Selection of Polymer Index Names for Chemical Abstracts

Classes of polymers, natural and synthetic, are indexed in the *Chemical Abstracts (CA) General Subject Index*.

Specific polymers are named on the basis of the monomers from which they are formed and/or on the basis of their structure, as represented by a structural repeating unit (SRU), and indexed in the *CA Chemical Substance Index*. Since original documents do not always provide sufficient structural information to allow generation of the SRU name, the method most frequently used for describing polymeric substances is by citation of the component monomers. A few commercial polymers, each of which accounts for a large number of index entries, are indexed only at the SRU-based systematic polymer name. (Cross-references at the monomer names appear in the *CA Index Guide*). Systematic nomenclature is discussed first in the following paragraphs, followed by monomer-based polymer nomenclature.

Systematic (SRU) nomenclature for polymers has been adapted from the system developed by the Committee on Nomenclature of the Division of Polymer Chemistry of the American Chemical Society*. Names derived by this system, in addition to monomer-based entries, are cited for polymers whose structural repeating units are well-documented or can confidently be assumed. "Expected," "idealized," or "drawn-for-convenience" SRUs are not given systematic polymer names. Occasionally, when there is no information on the component monomers in the original document, an entry derived from the SRU name is the only index entry available.

The SRU is named by citation of one or more multivalent radicals of regular substitutive nomenclature. Many of these radical names will be found in the Illustrative List of Substituent Prefixes (*CA Index Guide*, Appendix IV, Section H, ¶ 294); others are supplied in the various Appendix IV sections dealing with classes of compounds from which the radicals are derived. The SRU name is enclosed in parentheses or brackets, and prefixed by the term "Poly". Each multivalent radical retains its own numbering and is oriented, if possible, so that the point of attachment written at the left end of the repeating unit is assigned the lowest possible number. This permits the naming of the SRU in a directional manner, reading from left to right. The largest possible multivalent radicals are chosen as all or part of the name, and naming proceeds from left to right, starting with the most preferred multivalent radical. (See the following sections for the choice of most preferred radical.) Unsaturation and substituents are indicated by appropriate locants. Functional derivatives, such as esters and hydrazones and oxides of hetero atoms which are an integral part of the repeating unit are expressed by prefixes rather than by modification terms, and are numbered as low as possible while preserving the preferred names of the parent radicals. Salts of acids and anions of quaternary "-onium" compounds, and oxides of hetero atoms which are an integral part of the repeating unit are cited following the name of the SRU. The number of free valencies between units is minimized; i.e., unsaturated radicals are preferred.

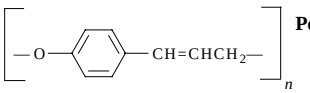
Polymers of unspecified length and chains of reported "average" length, are named by the methods described above. The prefix "oligo-" is not used to differentiate polymers of relatively low molecular weight from high polymers. When, however, the number of structural repeating units is exactly specified, the oligomer is usually named according to the principles of substitutive nomenclature.

Examples:

$(-CH_2-)_n$	**Poly(methylene)**
$(-CHMeCH_2-)_n$	**Poly(1-methyl-1,2-ethanediyl)**
$(-CH=CH-)_n$ (not $(=CHCH=)_n$)	**Poly(1,2-ethenediyl)** (not Poly(1,2-ethanediylidene))
$[-(CO)_2(CH_2)_2-]_n$	**Poly(1,2-dioxo-1,4-butanediyl)** (not Poly(1,4-dioxo-1,4-butanediyl))
$(-CH=CHCHMeCH_2-)_n$	**Poly(3-methyl-1-butene-1,4-diyl)**

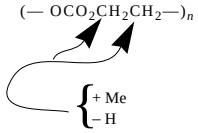
For more complex examples, further criteria for arranging the components of an SRU are required. The descending order of priority of citation (and of structuring of the SRU) is (*a*) heterocyclic rings, (*b*) acyclic hetero atoms in the order: O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Hg, (*c*) carbocyclic rings, (*d*) acyclic carbon chains. If substituents are present, otherwise identical parent radicals in the SRU are chosen by the principles, in turn, of maximum number, lowest locants, and earliest alphabetical order of substituents. The shortest path (smallest number of atoms) is taken from the most preferred multivalent radical to another occurrence of the same radical (if present) within the SRU, then to the next most preferred radical, and so on.

Examples:



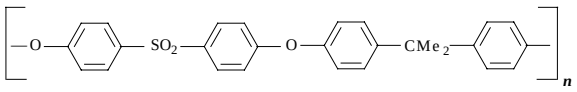
Poly(oxy-1,4-phenylene-1-propene-1,3-diyl)

$[-NHCO(CH_2)_2-]_n$	**Poly[imino(1-oxo-1,3-propanediyl)]**
$[-(SO_2)_2(CH_2)_2-]_n$	**Poly(disulfonyl-1,2-ethanediyl)**



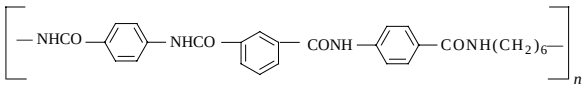
Poly[oxycarbonyloxy(methyl-1,2-ethanediyl)] (The position of the methyl group is not assumed in this polyester from carbonic acid and 1,2-propanediol.)

*"A Structure-based Nomenclature for Linear Polymers", *Macromolecules* **1968**, 1(3), 193-198. The IUPAC recommendations (*Pure Appl. Chem.* **1976**, 48, 373-385; **1993**, 65 (7), 1561-1580) are in full agreement with CAS practice. The IUPAC term "constitutional repeating unit" (CRU) corresponds to *CA*'s SRU.

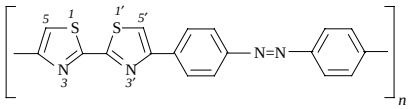


Poly[oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,4-phenylene(1-methylethylidene)-1,4-phenylene] (With equal numbers of atoms between the oxygen atoms in two possible arrangements, the preferred path includes the other hetero atom, sulfur, as early as possible.)

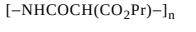
Poly(oxymethylenethioimino-1,2-ethanediyloxymethylenethiomethyleneiminomethylene) (With equal distances between the two oxygen atoms and between the oxygen and sulfur atoms, the direction is determined by the shortest distance between the oxygen atom and the hetero atom of third preference (nitrogen).)



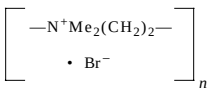
Poly(iminocarbonyl-1,4-phenyleneiminocarbonyl-1,3-phenylenecarbonylimino-1,4-phenylenecarbonylimino-1,6-hexanediyl) (The citation proceeds in the increasing order of distances between the nitrogen atoms: 5,5,5, and 6 intervening carbon atoms.)



Poly([2,2′-bithiazole]-4,4′-diyl-1,4-phenyleneazo-1,4-phenylene)



Poly[imino[1-oxo-2-(propoxycarbonyl)-1,2-ethanediyl]] (not Poly-[imino(1-carboxy-2-oxo-1,2-ethanediyl)], propyl ester)

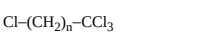


Poly[(dimethyliminio)-1,2-ethanediyl bromide] (the ionic derivative term is included in the SRU)

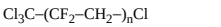
When SRUs are bridged only by metals, systematic polymer nomenclature is not used; instead, the substance is indexed either at the monomeric salt name or by coordination nomenclature (*CA Index Guide*, Appendix IV, ¶ 215), with a modification phrase, in either case, such as "homopolymer" or "polymer with" (see below).

End groups, when known, are specified by means of appropriate radical names, together with Greek letters "α-" and "ω-" expressed as substituents. The α-end group is the group attached to the left end of the SRU when the structure is ordered by the specified rules; it is cited first, regardless of alphabetical order.

Examples:



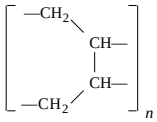
Poly(methylene) α-chloro-ω-(trichloromethyl)-



Poly(1,1-difluoro-1,2-ethanediyl) α-(trichloromethyl)-ω-chloro-

Linear double-strand ("ladder" and "spiro") polymers may sometimes be named as a chain of quadrivalent radicals. Two pairs of locants, separated by a colon, indicate the distribution of bonds.

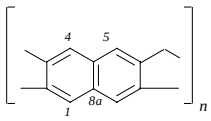
Example:



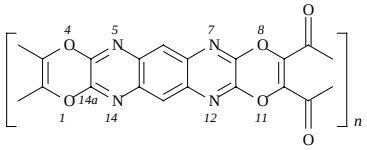
Poly(1,4:2,3-butanetetrayl)

When a ladder polymer must be named as an SRU of one or more quadrivalent radicals linked through one or more bivalent radicals (here, these terms are extended to mean radicals attached to four or two different atoms, not only to radicals with four or two free valence bonds) the direction of citation is from the most favored quadrivalent radical by the shortest path to the next most favored quadrivalent radical, and so on; then toward the most favored bivalent radical. Rings are broken (*a*) to minimize the number of free valencies of the total "mer," (*b*) to maximize the number of most preferred hetero atoms in the ring system, (*c*) to maintain intact the most preferred ring system (*CA Index Guide*, Appendix IV, ¶ 138). End groups, when known, are identified by α and α′ (at the left terminus as the structure is drawn) and by ω and ω′ (at the right terminus) as locants for substituent prefixes, e.g., α,α′-dihydroxy-ω,ω′-dihydro-.

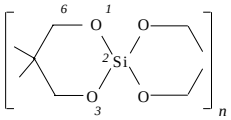
Examples:



Poly(2,3:6,7-naphthalenetetrayl-6-methylene)

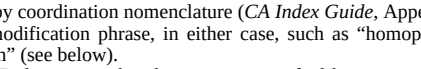


Poly([1,4]dioxino[2,3-*b*]-1,4-dioxino[2′,3′:5,6]pyrazino[2,3-*g*]-quinoxaline-2,3:9,10-tetrayl-9,10-dicarbonyl) (The same number of free valences can be expressed by breaking the oxygen ring or the partially saturated hydrocarbon ring; the latter course keeps intact the maximum number of heterocyclic rings.)



Poly[1,3-dioxa-2-silacyclohexane-5,2-diylidene-2,2-bis(oxymethylene)] (not Poly[1,3-dioxa-2-silacyclohexane-2,5-diylidene-5,5-bis(methyleneoxy)] (The direction is determined by the shortest path from the hetero atom in the ring to the acyclic hetero atom.)

Linear polymers composed of SRUs within SRUs, e.g.,



are not assigned systematic names; they are indexed at the monomer names only.

The previous paragraphs described a systematic nomenclature for polymers of well characterized structure, and for polymers whose structural repeating unit (SRU) can be confidently assumed. The latter are restricted to (*a*) polyamides from a dibasic acid (or derivative) and a diamine, or from an amino acid or lactam; (*b*) polyesters from a dibasic acid (or derivative) and a dihydric alcohol, or from a hydroxy acid or lactone; (*c*) polyurethanes from a diisocyanate and a dihydric alcohol; and (*d*) polycarbonates from carbonic acid (or an ester or halide) and a dihydric alcohol.

Polymers manufactured from known monomers are generally indexed at the monomer names whether or not systematic (SRU) entries are also made. An exception is the treatment of a few very common industrial polymers, e.g., nylon 6, nylon 66, terephthalic acid polymer with ethylene glycol, which, to preclude inordinate repetition of a large number of index entries at various names, are cross-referred in the *Index Guide* from monomer names to SRU names.

Example:

Terephthalic acid
See *1,4-Benzenedicarboxylic acid*

1,4-Benzenedicarboxylic acid, polymers
polymer with 1,2-ethanediol—see *Poly(oxy-1,2-ethanediyloxycarbonyl-1,4-phenylenecarbonyl)*

A cross-reference appears also at **1,4-Benzenedicarboxylic acid, esters, dimethyl ester, polymer with 1,2-ethanediol;** and two corresponding cross-references at **1,2-Ethanediol, polymers.**

Polymers from a single monomer are indexed at the monomer name with the term "homopolymer" cited in the modification. (The terms "peptides," "polyamides," and "polyesters" are not used for specific homopolymers at monomer headings.)

Examples:

$(BuCH{=}CH_2)_n$ — **1-Hexene**
homopolymer (only index entry)

$[H_2C{=}CMeCO_2(CH_2)_{12}Me]_n$ — **2-Propenoic acid, 2-methyl-tridecyl ester, homopolymer** (only index entry)

$[H_2N(CH_2)_{10}CO_2H]_n$ — **Undecanoic acid, 11-amino-homopolymer** (the *Formula Index* entry appears at $C_{11}H_{23}NO_2$; a systematic entry is also made at the assumed SRU name: **Poly[imino-(1-oxo-1,11-undecanediyl)],** $(C_{11}H_{21}NO)_n$)

Polymers formed from two or more monomers are indexed at each monomer name with the modification term "polymer with" followed by the other monomer names in alphabetical order. No attempt is made to indicate the percentage composition of copolymers. The preferred index name is determined by the usual rules for selection of a heading parent (*CA Index Guide*, Appendix IV, ¶ 138) but a stereoparent is preferred over a nonstereoparent, e.g., D-**Glucose**, polymer with butanedioic acid. For identical heading parents, the choice is determined by (*a*) maximum number of substituents, (*b*) lowest locants of substituents, (*c*) maximum number of occurrences of the index heading parent (in a multiplicative name), (*d*) earliest index position of the index heading. When the choice is dependent on modification terms, it is determined as follows: (*a*) underivatized heading preferred over derivatives cited in the modification; thus, a free acid is preferred over an ester; (changes in format caused by elevation of modification terms into the heading for purposes of subdivision *(CA Index Guide*, Appendix II, ¶ 10B) are ignored in applying this rule; thus **Acetic acid** is preferred over **Acetic acid ethenyl ester);** (*b*) class of derivative in the descending order: anhydride, ester, hydrazide, hydrazone, oxime; (*c*) largest number of (most preferred) derivative; thus, monoester preferred over dioxime preferred over monooxime; (*d*) lowest expressed locants of derivative terms; thus, for **1,2,4-Benzenetricarboxylic acid,** a 1,2-diester is preferred over a 1,4-diester; (*e*) the earliest alphabetical order; thus, "ethyl ester" preferred over "propyl ester."

Examples:

1(*a*) **1-Heptene**
polymer with 1-hexene (preferred index entry)

1(*b*) **1-Hexene**
polymer with 1-heptene (additional *Chemical Substance* and *Formula Index* entry)

2(*a*) **2-Propenoic acid**
butyl ester, polymer with 1-ethenyl-4-methylbenzene and 2,5-furandione (preferred index entry)

2(*b*) **2,5-Furandione**
polymer with butyl 2-propenoate and 1-ethenyl-4-methylbenzene (additional *Chemical Substance* and *Formula Index* entry)

2(*c*) **Benzene, 1-ethenyl-4-methyl-**
polymer with butyl 2-propenoate and 2,5-furandione (additional *Chemical Substance* and *Formula Index* entry)

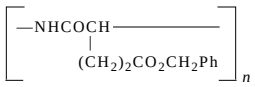
Peptides of established structure are indexed at systematic peptide names such as **Glycine**, **glycylglycyl-** (see *CA Index Guide*, Appendix IV, ¶ 206). Peptides of unknown structure are indexed as polymers.

Example:

$[HO_2CCH(NH_2)(CH_2)_2CO_2CH_2Ph]_n$

L-**Glutamic acid**
5-(phenylmethyl) ester, homopolymer

and the assumed structural repeating unit:



Poly[imino[(2*S*)-1-oxo-2-[3-oxo-3-(phenylmethoxy)propyl]-1,2-ethanediyl]]

When more than one amino acid is present and the sequence is unknown, each amino acid is indexed, and a "polymer with . . ." phrase is cited in the modification.

Alternating, block, and graft polymers are distinguished from random polymers by indexing as copolymers at the monomer names. The term "alternating", "block", or "graft" (or a combination thereof) is cited in a special modification after all other structural information but before descriptive phrases relating to properties, uses, etc. Differentiation between the polymeric substrate and the applied monomer is not made; e.g., whether 1-hexene is grafted on 1-heptene homopolymer or vice versa, the preferred index entry is at **1-Heptene**, polymer with 1-hexene, graft, with an additional entry at **1-Hexene**, polymer with 1-heptene, graft. The term "random" is not employed by *CA* in indexing specific polymers.

Siloxanes prepared by hydrolytic polymerization of chlorosilanes are indexed at the monomer names with the term "hydrolytic" cited in the modification to indicate the essential role of water in forming a polymer chain of -Si-O- units. The term "hydrolytic" is used in addition to the term "homopolymer" or "polymer with".

Example:

Silane, dichlorodimethyl-
polymer with dichlorodiphenylsilane, hydrolytic

Polymers of specific compounds with classes of compounds are indexed at the specific monomers in the *Chemical Substance Index* and at the class name, e.g., **Aldehydes** or **Nitriles,** in the *General Subject Index*.

Example:

1-Hexene, 5-methyl-
polymer with unsatd. nitriles
Nitriles
unsatd.; polymers with 5-methyl-1-hexene

Formaldehyde homopolymers containing only oxymethylene repeating units are indexed only at the heading **Poly(oxymethylene)** in the *Chemical Substance Index*. Commercial and impure polyformaldehydes are indexed at **Polyoxymethylenes** (a plural class heading in the *General Subject Index*) unless author emphasis is centered on **Paraformaldehyde.** Formaldehyde copolymers are indexed as polymers formed from two or more monomers (except **Formaldehyde** copolymers with **Phenol, Urea,** or **1,3,5-Triazine-2,4,6-triamine** which are cross-referred in the *Index Guide*).

Oligomers of definite structure are indexed as specific compounds by the regular principles of index nomenclature. When the precise structure is not known but the number of units is specific, "dimer," "trimer," etc., is expressed in the modification at the name of the monomer. The term "oligomeric" may be cited after "homopolymer" or "polymer with . . ." if this aspect is stressed in the original document.

Telomers with a definite structure are named systematically.

Examples:

$Cl\text{-}(CH_2)_6\text{-}CCl_3$ — **Heptane, 1,1,1,7-tetrachloro-**

$Cl\text{-}(CF_2\text{-}CH_2)_n\text{-}CHCl_2$ — **Poly(1,1-difluoro-1,2-ethanediyl) α-chloro-ω-(dichloromethyl)-**

Telomers of unknown structure are indexed as copolymers with the term "telomer with . . ." cited in the modification.

Example:

1-Hexene
telomer with tetrachloromethane
Methane, tetrachloro-
telomer with 1-hexene

Post-treated polymers are described by modification terms after the polymer has been described.

Examples:

2-Propenoic acid
homopolymer, sodium salt

Benzenamine, 4-ethenyl-
polymer with ethenylbenzene, hydrochloride

2-Propenoic acid, 2-methyl-
decyl ester, homopolymer, hydrolyzed

Poly[1-(4-sulfophenyl)-1,2-ethanediyl]
propyl ester

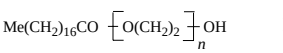
Ethenol (vinyl alcohol) polymers that are indexed at that heading are exceptions (they are prepared by hydrolysis of ethenol ester polymers). Also, acetals of ethenol polymers are entered in the *General Subject Index* at the trivially named class terms **Polyvinyl acetals** and **Polyvinyl butyrals** with a modification, e.g., "chlorobenzals," to indicate the type of acetal when appropriate. Cross-references or additional entries (in the *Chemical Substance Index*) are found at the aldehyde names.

Molecular addition compounds of polymers are indexed in the usual way (*CA Index Guide*, Appendix IV, ¶ 192), e.g., **Ethenesulfonic acid,** homopolymer, compd. with 4-ethenylpyridine homopolymer, with an additional entry for the other component.

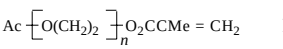
Polyethylene and polypropylene glycols are indexed as specific compounds when the precise structure is reported and not more than ten repeating units are present, e.g., **3,6,9,12,15-Pentaoxaheptadecane-1,17-diol, hexamethyl-** (a cross-reference will be found in the *Index Guide* at **Hexapropylene glycol**). The position of methyl substituents is not assumed; if it is reported, locants are cited. Glycol polymers of eleven units or more are indexed at **Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-**, and **Poly[oxy(methyl-1,2-ethanediyl)], α-hydro-ω-hydroxy-**. The class term **Polyoxyalkylenes** in the *General Subject Index* is used as an additional entry for all specific polyalkylene glycols except when the alkanediyl group is ethanediyl or propanediyl and for cases where the nature of the alkanediyl group is unknown. When it is known, the SRU can be named specifically; thus, **Poly[oxy(2-phenyl-1,3-propanediyl)], α-hydro-ω-hydroxy-**. Polyethylene-polypropylene glycols are named as copolymers: **Oxirane, methyl-**, polymer with oxirane, with an additional *Chemical Substance* and *Formula Index* entry at **Oxirane**.

Esters and ethers of polyalkylene glycols containing not more than ten repeating units are indexed by the regular principles of substitutive nomenclature. For larger polymers, the ester or ether is expressed as a substituent at the SRU-based heading. Mono derivatives are cited in the α-position, with ω-hydroxy at the other terminus. Dissimilar diesters or diethers are expressed in alphabetical order. Ester-ethers have the acyl group assigned to the α-position, and the ether at the ω-end. When appropriate information is lacking, an ester or ether term is cited without locant. When multiplying radicals must be employed, they are given α-locants.

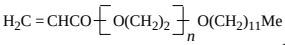
Examples:



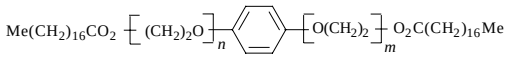
Poly(oxy-1,2-ethanediyl)
α-(1-oxooctadecyl)-ω-hydroxy-



Poly[oxy-1,2-ethanediyl]
α-acetyl-ω-[(2-methyl-1-oxo-2-propenyl)oxy]-



Poly(oxy-1,2-ethanediyl)
α-(1-oxo-2-propenyl)-ω-(dodecyloxy)-



Poly(oxy-1,2-ethanediyl)
α,α′-1,4-phenylenebis[ω-[(1-oxooctadecyl)oxy]-

Polynucleotides (cf. *CA Index Guide*, Appendix IV, Nucleotides, ¶ 210) are indexed as "homopolymer" or "polymer with . . ." at the "-ylic acid" monomers (5′-isomers).

Examples:

5′-Adenylic acid
homopolymer

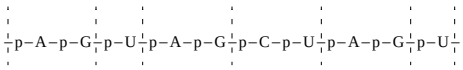
Cytidine, 5′-*O*-phosphonoadenylyl-(3′→5′)-
homopolymer

5′-Guanylic acid
polymer with 5′-adenylic acid and 5′-cytidylic acid (additional *Chemical Substance* and *Formula Index* entries at 5′-**Adenylic acid** and 5′-**Cytidylic acid**

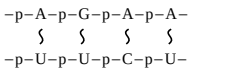
Polynucleotides in which different primary chains are associated intermolecularly by hydrogen bonds are indexed as molecular addition compounds at each component (the modification term "complex" is used in this special case); e.g., **5′-Adenylic acid, homopolymer, complex with 5′-uridylic acid homopolymer (1:1).**

In more complicated cases, a combination of policies is applied.

Examples:



Guanosine, 5′-*O*-phosphonoadenylyl-(3′→5′)- polymer with 5′-cytidylic acid and 5′-uridylic acid (additional *Chemical Substance* and *Formula Index* entries at **5′-Cytidylic acid** and **5′-Uridylic acid)**



5′-Guanylic acid
polymer with 5′-adenylic acid, complex with 5′-uridylic acid, polymer with 5′-cytidylic acid (1:1) (three additional *Chemical Substance* and *Formula Index* entries at the names of the other components)

Trade names are frequently used for polymers and are cross-referred to specific polymers if the components can be structurally defined. If the polymer components are unknown, or only partially known, or cannot structurally be defined, an index citation is made at the trade name and at the appropriate polymer class name.

Natural *rubber* is indexed at the *General Subject Index* heading **Natural rubber** and chlorine-treated rubber at **Chlorinated natural rubber**. When a synthetic rubber is indexed at **Butadiene rubber, Isoprene rubber,** etc., no additional entry will be found in the printed *Chemical Substance Index*, but for studies indexed at **Synthetic rubber, Urethane rubber,** or at **Polysulfide rubber,** information will also be found, when available, at the appropriate printed chemical compound or polymer heading, with "rubber" cited in the index modification.

Examples:

Synthetic rubber
styrene-vinyl bromide
(*General Subject Index* entry)
Benzene, ethenyl-
polymer with bromoethene, rubber
(preferred *Chemical Substance Index* entry)
Ethene, bromo-
polymer with ethenylbenzene, rubber
(additional *Chemical Substance Index* entry)

General subject headings for fibers are presented under the Top Term **Fibers** in *CA Index Guide*, Appendix I. For studies indexed at **Rayon, Acetate fibers,** etc., no additional index entries will be found, but for studies of fibers of specific chemical composition entered at **Polyamide fibers, Synthetic polymeric fibers,** etc., additional information is entered at the appropriate chemical substance name, except where a cross-reference to the fiber class appears.

Example:

Synthetic polymeric fibers
adipic acid-butanediol (*General Subject Index* entry)

Hexanedioic acid
polymer with 1,4-butanediol, fiber (additional *Chemical Substance Index* entries at **1,4-Butanediol** and at the SRU name)

Stereochemistry of polymers is expressed by special modification terms when the necessary information is reported; such terms include isotactic, syndiotactic, threo-diisotactic, erythro-diisotactic, and disyndiotactic. The term "atactic" (for a random configuration) is not employed by *CA* in indexing specific polymers.

In addition to the special terms above, polymer stereochemistry is defined, when appropriate, by the regular descriptors *E, Z, R, and S* (*CA Index Guide*, Appendix IV, ¶ 203 I). For commercial elastomeric polymers, which cannot generally be assumed to be stereochemically homogeneous, terms such as "1,2-configuration," and "cis-1,4-configuration" are included in the descriptive portions of index modifications, but are not made part of the unique preferred *CA* index names.