methods are available and where they are located.

### CA ABSTRACTS

The basis for the slogan, "Key to the World's Chemical Literature", is the abstract (Figure 1). The CA abstract summarizes, but does not critically evaluate, the results and conclusions reported in the primary journal documents. The information printed in the heading identifies the document being summarized, i.e., its title, author name(s), work location of the first author listed, bibliographic citation, and language of the original document. Evaluation of the merit of the investigation is left to the scientific community. An example of this is the recent controversy over the existence of "polywater". At the time "polywater" was reported, CAS abstracted papers on the subject and indexed "polywater". CAS made no attempt to determine whether the reported findings were valid, in keeping with CAS standard policy. The main purpose of the abstract is to help the searcher answer the question, "Does this document contain the information I need?"

Most abstracts of polymer-related documents can be found in the Macromolecular Chemistry Sections of *Chemical Abstracts* which are published biweekly in even-numbered issues (Figure 2). The polymer literature covered by CA ranges from purely theoretical studies of model chains to patents for commercial rubbers, fibers, plastics, and coatings. A detailed explanation of the content of each section, including a listing of topics that are covered in another section or are not covered at all by CA, can be found in the publication

"Subject Coverage and Arrangement of Abstracts by Section in *Chemical Abstracts*".<sup>6</sup> A few specialized polymer topics do appear outside the Macromolecular Chemical Sections; for example, abstracts about photopolymerizable compositions used in printing plate manufacture appear in Section 74—Radiation Chemistry, Photochemistry, and Photographic Processes.

Since the number of abstracts published annually by CAS (over 428 000 in 1978) is too large to read or scan when actually searching for information, the abstracts can be located using any of a variety of access routes. Some of these access routes appear in the weekly abstract issues of CA, and others are provided in the semiannual indexes.

### KEYWORD INDEX

The Keyword Index published at the back of each weekly abstract issue can be used to locate abstracts on a given topic within that issue. The Keyword Index is a natural language index that uses both author terminology and terminology current in the field. An abstract will typically have five to six access points in the Keyword Index, consisting of phrases derived from the title, text, or context of the abstract. Keywords can contain the standard abbreviations used in all CAS publications, generic and class terms, common names, acronyms, and trade names (Figure 3). Since the vocabulary is not standardized, a variety of synonyms is usually needed in searching. For example, the searcher interested in a fairly comprehensive search for information about poly(tetrafluoroethylene) would also include terms such as Teflon and PTFE as additional access points in a search of the Keyword Index.

Keyword Indexes provide rapid entry into current issues of CA, but are not in-depth indexes. That is, they do not necessarily refer to every subject or substance studied in the original document. In-depth access, however, is provided in the Volume Indexes: the Chemical Substance Index, the Formula Index, and the General Subject Index, published at the end of each semiannual volume of 26 weekly abstract issues.

### CHEMICAL SUBSTANCE INDEX

The Chemical Substance Index provides comprehensive access to every specific chemical substance for which actual information is presented in the original document, regardless of the number of such substances. The access point is the rigidly controlled CA Index Name. In the Keyword Index, as was previously mentioned, information about a specific polymer is often scattered among several access points, e.g., common names, acronyms, or trade names. Since the access

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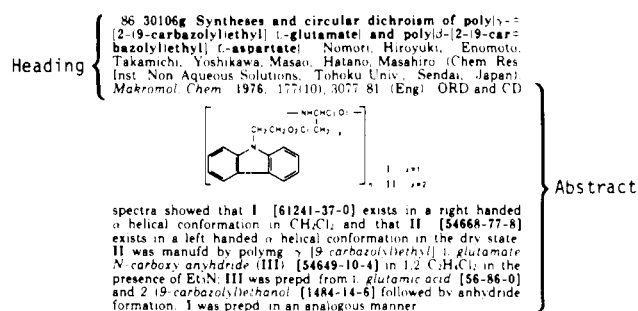


Figure 1. Sample abstract from *Chemical Abstracts* Section 35—Synthetic High Polymers (Volume 86, Issue 6).

35. Synthetic High Polymers
36. Plastics Manufacture and Processing
37. Plastics Fabrication and Uses
38. Elastomers, Including Natural Rubber
39. Textiles
40. Dyes, Fluorescent Whitening Agents, and Photosensitizers
41. Leather and Related Materials
42. Coatings, Inks, and Related Products
43. Cellulose, Lignin, Paper, and Other Wood Products
44. Industrial Carbohydrates
45. Fats and Waxes
46. Surface-Active Agents and Detergents

Figure 2. CA Macromolecular Chemistry Sections.

Polycarbonate polyolefin laminate 192236t  
 Polymer heterocyclic review 191812r  
 Polystyrene foam cup 192100u  
 PVC sulfonated coating reactor 191780d  
 Styrene polymn inhibitor 191997e  
 Teflon silver coating adhesive 192227r

Figure 3. Natural language access using the CA Issue Keyword Index.

Common Name	CA Index Name
Polyethylene	Ethene, homopolymer [9002-88-4]
Polypropylene	1-Propene, homopolymer [9003-07-0]
Isotactic polypropylene	1-Propene, homopolymer, isotactic [25085-53-4]
Syndiotactic polypropylene	1-Propene, homopolymer, syndiotactic [26063-22-9]
Polystyrene	Benzene, ethenyl-, homopolymer [9003-53-6]
Ethylene-propylene copolymer	Ethene, polymer with 1-propene [9010-79-1] 1-Propene, polymer with ethene [9010-79-1]
Butadiene-styrene copolymer	Benzene, ethenyl-, polymer with 1,3-butadiene [9003-55-8] 1,3-Butadiene, polymer with ethenylbenzene [9003-55-8]
ABS	Benzene, ethenyl-, polymer with 1,3-butadiene and 2-propenenitrile [9003-56-9] 1,3-Butadiene, polymer with ethenylbenzene and 2-propenenitrile [9003-56-9] 2-Propenenitrile, polymer with 1,3-butadiene and ethenylbenzene [9003-56-9]

Figure 4. Polymers in CA Chemical Substance Index.

point to the Chemical Substance Index is the unique CA Index Name, all information about a given polymer will be found consistently at a single location. For polymers, the CA Index Name is based on the monomer(s) from which the polymer was actually prepared (Figure 4). In the case of homopolymers, the CA Index Name of the monomer is followed by the modifying term "homopolymer" and the CAS Registry Number, a unique computer-checkable identification number which CAS has derived for each substance, which is enclosed in brackets. For copolymers, the CA Index Name of each monomer is followed by the phrase "polymer with..." and the uninverted CA Index Names of the other monomer(s) in alphabetical order. Since these multiple access points, available at each monomer name for copolymers, describe a single substance, the same CAS Registry Number is found at each

#### Benzene, ethenyl- [100-42-5], polymers

Coatings from homopolymers or unspecified copolymers are indexed at *Coating materials*, *Coating process*. Coatings from specific copolymers are indexed both at this heading and at *Coating materials*, *Coating process*

- • •
- polymer with 1,3-butadiene [9003-55-8]  
 adhesive binders, for color developing coatings, for copy paper, P 54641z
- • •
- block, absorbent contg., for oil spill collection, P 73196z  
 block, acoustic absorption and velocity in, 202227m
- • •
- graft, impact resistant, P 118735t  
 graft, impact-resistant, with improved gloss, P 202539q  
 graft, latexes, as finishing agents for textiles, prepn. of, 119135j
- • •
- oligomeric, PVC modified by, physicochem. properties in relation to, 6826s  
 oligomeric, contg. SBR, for strengthening wood, P 103528d
- • •
- triblock, solns. of, opalescence in micellization of, 136559t

Figure 5. Access to block and graft copolymers in CA Chemical Substance Index.

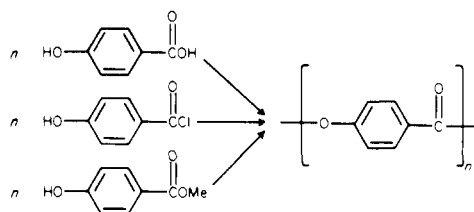


Figure 6. Structural repeating units for condensation polymers.

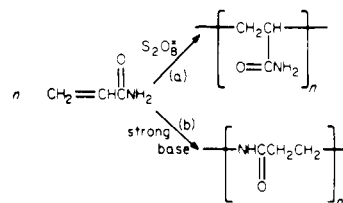


Figure 7. Structural repeating units for addition polymers.

of these names. This multiple access for copolymers also allows the searcher to find the homopolymer and all copolymers of a particular monomer at a single alphabetic location in the printed Chemical Substance Index.

Polymers with different tacticities, e.g., unspecified (atactic), syndiotactic, and isotactic polypropylene, have their own individual CAS Registry Numbers, but CA Index Names and CAS Registry Numbers for polymers are assigned without regard for molecular weight or molecular weight distribution. This means that butadiene-styrene copolymers with molecular weights 10000 and 10000000 have the same CA Index Name and CAS Registry Number. The term "oligomeric" may occur in the context of the index entry when stressed by the author (Figure 5). Similarly, graft and block copolymers have the same CA Index Names and CAS Registry Numbers as the random copolymers, with the terms such as "block", "graft", and "triblock" in the context of the index entry.

Since it is often possible to make a given polymer from a variety of starting materials (Figure 6), and since a single monomer may give rise to more than one final structure depending on the reaction conditions (Figure 7), some

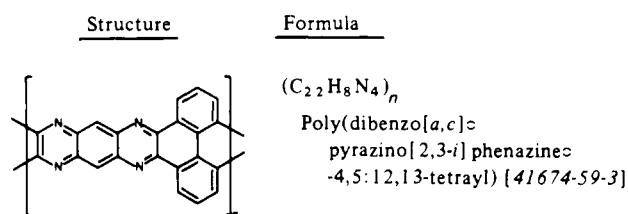


Figure 8. Structural repeating units for ladder polymers.

searchers prefer to have access to polymers on the basis of the structure formed, either in addition to or in place of access on the basis of the starting monomer(s). This additional access is available in the form of structural repeating units (SRU's) when the authors provide a structure of the final product accompanied by supporting data, but not when a single structure is drawn for convenience of discussion or to show the desired or predominant isomer. This additional access is also provided when a single structure can be reasonably inferred from the chemistry involved. For example, *p*-hydroxybenzoic acid or its derivatives polycondense to form a polyester with an unambiguous structure (see Figure 6). Access to information about this polyester is available at the name of the specific acid derivative used to prepare it, e.g., Benzoic acid, 4-hydroxy-, homopolymer [30729-36-3], and also at the name of the SRU formed, Poly(oxy-1,4-phenylene-carbonyl) [26099-71-8].

The monomer-based and SRU-based index entries (reflecting the two different structural viewpoints) represent different, although complementary, access points to a single chemical substance. These two access points, based on the extent of information reported on the starting materials used and the product formed, thus alleviate the ambiguity that may result from exclusive use of either approach alone. Since the structural representations associated with the monomer-based and SRU-based index entries are different, the CA Index Names, CAS Registry Numbers, and molecular formulas associated with each are also different. When the SRU is known, the searcher can find all references to that substance at a single place in the index, regardless of what starting materials were used.

Access at the SRU name is not provided routinely for addition homopolymers and copolymers, such as the polymer formed by reaction (a) in Figure 7. However, SRU entries can be found whenever the author provides evidence for the structure of the repeating unit. For example, if polymerization of acrylamide proceeded by reaction (b) in Figure 7 and the author substantiated the structure, access would be provided at Poly[imino(1-oxo-1,3-propanediyl)] [24937-14-2] as well as at the monomer-based name. Access is not usually provided at the SRU name for polymers prepared from unsymmetrical monomers or for condensation polymers prepared from more than two monomers.

The names for the SRU structures all begin with the term "poly" followed by the names of the multivalent radicals which make up the structure, in a preferred order derived from a well-specified set of rules.<sup>5</sup> This convention effectively collects all of the SRU entries, including those for complex double-strand chains of ladder polymers (Figure 8), in one general area of the Chemical Substance Index. Searchers who are familiar with CA Index Names may go directly to the Chemical Substance Index at either the monomer-based name or the SRU-based name to find the desired information. Those who may be less familiar with the nomenclature used by CAS have another access route, the CA Formula Index.

#### CA FORMULA INDEX

The principle for finding information about polymers in the Formula Index is analogous to that for using the Chemical

Common Name	Formula Index Entry
	$C_2H_4$ Ethene
polyethylene	homopolymer [9002-88-4]. See Chemical Substance Index
ethylene-propylene copolymer	polymer with 1-propene [9010-79-1]. See Chemical Substance Index
	$C_3H_3N$ 2-Propenenitrile
ABS	polymer with 1,3-butadiene and ethenylbenzene [9003-56-9]. See Chemical Substance Index
	$C_3H_6$ 1-Propene
polypropylene	homopolymer [9003-07-0]. See Chemical Substance Index
isotactic polypropylene	homopolymer, isotactic [25085-53-4]. See Chemical Substance Index
syndiotactic polypropylene	homopolymer, syndiotactic [26063-22-9], 39991v, 185088x
ethylene-propylene copolymer	polymer with ethene [9010-79-1]. See Chemical Substance Index
	$C_4H_6$ 1,3-Butadiene
butadiene-styrene copolymer	polymer with ethenylbenzene [9003-55-8]. See Chemical Substance Index
ABS	polymer with ethenylbenzene and 2-propenenitrile [9003-56-9]. See Chemical Substance Index
	$C_6H_6$ Benzene, ethenyl-
polystyrene	homopolymer [9003-53-6]. See Chemical Substance Index
butadiene-styrene copolymer	polymer with 1,3-butadiene [9003-55-8]. See Chemical Substance Index
ABS	polymer with 1,3-butadiene and 2-propenenitrile [9003-56-9]. See Chemical Substance Index

Figure 9. Polymers in CA Formula Index.

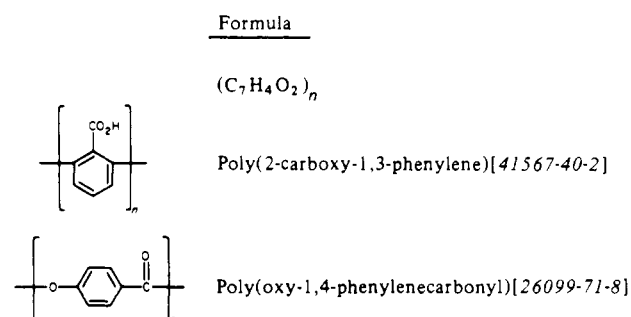


Figure 10. Structural repeating unit isomers.

Substance Index; i.e., the entry points are molecular formulas for each of the monomers (Figure 9) with the modifying phrases "homopolymer" and "polymer with..." for homopolymers and copolymers, respectively (Figure 9). This provides ready access to a monomer and all of its polymers at a single location in the Formula Index, just as there is ready access at the monomer name in the Chemical Substance Index. However, only the abstract number appears in the Formula Index, while the Chemical Substance Index provides contextual information about how the substance was studied in the document being cited. The SRU Formula Index entries are found (Figure 10) at the molecular formula entry for the repeating unit, enclosed in parentheses, and followed by a subscript *n*. Since molecular formulas are not unique, the searcher must verify that one of the names found at the molecular formula entry corresponds to the desired structure. For example, two different names are found at the molecular formula entry  $(C_7H_4O_2)_n$  (Figure 10), and the second name is the one which corresponded to the SRU of the polymer formed from *p*-hydroxybenzoic acid.

#### GENERAL SUBJECT INDEX

Information of a more general nature is often desired in addition to the information about specific polymers that is

**Glass temperature and transition**  
 of ABS polymer, compn. effect on, 122148a  
 of acrylamide-crotonic acid copolymers, crotonic  
 acid content effect on, 90280u

• • •

**Heat-resistant materials**  
 acetylene-terminated phenylquinoxaline oligomers,  
 crosslinked, 107378g  
 acetylene-terminated polyimides, 44331p

• • •

**Packaging materials**  
 ABS resins, with improved impact resistance, P  
 107428y  
 acrylonitrile-alkyl acrylate-vinylidene chloride  
 copolymer, flexible unplasticized, P 56232v

• • •

**Plasticizers**  
 R 55988j, R 90642p  
 absorption of, by PVC, improvement of, P 140941h

• • •

**Polycarbonates**  
 R 73847s  
 abrasion-resistant coatings for, vinyltrimethoxysilane  
 polymers as, 123035y

• • •

**Polymer degradation**  
 activation energy of, of PTFE and poly(Me  
 methacrylate), thermal, irradiation effect on,  
 44191t  
 anal. of, by laser microprobe techniques, 90521y

**Figure 11.** Controlled vocabulary access using the CA General Subject Index.

#### Lexan

See *Poly[oxycarbonyloxy-1,4-phenylene(1-  
 methylethylidene)-1,4-phenylene]*  
 [24936-68-3]

#### Polyamides

Amide group-containing polymers formed by the  
 polycondensation of polyamines or related  
 nitrogen compds. with polycarboxylic acids  
 acid halides, or related compounds, or by  
 polymerization of amino acids or lactams are  
 indexed at this heading. Polymers formed from  
 unsaturated amides, such as  
*N*-ethenylacetamide or 2-propenamide, by  
 addition polymerization are indexed at the  
 named amide or at *Amides, polymers*

See also *Peptides*  
 carboxy group-contg. — see *Polyamic acids*  
 fibers — see *Polyamide fibers*

#### Polyethylene

See *Ethene, polymers, homopolymer* [9002-88-4]

#### PVC

See *Ethene, chloro-, polymers, homopolymer*  
 [9002-86-2]

#### Styrene

See *Benzene, ethenyl-* [100-42-5]

#### Teflon

See *Ethene, tetrafluoro-, polymers, homopolymer*  
 [9002-84-0]

**Figure 12.** Search assistance from the CA Index Guide.

found in the Chemical Substance Index. Access to such diverse topics as classes of polymers, adjunct materials, and reactions and uses of polymers is provided in the General Subject Index (Figure 11). The boldface portion of each entry represents the primary controlled-vocabulary access points, while the lightface type gives free-text contextual information and the abstract number. Abstract numbers for patents and reviews

## 10. BUILDING MATERIALS

Building materials  
 . Adobe  
 . Bricks

• • •

Building materials treatment  
 . Adhesives  
 . Anodization  
 . Coating process  
 . Coloring  
 . Fireproofing  
 . Firing, heat treating process  
 . Firing of furnaces  
 . Hydration, chemical  
 . Molding  
 . (Reinforcement)  
 . Fibers  
 . Glass fibers  
 . Mineral wool  
 . Synthetic fibers  
 . Sealing  
 . Waterproofing  
 . Wetting

→

## 47. POLYMER APPLICATIONS

Building materials  
 . Adhesives

• • •

Fibers  
 . Fibrils  
 . Fibrous materials  
 . Ropes  
 . Synthetic fibers  
 . Hair substitutes  
 . Fur substitutes  
 . Wool substitutes  
 . Leather substitutes  
 . Paper substitutes  
 . Textiles  
 . Bands and Ribbons  
 . Carpets  
 . Flocks  
 . Rags  
 . Wearing apparel  
 . Web materials  
 . Threads  
 . Twine  
 . Leather

→

## 48. POLYMERIC COMPOSITIONS

Macromolecular compounds  
 . Carbohydrates  
 . Monosaccharides

• • •

. Polymers  
 . Acids, polymers  
 . Carboxylic acids, polymers

• • •

. Textiles  
 . Fibers  
 . (Natural fibers)  
 . (Animal fibers)  
 . Fur

• • •

→ . Synthetic fibers

. Acetate fibers  
 . Acrylic fibers  
 . Carbon fibers  
 . Phenolic resins  
 fiber

. Polyamide fibers

. Polyester fibers

. Polyimides

fiber

. Polyolefin fibers

. Polypropene fibers

. Polyoxymethylenes

fiber

. Polysulfones

fiber

. Polyureas

fiber

. Rayon

. Urethane polymers

fiber

. Spandex fibers

. Vinyl compounds, polymers

fiber

. Vinal fibers

. Vinyl acetal polymers

fiber

. Vinyon fibers

**Figure 13.** Hierarchies of CA General Subject headings for synthetic fibers.

are prefixed with P and R, respectively, as shown. An additional prefix, B for book, may also appear.

## CA INDEX GUIDE

As the science of chemistry has taken on an interdisciplinary nature and become more complex, the terminology used by chemists has changed. Chemical terminology has become more diverse, with large numbers of terms being associated with a given topic. At the same time, it has become more specialized, with a single term having highly specific meanings that may vary among the different branches of chemistry. The CA Index Guide has thus become an invaluable tool for determining the controlled vocabulary index headings used for topics of interest in the General Subject Index and for substances of interest in the Chemical Substance Index. The Index Guide also contains "See" cross-references to related headings and indexing policy notes which describe what is found at that heading and what is found elsewhere (Figure 12). All of these types of information are found in a single alphabetical listing which comprises the bulk of the Index Guide. The Index Guide Appendixes contain a wealth of additional information, such as hierarchies of general subject headings, a description of the organization and use of the CA indexes, and a detailed discussion of the selection of CA Index Names for chemical substances. This discussion of nomenclature has its own index so that it is not necessary to read the entire discussion, but only the portion(s) which describe(s)

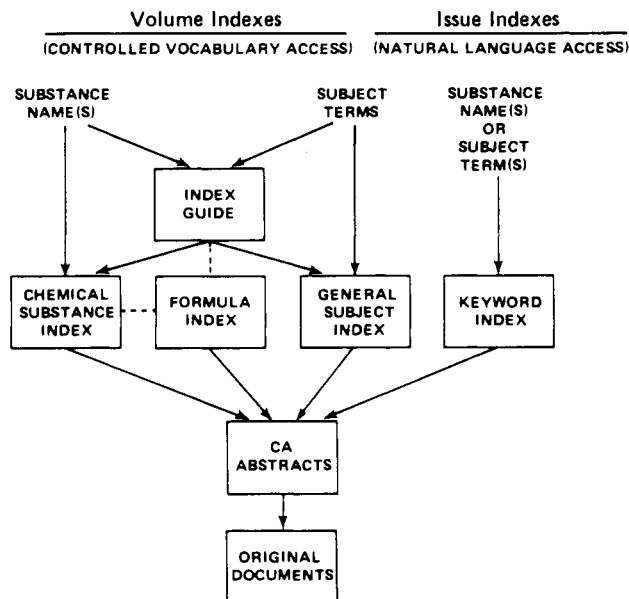


Figure 14. Access routes to documents through *Chemical Abstracts*.

the desired class of substances.

The hierarchies of General Subject Headings are found in Appendix I of the Index Guide. For each of 66 subject areas, CA index headings are listed in order of increasing specificity. An alphabetic index identifies the various hierarchies in which a given index heading may be found. Thus, a searcher who has a single topic in mind, e.g., synthetic fibers, may turn to it and find related headings, both more and less specific such as Fibers and Acetate Fibers, respectively (Figure 13). These will provide additional access points to the General Subject Index where information of interest may be found.

## SUMMARY

Figure 14 summarizes access to the chemical literature using printed CA issue and volume indexes. Access is available weekly in the natural-language Keyword Index using the terminology current in a given field of chemistry for both substances and general subjects. Access with a greater depth of indexing is available in the semiannual, controlled-vocabulary Chemical Substance, Formula, and General Subject Indexes. The existence of controlled access points in these indexes requires use of the Index Guide for effective and efficient use of the indexes. All of these access points lead back to the CA abstract which identifies a document and summarizes its technical content, thus allowing printed CA to fulfill its role as "Key to the World's Chemical Literature".

The title of the original document, the name(s) of the document's author(s), all the bibliographic information necessary to identify the document, the Keyword Index entries, and all of the in-depth volume index entries are also available in *CA Search*, a new biweekly computer-readable service offered by CAS. Use of this file for computer-assisted access to the polymer literature will be the topic of a subsequent paper.

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## POLIDCASYS: The Polymer Documentation System of IDC<sup>†</sup>

ROBERT FUGMANN

Hoechst A.-G., 6230 Frankfurt/M, Postfach 80 03 20, Federal Republic of Germany

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The IDC indexing system was adapted to the requirements of the polymer field. Polymer structures and the important syntactical relations between structures, including monomers, can be encoded precisely and searched as well. For nonstructural concepts (properties, etc.), a novel kind of controlled vocabulary, which can be supplemented continually by free terms, was developed.

## INTRODUCTION

In the indexing and retrieval of polymer literature we encounter some problems that play only a minor part in the nonpolymer literature.

First, the *structure* of a polymer is less clearly defined than that of a nonpolymer compound. An indexing language for polymers must therefore cope with various degrees of structural uncertainty and vagueness and must not be limited to precisely defined structures (cf. refs. 1-3, 9-13).

Secondly, polymers most often are not defined structurally, but rather by their route of preparation. In such cases, one should not be obliged to resort to assumptions regarding the structure of the polymer. Rather, it should be possible to represent this specific route of preparation as precisely as

possible. This includes indexing the monomers involved as well as the particularities of their *logical and syntactical relations* just as they are recorded in a document.

Thirdly, the indexing of properties, processes, and uses deserves particular attention in the polymer literature, for the essence of a document frequently consists precisely of these *nonstructural concepts*, and much less of statements regarding structures and syntheses.

Consequently, if one has at his disposal an indexing system developed specifically for the nonpolymer literature, he will encounter serious difficulties in using that system in the polymer field. This was the plight of IDC (International Documentation in Chemistry, Frankfurt/M., Hamburger Allee 26, Federal Republic of Germany) and, in particular, of our company as a member firm of IDC 11 years ago. At that time, it was also realized, that no indexing system was available that satisfied the relatively high requirements of the IDC firms with respect to the effectiveness of machine searches, in particular

<sup>†</sup> Presented before the Division of Chemical Information, Symposium on "Retrieval of Polymer Information", 176th National Meeting of the American Chemical Society, Miami Beach, Fla., Sept 13, 1978.