Indexing of Polymers in *Chemical Abstracts**

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Polymers can be indexed on the basis of the monomers from which they are formed or on the basis of their actual structure as represented by a structural repeating unit (SRU). Since the primary literature does not always provide sufficient information on actual structures, all polymers are indexed in the *CA* volume indexes and registered in the CAS Registry System on the basis of their monomers. All specific homopolymers, copolymers, and polymeric reaction products are indexed separately at every component in both the subject and formula indexes. Additional entries based on the new polymer rules of the American Chemical Society are made in both the subject and formula indexes and the CAS Registry System for polymers whose structures are well defined or can be clearly assumed.

The indexing of chemical compounds in the *Chemical Abstracts* (*CA*) volume indexes has always conformed to accepted nomenclature practices in a given field of chemistry, as far as these practices have been consistent with good indexing. Polymer chemists, like all chemists, have developed specialized practices which *CA* has attempted to incorporate within the framework of existing nomenclature. Although preferring to index a substance or a concept at the place a specialist may first logically search for it, *CA* has at times deviated from the practices of a particular field in order to better serve the entire scientific community.

Hence, although CAS continues to index all polymers on the basis of their component monomers, both the subject and formula indexes have provided structure-based (SRU) index entries for polymers beginning with Volume 66 (January-June 1967). These entries, which use systematic names based on new ACS polymer rules,[1] are offered as supplements to the monomer-based index entries. This paper describes the basis for both monomer- and structure-based indexing in the *CA* indexes, and presents general indexing policies and specific examples of the new index entries.

MONOMER *vs.* SRU AS A BASIS FOR NAMING POLYMERS

The 1952 IUPAC "Report on Nomenclature in the Field of Macromolecules"[2] gave three methods for naming high polymers. First, polymers may be named on the basis of their real or hypothetical method of preparation from monomers, for example, poly(methyl methacrylate) (prepared by polymerization of methyl methacrylate) and poly(vinyl alcohol) (prepared from the hypothetical vinyl alcohol). Second, polymers may be named on the basis of their relationship to well-known substances with trivial names, for example, cellulose acetate. Third, polymers may be named by assignment of a trivial name, for example, nylon. Under this system, copolymers are designated by inserting "co" between the names of the monomers enclosed in parentheses and prefixed by "poly," for example, poly(butadiene-*co*-styrene) and poly(vinyl acetate-*co*-vinyl chloride). The 1952 IUPAC report further stated that these methods were to be used when there was any doubt about the structure of the polymeric product, when it was desired to emphasize the method of preparation, or when the structure was too complicated to be represented by a simple name.

The traditional methods for polymer nomenclature given in the 1952 IUPAC report are used in the *CA* volume indexes with one major difference—the prefix "poly" is not used. Rather, a polymer is indicated by a descriptive phrase such as "polymer," "polyamide," or "polyester," following the name of the monomer. Similarly, copolymers are indexed at each of the component monomers, indicating the copolymer by phrases like "polymer with. . ." or "polyamide with. . ." In this manner, the subject index collects at a single location information concerning a monomer and its polymers.

Among the disadvantages of monomer-based nomenclature,[3] however, is the problem of ambiguity. That is, one monomer can lead to more than one polymer, and one polymer may be formed from a variety of monomers. Accordingly, the 1952 IUPAC report noted the desirability of naming macromolecules on the basis of total structure, but the structure-based system proposed in the report was never widely used. Recently, the American Chemical Society, through the Nomenclature Committee of its Division of Polymer Chemistry, has developed a structure-based nomenclature for linear polymers. These rules have been published[1] and are under study by the Nomenclature Commission of the IUPAC Macromolecular Division. CAS, responding to this renewed emphasis on structure-based polymer nomenclature, has added systematic polymer names based on this latter system to the *CA* subject and formula indexes beginning with Volume 66 (1967). This volume is the first of the eighth collective

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period, which will cover the years 1967–71. The systematic polymer names will supplement the traditional monomer-based indexing wherever the structural repeating unit (SRU) of a polymer is known or can be assumed.

Since papers and patents on polymers vary greatly in the detail of polymer structural information, CAS will continue monomer-based indexing in order to maintain a complete and consistent literature record. The new ACS polymer names based on the structural repeating units, although supplementary at this stage, will become more important as methods for characterization of polymer structure are refined and as methods for preparation of controlled structures are developed. Additional emphasis on structure-based nomenclature will occur as the registration of polymers proceeds in the structure-oriented CAS Chemical Registry System.[4] The use of the new ACS polymer nomenclature will be continually re-evaluated. As the field of polymer chemistry advances and as we gain experience with structure-based names, more of these names may be used in the next collective period (1972–76).

GENERAL INDEXING POLICIES

Before discussing specific examples of polymer nomenclature and indexing, some general indexing policies are illustrated by the examples in Figures 1 and 2 taken from the *CA* Vol. 66 Subject and Formula Indexes, respectively. Each subject index entry (Figure 1) consists of a heading (in bold-face type), a modification (in light-face type), and a *CA* reference (volume and abstract number). The first part of the modification completes the chemistry, for example, "polymers," and "polymer with ethylene;" the rest of the modification relates the subject matter as discussed in the document, for example, use, properties, or methods of preparation. A new feature of the *CA* subject indexes, starting with Volume 66, is the subdivision of the headings of common chemical compounds into categories such as "analysis," "preparation," or "reactions," in order to lead a searcher more rapidly to his particular point of interest at a given subject. "Polymers" is a category used for commonly occurring monomers. Thus, polymers of very common chemical compounds are grouped together under a separate subject index heading, such as **Butadiene polymers**, which in turn may be categorized.

The first example in Figure 1 shows a homopolymer of a relatively uncommon monomer. The second example shows two chemically different condensation-type adipic acid polymers. The fifth, seventh, and eighth examples are the index entries for the polymers of adipic acid at the headings for the other components.

The third example is an addition-type copolymer, and the modification for this entry illustrates a change from previous indexing practice. The modification under the name of a monomer prior to Volume 66 began with "polymerization of" in a case of polymer preparation and with "polymer with..." in case of property studies. This led to scattering of similar information in the *CA* indexes. Beginning with Volume 66, every polymer and copolymer is indexed in the same way, with the information "prepn. of" or "manuf. of" given later in the modification. The heading **Polymerization** is retained for information on the general reaction, but is not used for every individual polymerization reaction.

1. **Acrylamide, *N*-(2-morpholinoethyl)-**
   polymers, photographic emulsions contg., **66**:P 100201x
2. **Adipic acid polymers**
   polyamide with 1,6-hexanediamine and sebacic acid, hosiery from nylon 66 and, **66**:P 29974u
   polyester with 2,2-dimethyl-1,3-propanediol, prepn. of, kinetics of, **66**:86060s
3. **Ethylene, fluoro-**
   polymer with ethylene, prepn. of, reactivity ratios in, **66**:29190k
4. **Ethylene polymers, preparation**
   polymer with fluoroethylene, reactivity ratios in, **66**:29190k
5. **1,6-Hexanediamine polymers**
   polyamide with adipic acid and sebacic acid, hosiery from nylon 66 and, **66**:P 29974u
6. **Poly[oxy(2,2-dimethyltrimethylene)oxyadipoyl]**
   prepn. of, kinetics of, **66**:86060s
7. **1,3-Propanediol, 2,2-dimethyl-**
   polyester with adipic acid, prepn. of, kinetics of, **66**:86060s
8. **Sebacic acid polymers**
   polyamide with adipic acid and 1,6-hexanediamine, hosiery from nylon 66 and, **66**:P 29974u

Figure 1. CA subject index entries

1. **C_2H_3F**
   Ethylene, fluoro-
   polymer with ethylene, **66**:29190k
2. **C_2H_4**
   Ethylene
   polymer with fluoroethylene, **66**:29190k
3. **$C_5H_{12}O_2$**
   1,3-Propanediol, 2,2-dimethyl-
   polyester with adipic acid, **66**:86060s
4. **$C_6H_{10}O_4$**
   Adipic acid
   polyamide with 1,6-hexanediamine and sebacic acid, **66**:P 29974u
   polyester with 2,2-dimethyl-1,3-propanediol, **66**:86060s
5. **$C_6H_{16}N_2$**
   1,6-Hexanediamine
   polyamide with adipic acid and sebacic acid, **66**:P 29974u
6. **$(C_9H_{16}N_2O_2)_n$**
   Acrylamide, *N*-(2-morpholinoethyl)-
   polymers, **66**:P 100201x
7. **$C_{10}H_{18}O_4$**
   Sebacic acid
   polyamide with adipic acid and 1,6-hexanediamine, **66**:P 29974u
8. **$(C_{11}H_{18}O_4)_n$**
   Poly[oxy(2,2-dimethyltrimethylene)oxyadipoyl], **66**:86060s

Figure 2. CA formula index entries

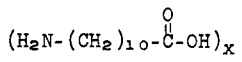
The fourth example shows the same copolymer as the third example, but indexed under the other component. **Ethylene polymers** is a subject heading where a large number of studies are reported, and it has been subdivided into categories as described above.

The sixth example is the added structure-based subject index entry for the assumed SRU of the adipic acid polyester shown in example 2. Assumption of SRU's are made for polymers and hydroxy acids, lactones, lactams, and for simple two-component polyamides and polyesters. In general, assumptions of SRU's are made for those two-component condensation polymers where only one type of SRU can be formed. No assumptions are made for addition polymers or for condensation polymers of three or more components. Index entries based on the SRU for these polymers are made only when the structure of the repeating unit is accompanied by supporting data.

Figure 2 shows formula index entries for the examples described above. Beginning with Volume 66, all polymers are fully and separately described under every component in the formula index, as well as the subject index. Under

each monomer formula, the text entry completes the chemistry and gives the *CA* reference. The subject matter, such as use or preparation, is not included. The sixth example illustrates a formula index entry for a homopolymer. The homopolymer is in parentheses with a subscript "*n*", thus distinguishing it from the formula of the monomer. The last example shows the formula of an SRU, again in parentheses with subscript "*n*".

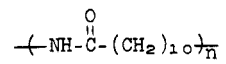
Monomer entries:



Subject Index: **Undecanoic acid, 11-amino-** polyamides

Formula Index: $(C_{11}H_{23}NO_2)_n$
Undecanoic acid, 11-amino-polyamides

SRU entries:



Subject Index: **Poly(iminocarbonyldecamethylene)**

Formula Index: $(C_{11}H_{21}NO)_n$
Poly(iminocarbonyldecamethylene)

Figure 3. 11-Aminoundecanoic acid homopolymer

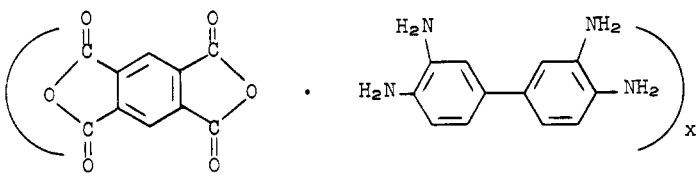
SPECIFIC EXAMPLES OF POLYMER INDEXING

The above discussion dealt with general indexing policies and illustrated how various index entries appear in the subject and formula indexes. Figures 3 through 6 illustrate the index entries for some specific polymers.

Figure 3 is an example of a one-component condensation polymer, showing that a monomer-based formula index entry is different from the SRU-based formula index entry. Figure 4 is an example of a two-component copolymer illustrating the usefulness of the SRU entry, since the structure of the final polymer differs considerably from the starting materials. Both monomers are indexed, as is the SRU given by the author. An index entry of a general nature is also found at the ring name in order to provide coverage for the user interested in ring systems.

Figure 5 illustrates the indexing of a telomer. Indexing of telomers is analogous to polymer indexing, with the exception that the descriptive phrase "telomer with" is used in place of "polymer with." Also, when end groups are known, subject and formula index entries are made at the compounds from which these groups were derived. This example also illustrates the application of the new ACS polymer rules in the citation of end groups of SRU units. End groups are designated by radicals cited in the modification of the *CA* index name. The SRU, when written according to the prescribed rules, is terminated by the α group on the left, the ω group on the right.

Monomer entries:



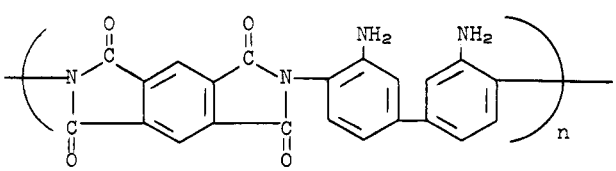
Subject Index: **1,2,4,5-Benzenetetracarboxylic 1,2:4,5-dianhydride** polymer with 3,3′,4,4′-biphenyltetramine

3,3′,4,4′-Biphenyltetramine polymer with 1,2,4,5-benzenetetracarboxylic 1,2:4,5-dianhydride

Formula Index: $C_{10}H_2O_6$
1,2,4,5-Benzenetetracarboxylic 1,2:4,5-dianhydride polymer with 3,3′,4,4′-biphenyltetramine

$C_{12}H_{14}N_4$
3,3′,4,4′-Biphenyltetramine polymer with 1,2,4,5-benzenetetracarboxylic 1,2:4,5-dianhydride

SRU entries:



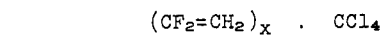
Subject Index: **Poly[(5,7-dihydro-1,3,5,7-tetraoxobenzo[1,2-*c*:4,5-*c*′] dipyrrole-2,6(1*H*,3*H*)-diyl)-(3,3′-diamino-4,4′-biphenylylene)]**

Benzo[1,2-*c*:4,5-*c*′] dipyrrole derivs., polymers

Formula Index: $(C_{22}H_{12}N_4O_4)_n$
Poly[(5,7-dihydro-1,3,5,7-tetraoxobenzo[1,2-*c*:4,5-*c*′] dipyrrole-2,6(1*H*,3*H*)-diyl)(3,3′-diamino-4,4′-biphenylylene)]

Figure 4. Two-component copolymer

Monomer entries:



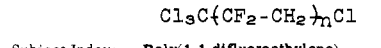
Subject Index: **Ethylene, 1,1-difluoro-** telomer with carbon tetrachloride

Carbon tetrachloride polymers telomer with 1,1-difluoroethylene

Formula Index: $C_2H_2F_2$
Ethylene, 1,1-difluoro- telomer with carbon tetrachloride

CCl_4
Carbon tetrachloride telomer with 1,1-difluoroethylene

SRU entries:



Subject Index: **Poly(1,1-difluoroethylene)** α-(trichloromethyl)-ω-chloro-

Formula Index: $(C_2H_2F_2)_n$
Poly(1,1-difluoroethylene) α-(trichloromethyl)-ω-chloro-

Figure 5. Telomer

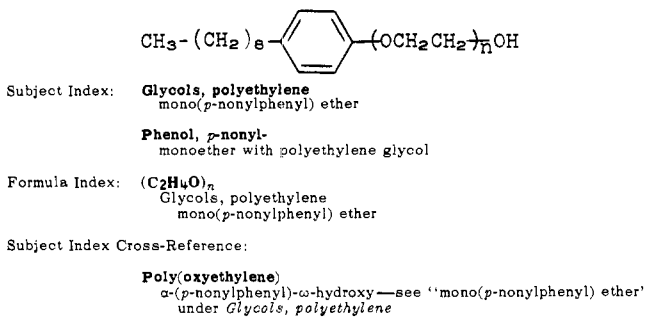


Figure 6. Poly(oxyethylene) derivatives

The indexing of polyalkylene glycols is illustrated in Figure 6. Additional entries or cross-references are found at the systematic poly(oxyalkylene) name to serve the increasing number of polymer chemists that are now using this type of nomenclature. A number of commercial products being reported are not characterized well enough to be systematically named. As a result, both well-defined and less specific derivatives of polyalkylene glycols are grouped together in the subject index.

POLYMER REGISTRATION

Registration of polymers in the CAS Registry System[4] involves the recording of both the structure and the names for a particular polymer. The computer file stores not only approved names—both monomer-based and structure-based—as they appear in the *CA* subject and formula indexes, but also trade names, names based on non-systematically-named monomers, etc.

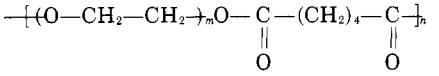
The new polymer rules for naming the SRU's are based on a strict order of precedence for bivalent radicals. However, for retrieval of structural information from the computer file, component biradicals need not be expressed in the same order. An SRU such as Poly(thioiminoethylene) can be drawn in several ways; $-(S-NH-CH_2-CH_2)_n-$, $-(CH_2-CH_2-S-NH)_n-$, $-(CH_2-NH-S-CH_2)_n-$, etc. All these structures will be recognized as identical.

Substructure search programs used for registered organic compounds can be applied to the SRU's of polymers as well. This capability will make it possible to retrieve information on all polymers containing a specific organic group, such as benzodipyrrole ring.

SOME REMAINING PROBLEMS

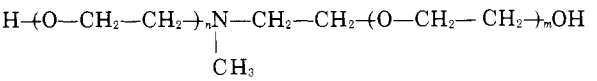
The new polymer nomenclature rules are in an early stage of development. At present, they will handle organic linear polymers, both of the single and double stranded types. CAS experience with the use of these rules has been very encouraging. However, there are areas for which the new polymer rules must be extended.

One example is a polymer within a polymer, such as:



This formula represents a polymer prepared by polyesterification of adipic acid with polyethylene glycol.

Another example is a polymer composed of two SRU's linked through a bivalent radical, for example:



Polymers of this type result by oxyethylation of an organic amine. The problem becomes even more complex when the two SRU moieties are not identical.

In addition, the applicability of the new ACS polymer rules to inorganic polymers, coordination polymers, etc., must be determined. Methods for naming "net" (cross-linked) polymers, block and graft polymers, and "post-treated" polymers need to be devised. At present, these types of polymers are described in the subject index by descriptive terms or phrases cited in the modification.

Finally, in indexing the chemical literature from a wide variety of sources, the recognition and interpretation of author names also remains a problem. For example, the description of a polymer only by the code PMA may result in its loss to the index user unless its structure is more fully identified. The code PMA can indicate poly(methyl acrylate), poly(maleic anhydride) or poly(methacrylic acid). The same abbreviation has also been used for pyromellitic acid.

It is the desire of CAS to develop better and more complete means for documenting the important progress that is being made in polymer chemistry. We hope the nomenclature and indexing policies presented in this paper, supplemented by increasingly more complete product descriptions from polymer chemists, will help achieve this goal.

LITERATURE CITED

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