Polymer Nomenclature and Structure: A Comparison of Systems Used by CAS, IUPAC, MDL, and DuPont. 1. Regular Single-Strand Organic Polymers

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Polymer nomenclature styles and structure representation systems described, recommended, or used by Chemical Abstracts Service (CAS), the International Union of Pure and Applied Chemistry (IUPAC), MDL Information Systems, Inc. (MDL), and DuPont are compared and contrasted. Structure-based versus source-based nomenclature and structural representations are discussed. The types covered in this paper (part 1 of 4) are regular single-strand organic homo- and copolymers. Nomenclature styles and structural representations of end groups are included.

1. INTRODUCTION AND SCOPE

The International Union of Pure and Applied Chemistry (IUPAC) defines a polymer as a substance composed of molecules characterized by the multiple repetition of one or more species of atoms or group of atoms (constitutional units) linked to each other in amounts sufficient to provide a set of properties that do not vary markedly with the addition or removal of one or a few constitutional units.[1]

Real polymers, as synthesized, are seldom structurally perfect. Depending upon the type of polymer, various kinds of structural irregularities may arise.

- Poly(ethylene terephthalate) is likely to contain irregularities known as "ether defect", a colloquial name indicating the presence of some $-O-CH_2-CH_2-O-CH_2-CH_2-O-$ moieties.
- Depending upon polymerization concentration, difunctional acrylic compounds (e.g., ethylene diacrylate) may give polymers that are hyperbranched, hypercross-linked, or both.
- Low-density polyethylene is irregularly branched.
- Polymers formed between simple diamines (e.g., 1,5-pentanediamine) and simple dihalo compounds (e.g., 1,5-dichloropentane) are frequently branched, cross-linked, or both.

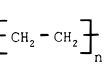
These irregularities, which can have a profound effect upon polymer properties, may vary from polymer batch to batch.

In contrast, polymer structures stored in a database are frequently an ideal or theoretical representation, rather than a true representation of the actual polymer structure.

It is precisely because of different attempts to represent real polymers that different methods of representation have arisen as idealizations of polymers. Probably the most prominent example in polymer literature is polyethylene. Should it be represented as

(a) 

because this is the largest fragment that can be written without repetition,

(b) 

because it is made by opening the double bond in ethylene, or

(c) 

because the structure of the monomer from which it is made is known, whereas the complete structure of the polymer is not known?

Note: in pictorial representations of structural repeating units (SRUs) and polymers in this paper, conventions are as follows: in the CAS, IUPAC, and SCION discussion segments, an SRU is enclosed in brackets with a subscript *n* outside the closing bracket, and a polymer is enclosed in parentheses with a subscript *x* outside the closing parenthesis. CAS online displays showing parentheses or brackets are left unaltered. All MDL structures are depicted with brackets, as shown in the MDL source document.[2]

This example illustrates a fundamental point: a polymer should have a unique, unambiguous structural representation, even if it fails to depict fully the complete structure of the polymer. Failure to follow this seemingly simple rule has resulted in decades of redundant registration of many polymers by different methods, and the dilemma is not likely to be resolved in the near future. If a polymer is represented by more than one structure in a database, it follows that retrieval of one structure may result in others not being retrieved because they were not sought.

In a brief article called "What's in a Name?",[3] Chemical Abstracts Service (CAS) published a spectacular example of redundant registration; the same polymer is documented as being registered with seven different structures and seven different registry numbers. One of these registrations is a structure-based representation, and the other six are source-based representations from different monomers; the representations, and some comments by the author of this paper, are given in Table 1.

Many polymer nomenclature and/or registration systems exist; three of the most prominent are those recommended or used by CAS, IUPAC, and MDL. Others include

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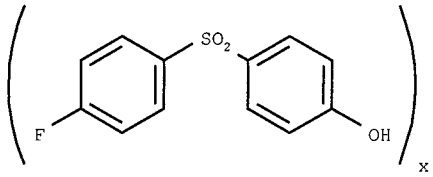
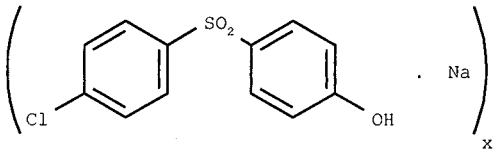
Table 1. Summary of Polymers Presented under the Title "What's in a Name?"[3]

CAS Registry Numbers and structures (examples 1-6 are source-based; example 7 is structure-basec
Note that the graphic representations shown are **not** necessarily identical with CAS online displays):

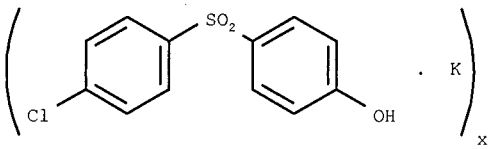
[1] RN 52661-08-2 REGISTRY
CN Phenol, 4-[(4-fluorophenyl)sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)
:
MF (C12 H9 F O3 S)x
:



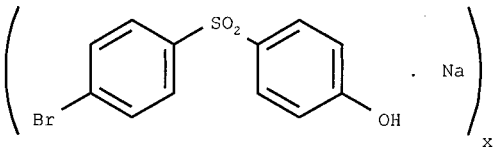
[2] RN 36313-65-2 REGISTRY
CN Phenol, 4-[(4-chlorophenyl)sulfonyl]-, sodium salt, homopolymer (9CI) (CA INDEX NAME)
:
MF (C12 H9 Cl O3 S . Na)x
:



[3] RN 36313-64-1 REGISTRY
CN Phenol, 4-[(4-chlorophenyl)sulfonyl]-, potassium salt, homopolymer (9CI) (CA INDEX NAME)
:
MF (C12 H9 Cl O3 S . K)x
:

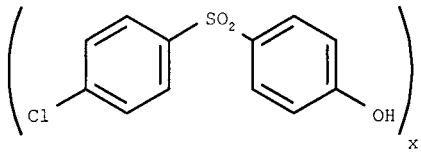


[4] RN 30706-34-4 REGISTRY
CN Phenol, p-[(p-bromophenyl)sulfonyl]-, sodium salt, polymers (8CI) (CA INDEX NAME)
MF (C12 H9 Br O3 S . Na)x
:

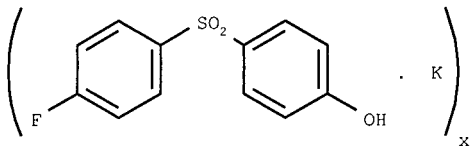


[5] RN 27400-52-8 REGISTRY
CN Phenol, 4-[(4-chlorophenyl)sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)
:
MF (C12 H9 Cl O3 S)x
:

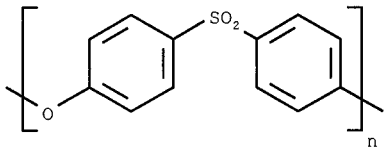
Table 1 (Continued)



[6] RN 26220-27-9 REGISTRY
CN Phenol, 4-[(4-fluorophenyl)sulfonyl]-, potassium salt, homopolymer (9CI) (CA INDEX NAME)
:
MF (C12 H9 F O3 S . K)x
:



[7] RN 25667-42-9 REGISTRY
CN Poly(oxy-1,4-phenylenesulfonyl-1,4-phenylene) (9CI) (CA INDEX NAME)
:
MF (C12 H8 O3 S)n
:



[a] *Author's comments:* It is the policy of Chemical Abstracts to provide polymer access to users either in terms of the monomer(s) or the SRU because different users have different interests and needs.[20] This policy conflicts strongly with SCION rules, which state that a polymer must have one, ***and only one***, structural representation. (SCION is a proprietary database.) It is SCION policy that: (1) polyethers (see Table 3) and polysulfones (and therefore polyethersulfones) shall be structured ***only*** as SRUs and ***never*** as source-based polymers; and (2) a polymer shall ***never*** be structured in SCION as both structure-based and source-based. This is why, with regard to the polymers in this table, the author of this paper reacts so strongly to CAS's representation of what is essentially the same polymer by seven different representations; cross-referrencing at the polymer level is long overdue and would be a most welcome addition to File Registry. The practical solution offered[20] to resolve this situation is to provide links between the registrations.

Derwent, which has a system that operates by means of polymer fragmentation codes; Information for Industry (IFI)/ Plenum; the Rubber and Plastics Association of Great Britain (RAPRA); the German Plastics Institute (DKI); polymer modeling systems; and proprietary storage and retrieval systems operated by private companies, e.g., Dow, DuPont, Eastman, and Kodak.

In a previous publication,[4] Herz compared polymer searching in different databases—CAS, Derwent, IFI/Plenum, RAPRA, and DKI.

In this comparison, which will be published in four parts, the polymer nomenclature styles and structural representations described, recommended, or used by CAS, IUPAC, MDL, and SCION, a DuPont proprietary database, are presented, compared, and contrasted. Each of the systems described seeks to represent as accurately as possible the polymers of the real world. Comments are made on the naming by CAS or organic esters, some of which are used as polymer intermediates.

Within each section of the four parts the four systems—CAS, IUPAC, MDL, and SCION—are discussed strictly in alphabetical order. The paper does not attempt to provide a comprehensive guide to polymer nomenclature, exhaustive analyses of all four systems, or descriptions of how to register and/or search polymers in them. The broad concepts are covered, and references are given as pointers to more detailed descriptions. Both structure-based and source-based nomenclature are discussed.

The four parts cover 11 sections. Part 1 (sections 1 through 5) covers single-strand organic homopolymers and copolymers. Part 2 (sections 6.1 through 6.3) will cover some irregular single-strand organic polymers: aftertreated (posttreated); alternating and other periodic; and block. Part 3 (sections 6.4 through 6.6) will cover more irregular single-strand organic polymers: comb and graft; cross-linked; and dendritic, hyperconnected (i.e., hyperbranched and/or hypercross-linked), and star polymers. Part 4 (sections 7 through 11) will cover stereochemistry in polymers, regular and quasi-single-strand inorganic and coordination polymers, regular double-strand (ladder and spiro) organic polymers, polysiloxanes, and oligomers and telomers. Only synthetic polymers are discussed, and the following are excluded: macrocycles (such as catenanes and knots), natural polymers, polymer aggregates, polymer blends (alloys), micronetworks, rotaxanes, and interpenetrating and semi-interpenetrating networks.

Table 2. Glossary of Acronyms and Terms

acronym or term	name or explanation	source(s)
ASM	"Actual starting material" (polymer type)	SCION
configuration of SMUs and mers	An SMU Sgroup has no crossing bonds because the connectivity of the Sgroup is unknown. SMU configuration can be specified as hh, ht, or eu. The configuration of a mer is always eu	MDL
configuration of SRUs	The configuration of the SRU with respect to the next SRU in sequence can be head-to-tail (ht), head-to-head (hh), or either-unknown (eu)	MDL
connectivity	A crossing bond implies that the connectivity (the chemical bond connecting the SRU to another SRU in the polymer) is known	MDL
crossing bond	Bond connecting an atom inside an Sgroup to an atom outside the same Sgroup; generally crosses an Sgroup bracket	MDL
CRU	constitutional repeating unit	IUPAC
mer	a group that cannot (or does not in the situation in which the word is seen) repeat adjacent to itself	MDL
mon	monomer; a group that can (or does in the situation in which the word is seen) repeat adjacent to itself	MDL
PMC	"prescribed monomer condensation" (polymer type)	SCION
SMU	source materials unit	MDL
Sgroup	collection of structural fragments that defines the repeating unit of a polymer	MDL
SRU	structural repeating unit	CAS, MDL, SCION

2. POLYMER NOMENCLATURE AND STRUCTURE REPRESENTATION SYSTEMS

On the assumption that the names and/or structures of chemical substances that were used to prepare a polymer are known, almost every synthetic polymer can be represented by a source-based name and/or structure. For some polymers, a name that indicates the actual repeating unit, together with a structural representation that depicts the precise atom sequence in the polymer, may be preferable to a name and molecular expression based on names and/or structures of monomers used to form the polymer.

For polymers that can be registered both by component monomers (i.e., source-based representation) and by repeating unit (i.e., structure-based representation), the relative merits of these two formats for nomenclature and graphic representation are discussed endlessly, and the debate may never be resolved.

CAS has developed comprehensive sets of nomenclature rules and structure conventions that, in spite of their irregularities, exceptions, and duplications (i.e., naming polymers by both source-based and structure-based methods), have become standards in the world of chemical literature. CAS maintains an online chemical file, called File Registry, that is remotely searchable via the Scientific and Technical Network (STN) system in Columbus, OH. Anyone with an STN account and a computer equipped with the necessary hardware and software may access the registry file. As of November, 1996, File Registry contains names and structures for over 15.6 million substances, of which approximately 687 000 are polymers; nearly 600 000 of these have structure records.

IUPAC is an international consortium comprised of professional scientists who propose and recommend standards for chemical nomenclature and structure representation.

MDL is a computer software company that offers for sale computer programs and systems such as MACCS, REACCS, and ISIS; these are suitable for either mainframe or personal computers, and many companies use them to create databases containing polymers, pharmaceuticals, agricultural chemicals, etc. Some computer programs are for chemical structures only, while others are for text data only. ISIS is a computer program that enables users to combine chemical structures from one file with text data from another to produce an integrated product. MDL names some polymer examples,[2] but offers no polymer nomenclature rules or recommendations, and users of their software are free to use polymer nomenclature rules of their own choice.

SCION is a proprietary database that is maintained in Columbus, OH by CAS exclusively for DuPont. For searching, SCION uses CAS Messenger software. DuPont's polymer nomenclature and structure conventions are based partly on the nomenclature rules and structure conventions of CAS and partly on DuPont Company internal rules. A polymer is registered only once; dual registration (structure-based *and* source-based) is prohibited. Whenever possible (see point 2.1), except for the categories that are *always* structured as source-based (see point 2.2), each polymer is registered and named on the basis of its SRU. New nomenclature and structure rules are devised for new polymer types as they are reported.[5−11]

Point 2.1: Exceptions are asymmetrical SRUs with odd numbers of crossing bonds (see Table 2) that have to be registered as source-based because of CAS Registry System limitations.

Point 2.2: The following are *always* registered as source based, even when structure-based representation is possible: (i) condensation types (polyamides, polyesters, polyimides, polyurethanes, and combinations of these); (ii) carbon−carbon multiple-bond types (acetylenic, acrylic, ethylenic, and vinyl); (iii) polymers for which no representative structure can be drawn (e.g., those from formaldehyde, melamine, phenol, urea, etc.).

CAS, IUPAC, and MDL polymer examples given are taken from the published literature; SCION polymer examples given are theoretical and may or may not have been reduced to practice.

3. NOMENCLATURE STYLES

The four different systems—CAS, IUPAC, MDL, and SCION—use different polymer nomenclature styles and rules. Polymer names in this paper that are taken from literature references are given in the style of the original reference. For example, CAS[12a] uses 1,3-butadiene, homopolymer; IUPAC[13,14,15] uses polybutadiene, poly(but-1-ene-1,4-diyl), 1,4-polybutadiene, or poly(buta-1,3-diene); MDL[2] uses polybutadiene; and SCION[16] uses POLY-1,3-BUTADIENE (see point 3.1).

Point 3.1: By SCION polymer nomenclature rules, noncondensation type polymer names begin "POLY-..." not "POLY(...". Polymer names are always capitalized.

3.1. CAS Ninth Collective Index versus Earlier Collective Indexes. In spite of the sweeping changes made by CAS with their introduction in 1972 of the Ninth Collective Index (9CI) nomenclature rules, many scientists still use monomer and polymer names from earlier Collective Index periods, especially the Seventh (1962−1966) and Eighth (1967−1971) (8CI). Thus the monomer MMA, which has the formal CAS 9CI index name "2-propenoic acid, 2-methyl-, methyl ester", is still frequently called by its 8CI index name "methacrylic acid, methyl ester" or the common synonym "methyl methacrylate". Even in the 1990s, IUPAC publications still largely use pre-9CI names, e.g., styrene vice ethenylbenzene.

3.2. Inversion versus "National-Language" for Chemical Names. A key difference between CAS and IUPAC nomenclature philosophy is that CAS inverts names for indexing purposes, whereas IUPAC does not. Thus PABA has the CAS index name "benzoic acid, 4-amino-", whereas IUPAC names it "*p*-aminobenzoic acid". IUPAC now prefers numerals,[17] but continues to permit use of "*o*-", "*m*-", and "*p*-" for disubstituted benzene derivatives. Comprehensive texts are available for current CAS and IUPAC nomenclature.[12,17]

Chemical names cited in this comparison are a mixture of Eighth and Ninth Collective Index names, and some are inverted while others are not. Various name styles are used deliberately to illustrate points of similarity and difference in nomenclature. CAS's polybutadiene vs SCION's POLY-1,3-BUTADIENE, the example given above, illustrates this.

3.3. Esters from "Class I" versus "Class II" Acids and Alcohols. The nomenclature of esters is discussed in some detail because it inevitably affects polymer nomenclature. On the argument that it makes names of certain esters easier to find, CAS modifies the usual name-index rules.[12b] The chemical functionality precedence of certain very common acids, called "Class I" acids, is disregarded for the purposes of naming their esters unless the alcohol from which the ester is formed is also "Class I" (i.e., very common); in this case the substances are indexed at the name of the uncommon ("Class II") alcohol, despite its lower functionality. Thus, "common acid" esterified with "common alcohol" is named "common acid, commonyl ester"; "exotic acid" esterified with "common alcohol" is named "exotic acid, commonyl ester"; and "exotic acid" esterified with "exotic alcohol" is named "exotic acid, exoticyl ester". However, "common acid" esterified with "exotic alcohol" is named "exotic alcohol, commonate". While this rule has some merit, it flies in the face of consistent nomenclature and it is hard to apply because it is unrealistic of CAS to expect end-users to remember lists of "Class I" acids and "Class I" alcohols and to do the necessary mental gymnastics every time they wish to locate esters by name. One rule that names all esters in the same way would greatly facilitate their location by index name.

Neither IUPAC nor SCION nomenclature follows these rules. In SCION, all esters are named in the uniform style "ACID, ALCOHOLIC ESTER". Common synonyms are frequently added to substance text records, e.g., ETHYL ACETATE for ACETIC ACID, ETHYL ESTER. Examples 3.3.1 through 3.3.4 illustrate the method.

Example 3.3.1. Class I acid + class I alcohol

8CI CAS name	SCION name
Acetic acid, ethyl ester	ACETIC ACID, ETHYL ESTER

Example 3.3.2. Class II acid + class I alcohol

8CI CAS name	SCION name
Arachidonic acid, methyl ester	ARACHIDONIC ACID, METHYL ESTER

Example 3.3.3. Class I acid + class II alcohol

8CI CAS name	SCION name
Silanol, trimethyl-, acetate	ACETIC ACID, TRIMETHYLSILYL ESTER

Example 3.3.4. Class II acid + class II alcohol

8CI CAS name	SCION name
Arachidonic acid, cholesteryl ester	ARACHIDONIC ACID, CHOLESTERYL ESTER

Note on example 3.3.1: The CAS examples used here are strictly 8CI. Beginning with the 9CI in 1972, CAS nomenclature became more systematic than it was in the Eighth; however, the CAS policy of naming esters based on a classification of Class I and Class II acids and alcohols was not changed.

4. NOMENCLATURE AND GRAPHIC REPRESENTATION OF REGULAR, SINGLE-STRAND, ORGANIC HOMOPOLYMERS

This section deals with structure-based and source-based representations of single-strand, organic homopolymers. The word "regular" in the heading is used by the author to mean "ordinary", random, or statistical copolymers, *expressed by either source-based or structure-based names*, with no special attributes such as "non-polymeric spacer groups" (also called "junction units"). This differs from the IUPAC definition of a "regular" polymer as "a polymer whose molecules can be described by only one species of constitutional unit in a sequential arrangement";[1] this definition covers homopolymers and copolymers, but only in the context of their structural representations, because CAS and IUPAC source-based names cannot reflect that kind of "regularity".[18]

Structure-based homopolymers are represented by a repeat unit called a constitutional repeating unit (CRU) or structural repeating unit (SRU). IUPAC prefers CRU; CAS, MDL, and SCION prefer SRU. In this paper, SRU is used as the abbreviation for a constitutional or structural repeating unit. The basics of SRU homopolymers are dealt with in some detail. A comparison of CAS, IUPAC, MDL, and SCION structural representations of these polymer types is made.

Source-based homopolymers are represented by the monomer or monomers that form the polymer.

End groups are discussed for both structure-based and source-based homopolymers.

Table 3. Summary of Classification of Some Linear, Single-Strand Polymer Types by CAS, IUPAC, and SCION, Structure-Based (SRU) versus Source-Based (non-SRU) Format

	structured as SRU by:		
polymer type	CAS	IUPAC	SCION
acrylic/methacrylic	NO[a]	YES	NO
anhydride, e.g., −[−O−CO−CO−]$_n$−	YES	YES	YES
carbonate, e.g., −[−O−CO−O−CH_2−CH_2−]$_n$−	YES	YES	NO
ether, e.g., −[−O−CH_2−CH_2−]$_n$−	YES	YES	YES
Ethylenic	NO[a]	YES	NO
sulfide, e.g., −[−S−C_2H_4−]$_n$−	YES	YES	YES
urea, e.g., −[−NH−CO−NH−CH_2−CH_2−]$_n$−	YES	YES	NO
1-component condensation[b]	YES	YES	NO
2-component condensation[b]	YES	YES	NO

[a] ACS presented the concept of structure-based acrylic, methacrylic, and ethylenic polymer names in a 1968 publication,[19] but CAS currently uses source-based nomenclature to index these types. However, in addition to monomer-based entries, structure-based names are cited for polymers whose SRUs are well-documented or can confidently be assumed.[12a] [b] Condensation is here defined as polyamic acid, polyamide, polyester, polyimide, polyurethane, or combinations of these basic types, e.g., polyamide-ester (also called polyesteramide).

MDL offers no nomenclature rules; users of computer programs such as the MACCS-II Substance Module may structure polymers in a variety of ways.[2]

4.1. General Approach: Structure-Based versus Source-Based Approach to Nomenclature and Representation. 4.1.1. Structure-Based Method. For structure-based representations, CAS, IUPAC, and SCION all approach the structuring and nomenclature of SRU homopolymers in the same fundamental manner:

STEP 1. The atom sequence that defines the SRU is identified.

STEP 2. The "head" atom or senior bivalent radical of the sequence is defined.

STEP 3. The SRU is oriented, i.e., a decision is made on which way to proceed along the atom sequence.

STEP 4. The SRU is named.

However, there are major differences in the polymer types classified as SRU by CAS and IUPAC versus types classified as SRU by SCION.[12,13,16,19] These are summarized in Table 3.

4.1.2. Source-Based Method. For source-based representations, CAS and SCION both approach the structuring of homopolymers in the same manner.

polymer structure: $(A)_x$

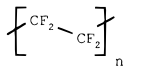
where A is a monomer, or

polymer structure: $(A.B)_x$

where A and B are monomers such that neither on its own can represent a polymer. However, CAS and SCION use different nomenclature for homopolymers; examples of these are given below in the sections on CAS and SCION.

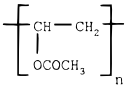
IUPAC makes no formal recommendations for source-based, one-component homopolymer nomenclature or structural representation. However, semisystematic or trivial names for many common polymers are approved for use in scientific work—see examples 4.1.2.1 and 4.1.2.2.

Example 4.1.2.1. IUPAC source-based semisystematic name for poly(difluoromethylene)



poly(tetrafluoroethylene)

Example 4.1.2.2. IUPAC source-based homopolymer name



poly(vinyl acetate)

4.2. CAS and IUPAC Structure-Based Nomenclature and Structure Representations. These two systems are discussed together because they are very similar in overall concept.

4.2.1. The Method. STEP 1 (identifying the atom sequence of the SRU): at least two complete sequences of the SRU are drawn.

STEP 2 (defining the "head" atom or senior bivalent radical): CAS and IUPAC follow the same set of rules. The SRU subunit seniority is (1) heterocyclic rings, (2) heteroatoms in chains, (3) carbocyclic rings, and (4) carbon chains. For SRUs with two or more dissimilar heterocyclic rings, further rules are defined for choosing the most senior heterocyclic ring. For example, a nitrogen-containing heterocycle is senior to a heterocycle containing any other heteroatom. For situations where a heteroatom in the chain is the SRU head atom, the most senior atom is O, followed in order by S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, etc.[12a,13]

STEP 3 (SRU orientation): CAS and IUPAC both currently use the principles, in turn, of maximum number, lowest locants, and earliest alphabetical order of substituents.[12a,13]

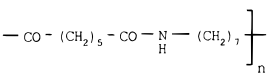
Example 4.2.1.1. Consider the sequence −O−CHF−CH_2−O−CHF−CH_2−: −[−O−CHF−CH_2−]$_n$− is preferred to −[−O−CH_2−CHF−]$_n$−, because in the first SRU the fluorine atom has a lower locant (1- versus 2-)

CAS and IUPAC both use the rule that the shortest path (smallest number of atoms) is taken from the most preferred multivalent radical to the next preferred radical, and so on.[12a,13] When two or more paths between the two heteroatoms are of equal length, the most highly substituted one, or the one with earliest substitution, takes precedence. Two examples illustrate these rules.

Example 4.2.1.2. Nylon-77, −[−NH−CO−$(CH_2)_5$−CO−NH−$(CH_2)_7$−]$_n$−: [CAS RN 32473-30-6]

The nitrogen atoms are equidistant by either path, i.e., NH−CO−$(CH_2)_5$−CO−NH versus NH−$(CH_2)_7$−NH.

The preferred path between the two N heteroatoms is via the two carbonyl groups. The current CAS structure-based name for nylon-77 is poly[imino(1,7-dioxo-1,7-heptanediyl)-imino-1,7-heptanediyl].



poly[imino(1,7-dioxo-1,7-heptanediyl)imino-1,7-heptanediyl]

Earlier records were less rigorous; thus, the 8CI index contains two SRU names:

poly(iminoheptamethyleneiminopimeloyl)

poly(iminopimeloyliminoheptamethylene)

It is therefore prudent to consider all possibilities when searching for SRUs by name in earlier indexes.

Example 4.2.1.3. Consider the 12-backbone-atom SRU sequence:

```
   -O-C-O-C-NH-C-C-S-C-NH-C-C-O-C-O-C-NH-C-C-S-C-NH-C-C-
Row A              ...8 7 6   5 4 3 2 1
Row B                         1 2 3 4 5   6 7 8...
```

Determination of the head atom, and subunit citation order, is as follows: O is senior to S, and S is senior to N; therefore, one of the two oxygen atoms must be the head atom. The SRU must therefore be either row A, atoms 1 to 12, or row B, atoms 1 to 12. The row A sequence places the N atom in position 6, whereas the row B sequence places it in position 5; the latter is therefore correct, and the final SRU is −[−O−C−O−C−NH−C−C−S−C−NH−C−C−]$_n$−.

STEP 4 (naming the SRU): CAS currently uses its own 9CI nomenclature rules;[12a] there have been a few minor changes in collective indexes following the 9th CI. Printed copies of Chemical Abstracts, of course, have polymer names in the nomenclature system in force at the time of printing. CAS selects one name as the index name and adds as many synonyms as necessary to facilitate polymer retrieval by name. The permutations of the index name are provided as additional access points in the printed index and may not be of great value for online retrieval.[20] Example 4.2.1.4 shows the text segment of the CAS online record for −[−O−CH_2−CH_2−CH_2−]$_n$−.

Example 4.2.1.4.

```
REGISTRY COPYRIGHT 1995 ACS
RN 26913-43-9 REGISTRY
CN Poly(oxy-1,4-butanediyl) (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Poly(n-butylene oxide)
MF (C4 H8 O)n
CI PMS
PCT Polyether
:
```

Note on example 4.2.1.4: In this and other CAS examples in this paper, the original CAS online display, as captured by a text-type terminal, is neatened to save space; additional data not pertinent to the discussion and omitted from the original display are indicated by colons.

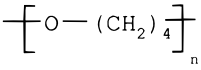
In 1976, IUPAC recommended structure-based names to accompany structure-based pictorial representations of polymers, e.g., poly(1-phenylethylene) for polystyrene.[13] However, the commission recognized that many common polymers have trivial or semisystematic names and acknowledged that these were unlikely to be displaced by structure-based names.

As part of a lengthy 1952 publication on linear high polymers, IUPAC introduced the "-amer" structure-based nomenclature system.[21] For example, names such as polymethamer, polyethoxamer, and polyphenyleneamer-4 were proposed for polyethylene, poly(oxyethylene), and poly(*p*-phenylene), respectively. The system was apparently neither liked nor accepted, for it has disappeared from use. Other IUPAC publications use a variety of styles when citing polymer names. Even as late as 1994, semisystematic or trivial names such as polystyrene and poly(methyl methacrylate) are used in publications;[22] however, these are allowed only for source-based names.[22,23]

4.2.2. CAS SRU Graphic Representations. CAS File Registry graphic representations for polymers may be retrieved with text-type terminals or terminals having graphic capabilities, e.g., by use of STN Express. With text-type terminals, the image for poly(oxytetramethylene) [RN 26913-43-9], for example, appears thus:

```
...                                  ..
.          O   (CH2)4                .
.  .....................  .....     .
...                                  .. n
```

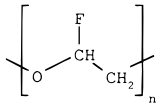
With terminals having graphic capabilities, the image appears thus:



The rigorous rules for structure representation used by CAS ensure that computer storage of only one structure occurs for a given SRU. The CAS Registry System has duplicate-structure detection, which means that an existing structure cannot be reregistered with a second registry number. Thus, poly(oxyethylene) is allowed to be registered only as −[−O−CH_2−CH_2−]$_n$−, and registration of −[−CH_2−O−CH_2−]$_n$− is forbidden. Were −[−CH_2−O−CH_2−]$_n$− to be submitted for registration, it would be "perceived" (by the computer) as a separate substance and not as a duplicate of −[−O−CH_2−CH_2−]$_n$−. The third structure, −[−CH_2−CH_2−O−]$_n$−, is accepted by the computer for registration, but it is "perceived" as being the same as −[−O−CH_2−CH_2−]$_n$−. A substructure search for −[−CH_2−O−CH_2−]$_n$− fails to retrieve −[−O−CH_2−CH_2−]$_n$−; searchers are taught that they must search specifically for oxygen on the left. However, a substructure search for −[−CH_2−CH_2−O−]$_n$− would retrieve −[−O−CH_2−CH_2−]$_n$−.[24]

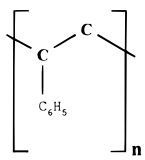
4.2.3. IUPAC SRU Graphic Representations. As stated earlier, IUPAC publishes recommendations for polymer names and structures but does not, per se, register polymers. The latest IUPAC recommendations[15] for structural or graphic representations of polymers (on paper or in a computer) are not in agreement with earlier recommendations.[13] The highly detailed description of derivation of the SRU for poly[oxy(1-fluoroethylene)][13] states that, of all the possibilities, the preferred graphical representation is as shown in example 4.2.3.1.

Example 4.2.3.1. IUPAC preferred representation for −[−O−CHF−CH_2−]$_n$−

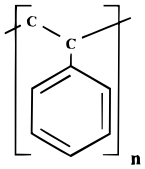


In contrast, polystyrene[15] is represented by the structures shown as examples 4.2.3.2, 4.2.3.3, or 4.2.3.4.

Example 4.2.3.2.



Example 4.2.3.3.



Example 4.2.3.4.

-[-CH(C$_6$H$_5$)-CH$_2$-]$_n$-

The structure of example 4.2.3.3 is in conflict with IUPAC's earlier recommendations. Furthermore, typical computer chemical database registration, e.g., in MACCS, of left- and right-handed versions (example 4.2.3.3 and its mirror image) would both be accepted, although intellectually one is a duplicate of the other. This could lead to multiple records being kept in a computer database for any polymer where more than one representation is possible for the same structure. If this situation leads to retrieval of only one specific structure at search, an unsatisfactory situation will exist because other structures for the same polymer will not be retrieved. Unless a computer program has a "duplicate detection at registration" feature, this situation places burdens on either structure-input personnel or searchers to check for possible duplicates. Therefore, IUPAC's latest recommendations[15] should be treated with caution in connection with creation of a chemical structure database.

4.3. CAS and IUPAC Source-Based Nomenclature and Structure Representations. As stated above, IUPAC makes no recommendations on source-based representation of one-component homopolymers. An earlier paper[25] states that CAS names homopolymers by citing the inverted name of the monomer and adding an appropriate descriptor. This is shown in examples 4.3.1 and 4.3.2 (corresponding 9CI names are given beneath each earlier name):

Example 4.3.1. undecanoic acid, 11-amino-, polyamides [25587-80-8] 8CI
undecanoic acid, 11-amino-, polymers [25587-80-8] 8CI
undecanoic acid, 11-amino-, homopolymer [25587-80-8] 9CI

Example 4.3.2. benzoic acid, p-hydroxy-, polyesters [30729-36-3] 8CI
benzoic acid, 4-hydroxy-, homopolymer [30729-36-3] 9CI

The CAS 1994 Index Guide[12a] states that 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 an SRU. Therefore, a comprehensive search for a polymer must include both source-based and structure-based formats.

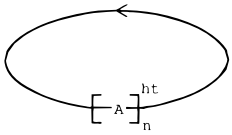
4.4. MDL Graphic Representations. 4.4.1. Structure-Based Method. MDL offers no rules for the identification, orientation, and naming of SRUs.[2] MDL offers a computer program called the MACCS-II Substance Module for consistent representation of polymers for database registration and searching. As part of this computer program, "polymer Sgroups" are used to represent structures of polymers. A polymer Sgroup is a collection of structural fragments that defines the repeating unit of a polymer.

For homopolymers, the Sgroup $-[-A-]-_n$ provides the means to represent the structure unambiguously; this represents the polymer ...AAAAAAAA... . This is an SRU Sgroup in which one or more molecular fragments, connected to form a single structure (the backbone or main chain), define the repeating unit of the homopolymer. The repeating unit is enclosed by two brackets; to the right of the closing bracket is a subscript *n*. Bonds cross the brackets and show how the repeating units connect to each other within the polymer (connectivity). Labels are attached to the brackets to show the orientation of the repeating units toward each other within the polymer (configuration).

A crossing bond connects an atom inside an Sgroup to an atom outside the same Sgroup, and generally crosses a bracket of the Sgroup. A crossing bond implies that the connectivity (the chemical bond connecting the SRU to another SRU in the polymer) is known. The configuration of the SRU with respect to the next SRU in sequence can be head-to-tail (ht), head-to-head (hh), or either-unknown (eu).

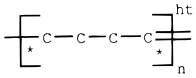
The crossing bonds of a head-to-tail SRU imply that the SRU (A) in example 4.4.1.1 can connect to an identical SRU if such a bond is chemically feasible; that is, crossing bonds indicate that ...AAAAAA... is possible. This is conveniently vizualized as a cyclization of the crossing bonds.

Example 4.4.1.1.



Mismatched crossing bonds can only be hh. Nonidentical bond types on crossing bonds are allowed only if the configuration is hh, i.e., the configuration cannot be eu—see example 4.4.1.2.

Example 4.4.1.2. (the two bonds marked with asterisks are mismatched bond types)



It is a key feature of MDL, e.g. in a MACCS structure database, that critical orientation of an SRU is not required; this is in sharp contrast to CAS rules. Thus, the poly(oxyethylene) SRU may be represented by any of the structures shown as examples 4.4.1.3, 4.4.1.4, and 4.4.1.5.

Example 4.4.1.3. -[-O-CH$_2$-CH$_2$-]$_n$-

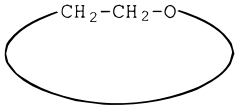
Example 4.4.1.4. -[-CH$_2$-O-CH$_2$-]$_n$-

Example 4.4.1.5. -[-CH$_2$-CH$_2$-O-]$_n$-

On the assumption that all three are registered, a "flexmatch" search for any one of these retrieves all three. A "duplicate detection" step at registration is optional, but the structures shown as examples 4.4.1.3, 4.4.1.4, and 4.4.1.5 could still all be registered, because they are not "perceived" as duplicates during registration.

The "flexmatch" search works on the principle that the computer "cyclizes" each of these three structures by means of an invisible bond; thus, the structures shown as examples 4.4.1.3, 4.4.1.4, and 4.4.1.5 all "look" like the structure of example 4.4.1.6.

Example 4.4.1.6.



In effect, structures 4.4.1.3, 4.4.1.4, and 4.4.1.5 are all "phase-shift" versions of one another.

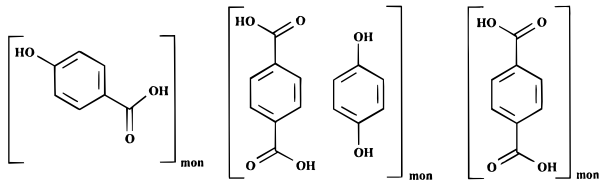
4.4.2. Source-Based Method. With regard to the configuration of source materials units (SMUs) and mers (see Glossary, Table 2), MDL states that an SMU has no crossing bonds because the connectivity of the Sgroup is unknown. However, the configuration of the SMU can be specified as hh, ht, or eu. The configuration of a mer is always eu.

Thus, polyA is represented as:

$[A]_{mon}$

Because an SMU Sgroup represents a polymer, all the functional groups necessary to produce the polymer should be present in the Sgroup. Thus, only substances that are capable of forming homopolymers of the required type should be used in SMU Sgroups. Examples 4.4.2.1 and 4.4.2.2 represent polyesters in the SMU Sgroup form; example 4.4.2.3 is the SMU representation of a polyanhydride.

Example 4.4.2.1. Example 4.4.2.2. Example 4.4.2.3.

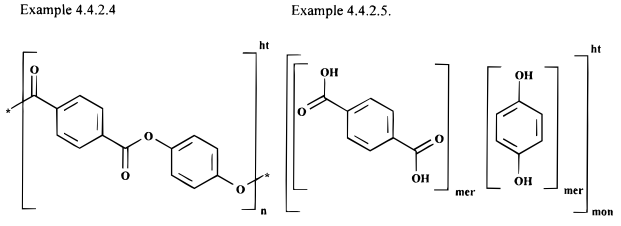


The representation in example 4.4.2.2 is useful in two contexts: during searching, to find addition or certain types of condensation homopolymers, represented as either multifragment SMU Sgroups (as shown in example 4.4.2.2) or their corresponding SRUs (as represented in example 4.4.2.4); at registration, to represent a polymer when the source chemicals are known but the connectivity is unknown or potentially complex.

The SMU anhydride representation (example 4.4.2.3) is source-based. (CAS registers polyanhydrides by both source-based and structure-based methods; SCION uses only the structure-based method.)

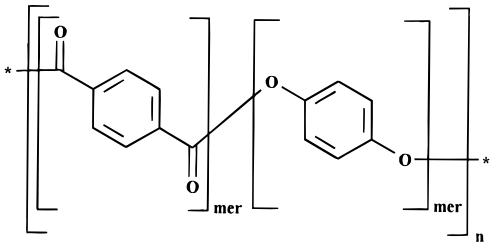
Example 4.4.2.5 shows an alternative, generally applicable way to represent the polymer of example 4.4.2.2.

Example 4.4.2.4 Example 4.4.2.5.



Example 4.4.2.5 represents a polyester as an SMU Sgroup with the two fragments of example 4.4.2.2 as complementary Sgroups. Example 4.4.2.6 shows the same polymer with an SRU representation; mer Sgroups are used to delineate the two fragments comprising the SRU.

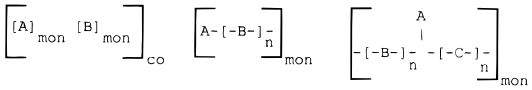
Example 4.4.2.6.



The capability of the MACCS-II "flexmatch" search tool is such that, on the assumption that both representations are in a file, a search for either the SMU or the SRU will find both structure 4.4.2.5 (SMU) and 4.4.2.6 (SRU). This is a distinct advantage over CAS's Messenger software search capabilities; with Messenger software, SMU and SRU representations are fundamentally different, and currently a search for one will not retrieve the other.

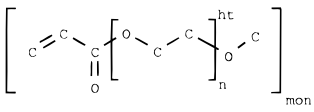
The value of the mer Sgroup is that it immediately signals that homopolymerization is precluded, even though the molecule or fragment defining the mer might be homopolymerizable under other conditions.

On the subject of nesting homopolymers, MDL states that nesting SMU Sgroups is allowed only if the sibling Sgroups are not on the "backbone" of the parent Sgroup, otherwise the parent Sgroup must be a copolymer. The following representations are permissable:



The first of these three examples is clearly a copolymer; whether the other two are homopolymers or copolymers is a moot point. Examples of SMU homopolymers:[2]

$[\,CH_2{=}CH\text{-}Ph\,]_{mon}$ polystyrene



homopolymer of an oligomer (homopolymerized macromonomer)

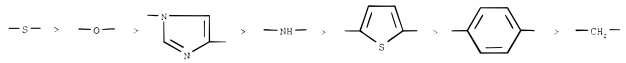
4.5. SCION Nomenclature and Structure Representation. 4.5.1. Structure-Based Method. SCION rules for identifying and orienting SRUs are appreciably different from those of CAS and IUPAC; nomenclature rules generally follow those of CAS 8CI, but they are used to name the SRU as defined by SCION rules.

STEP 1 (identifying the atom sequence of the SRU): At least two complete sequences of the SRU are drawn.

STEP 2 (defining the "head" atom): An exhaustive set of rules,[5a] the presentation of which is outside the scope of this paper, is used to determine SRU subunit seniority. Briefly, because (a) ring bonds cannot be broken in order to draw the SRU and (b) seniority is determined by the atomic numbers and environment of individual atoms, seniority usually works out as follows: (1) heterocyclic rings in which the heteroatom is also connected to at least one other backbone atom by an open-chain (nonring) bond; (2) heteroatoms in chains; (3) heterocyclic rings in which the heteroatom is not also connected to at least one other backbone atom by an open-chain (nonring) bond; (4) carbocyclic rings; (5) carbon chains (see point 4.5.1.1). For

SRUs with two or more dissimilar heterocyclic rings, there are further rules for choosing the senior heterocyclic ring. For situations where a heteroatom in the chain is the SRU head atom, the heteroatom with the highest atomic number is chosen. Thus, the most senior atom is Bi, followed in order by Pb, Hg, Te, Sb, Sn, Se, As, Ge, S, P, Si, O, N, B, etc.

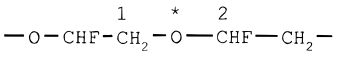
Point 4.5.1.1: SCION seniority examples (> means "is senior to").



STEP 3 (SRU orientation): SCION rules are based on the principle: "move in the direction of the heaviest/most crowded environment"; this means that the SRU citation direction is determined by, in order, the highest atomic number of an atom, and how many there are. This results in some SRUs having structures identical with those derived by CAS and IUPAC rules, but for different reasons, whereas other structures are different from CAS- or IUPAC-derived ones.

In example 4.5.1.1, the O atom marked with an asterisk is the head atom.

Example 4.5.1.1.



The asterisked oxygen atom is joined to two carbons (numbered 1 and 2); the two environments are thus equal, and no decision can be made yet. Therefore, it is necessary to consider atoms further from the head atom. Examination of the atoms joined to C-1 and C-2 shows that C-2 has a fluorine joined to it whereas C-1 does not. Therefore, C-2 is in a heavier environment, and the final SRU is $-[-O-CHF-CH_2-]_n-$.

Higher atomic number overrules lower atomic number, regardless of quantity; thus, $-[-O-CHBr-CCl_2-]_n-$ is correct, whereas $-[-O-CCl_2-CHBr-]_n-$ is not, because Br is heavier than Cl, regardless of the fact that there are two Cl atoms and only one Br atom. This is also seen in the structure of example 4.5.1.1, where, because F is senior to H, "H plus F" outranks "H plus H".

Application of SCION rules to the structure of example 4.5.1.2 results in an SRU appreciably different from that derived by CAS and IUPAC rules.

Example 4.5.1.2 (repeat of example 4.2.1.3).

```
   -O-C-O-C-NH-C-C-S-C-NH-C-C-O-C-O-C-NH-C-C-S-C-NH-C-C-
Row A        ..3  2  1
Row B              1  2 3...
```

S has higher atomic weight than O or N and is selected as the head atom. Starting from S, in one direction the path is S−C−C..., whereas in the other it is S−C−N... . N has higher atomic number than C. Moving in the direction of the heavier environment (i.e., toward the atom of higher atomic number) gives S−C−N... as the preferred path. Therefore, the final SRU is $-[-S-C-NH-C-C-O-C-O-C-NH-C-C-]_n-$.

STEP 4 (naming the SRU): After the SRU has been defined, it is named. SCION rules for naming the SRU follow CAS 8CI rules with two exceptions: (1) use of parentheses may be different; (2) even as a last resort, nomenclature is *never* used to make a decision between two very similar structures—the SRU is defined by structure alone. Creation of SCION was begun in the 1960s, when CAS 8CI nomenclature rules were in force. To maintain file uniformity 8CI rules are still used, even though CAS 9CI nomenclature rules have been in force for over 20 years. Table 4 shows comparisons between CAS, IUPAC, and SCION names for some SRU homopolymers.

Table 4. Comparison: CAS, IUPAC, and SCION Names for Some SRU Homopolymers

Anhydride	
polymer:	$-[-O-CO-CH_2-CH_2-CO-]_n-$
CAS 8CI polymer name:	poly(oxysuccinyl)
CAS 9CI polymer name:	poly[oxy(1,4-dioxo-1,4-butanediyl)]
IUPAC polymer name:	poly(oxysuccinyl)
SCION polymer name:	POLY-OXYSUCCINYL
Ether	
polymer:	$-[-O-CH_2-CH_2-]_n-$
CAS 8CI polymer name:	poly(oxyethylene)
CAS 9CI polymer name:	poly(oxy-1,2-ethanediyl)
IUPAC polymer name:	poly(oxyethylene)
SCION polymer name:	POLY-OXYETHYLENE
Sulfide	
polymer:	$-[-O-CH_2-CH_2-S-CH_2-CH_2-]_n-$
CAS 8CI polymer name:	poly(oxyethylenethioethylene)
CAS 9CI polymer name:	poly(oxy-1,2-ethanediylthio-1,2-ethanediyl)
IUPAC polymer name:	poly(oxyethylenethioethylene)
SCION polymer name:	POLY-THIOETHYLENEOXYETHYLENE[a]

[a] Head atom is S by SCION rules.

SCION uses the CAS Registry System for substance registration and Messenger software for searching and is therefore subject to the same rules and limitations as CAS's File Registry with regard to SRU orientation. It is somewhat confusing that, with respect to nomenclature and orientation of SRUs according to head atom priority rules, many SRUs such as that for poly(oxyethylene) appear *mirror-image* on the searcher's monitor screen. Thus, poly(oxyethylene) appears as $[...CH_2-CH_2-O...]_n$, as shown in example 4.5.1.3; C-Numbers (the CNUM field—the proprietary equivalent of the CAS RN) in all SCION examples are disguised for security reasons.

Example 4.5.1.3. Messenger software display for POLY-OXYETHYLENE in SCION

DUPONT PROPRIETARY INFORMATION

CNUM: 225391M
RN: 9002-90-8
CAS: Poly(oxy-1,2-ethanediyl)
DUP: POLY-OXYETHYLENE
MF: (C2 H4 O)n
CI: PMS, COM
$[.....CH_2CH_2O.....]_n$

It is probable that a substructure search for this exact structure would retrieve it, but, as for CAS's File Registry, searchers are taught that the SRU should be correctly oriented; in this example, the oxygen atom should be on the left.

4.5.2. Source-Based Method. Source-based homopolymers are divided into two broad categories:

•**Category 1:** Prescribed-monomer condensation (PMC) homopolymers are condensation polymers of the classes

Table 5. PMC Polymer Classes That Can Form Homopolymers

POLYAMIDE
POLYAMIDE-ESTER
POLYAMIDE-IMIDE
POLYAMIDE-URETHANE
POLYESTER
POLYIMIDE
POLYURETHANE

polyamide, polyester, polyimide, polyurethane, and combinations of these, e.g., polyamide ester.

According to SCION rules, one-component PMC polymers—homopolymers—are registered *only* by the source-based method, even when an SRU representation is possible. Two-component PMC polymers are also classified as homopolymers if the two comonomers are "complementary"—that is, neither can polymerize by itself; the PMC classes for which homopolymers are possible are summarized in Table 5. The definition of a homopolymer is therefore not simply "a polymer from one type of monomer"; the concept is "one ideal SRU", and this accords with the thinking of most polymer chemists.

Regardless of the actual reactants polymerized, monomers in this category are "stylized" to their parents; thus, if *p*-aminobenzoyl chloride is an actual reactant in a polymerization, *p*-aminobenzoic acid is the stylized monomer stored as the polymer component. This is a key point for SCION searchers; a search for polymers of a stylized monomer, e.g., phthalic acid, *automatically includes derivatives*, e.g., phthaloyl halides, phthalic esters, and phthalic anhydride. This makes searching easy compared with source-based polymer searching in other systems that store the actual monomers used; in these, searchers are usually faced with trying to guess what derivatives of a "parent" were used in polymerizations. Table 6 compares possible actual monomers of some typical condensation polymers with their corresponding stylized parents.

Chemical substances in the bibliographic file of the SCION database are indexed with one or more roles; thus, although polymers (7) and (8) in Table 6 are the same, it is possible to distinguish between syntheses of (7) and (8) because they have different reactants (see point 4.5.2.1). The file thus functions in a manner similar to CAS's file CASREACT.

Point 4.5.2.1: This is true when the reactants are unusual; customary or commonly used monomers, however, are generally not indexed as reactants.

Category 1 (PMC) homopolymer names from one monomer consist of the CAS 8CI name of the stylized monomer, preceded by a prefix that indicates the PMC polymer class, e.g., POLYAMIDE-.

Category 1 (PMC) homopolymer names from two monomers consist of the CAS 8CI names of the stylized monomers (see point 4.5.2.2), alphabetized, separated by slashes, and preceded by a prefix that indicates the PMC polymer class, e.g., POLYAMIDE-. Thioacids and thioalcohols are included in the polyamide class.

Point 4.5.2.2: SCION disregards the CAS policy of using the name of an exotic alcohol as the parent even when it is esterified with a common acid; see discussion in section 3.3.

There is only one systematic polymer name, and addition of systematic monomer-based synonyms is omitted. Synonyms such as trade names, acronyms, or trivial names are added. A few examples illustrate the nomenclature style.

POLYAMIDE-IMIDE-1,2,4-BENZENE-
TRICARBOXYLIC ACID/P-PHENYLENEDIAMINE

POLYESTER-ETHYLENE GLYCOL/
TEREPHTHALIC ACID

Synonyms: DACRON*; MELINEX*; MYLAR*; PET

(Note: in SCION, trade names are indicated by an asterisk, vice the more usual double quotation marks; thus, Dacron*, vice "Dacron", etc.)

POLYURETHANE-1,4-BUTANEDIOL/
1,6-HEXANEDIAMINE

Notice the absence of carbonic acid as a stylized component of a polyurethane; this is explained in note *a* under Table 6.

•**Category 2:** Homopolymers are formed from actual starting monomers (ASM) containing a carbon−carbon multiple bond (acetylenic, acrylic, ethylenic, vinyl).

Category 2 (ASM) homopolymer names consist of the CAS 8CI monomer name prefaced by POLY-. There is only one systematic name, and addition of systematic monomer-based synonyms is omitted. Synonyms such as trade names, acronyms, or trivial names are added. A few examples illustrate the nomenclature style.

POLY-ACRYLONITRILE

Synonyms: POLY-AN; AN HOMOPOLYMER

POLY-1,3-BUTADIENE

POLY-ETHYLENE

Synonym: POLYTHENE*

Table 6. Comparison of Actual and Stylized Monomers of Some PMC Homopolymers

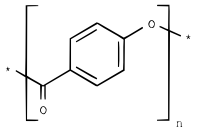
actual monomer(s) polymerized	polymer type[a]	stylized parent(s) [polymer component(s)]
(1) *p*-aminobenzoyl chloride	polyamide	*p*-aminobenzoic acid
(2) *p*-hydroxybenzoyl chloride	polyester	*p*-hydroxybenzoic acid
(3) monoethanolamine/phosgene	polyamide-ester[b]	carbonic acid/monoethanolamine
(4) 4-aminophthalic anhydride	polyimide	4-aminophthalic acid
(5) *p*-phenylenediamine/pyromellitic anhydride	polyimide	1,2,4,5-benzenetetracarboxylic acid/*p*-phenylenediamine
(6) monoethanolamine (ht)/phosgene	polyurethane	monoethanolamine
(7) ethylenediamine/ethylene glycol bis(chloroformate)	polyurethane	ethylenediamine/ethylene glycol
(8) ethylene diisocyanate/ethylene glycol	polyurethane	ethylenediamine/ethylene glycol

[a] Carbonic acid is always present as a stylized monomer in polyurethanes; its presence is unnecessary, and therefore it is omitted as a component. [b] For homopolymer (3) in this table to be classified as a polyamide-ester, every other monoethanolamine unit must be turned around with respect to the preceding unit.

Table 7. Selected Homopolymer Types: Summary of CAS, IUPAC, MDL, and SCION Graphic Representations and Names

(1) 1-COMPONENT POLYESTER: poly(p-hydroxybenzoic acid)
CAS structure: -[-O-p-C_6H_4-CO-]$_n$-
CAS 8CI polymer name: poly(oxy-p-phenylenecarbonyl)
CAS 9CI polymer name: poly(oxy-1,4-phenylenecarbonyl)

IUPAC structure: -[-O-p-C_6H_4-CO-]$_n$-
IUPAC polymer name: poly(oxy-1,4-phenylenecarbonyl)

MDL structure: 

SCION structure: (HO-p-C_6H_4-COOH)$_x$
SCION polymer name: POLYESTER-BENZOIC ACID, P-HYDROXY-

(2) 1-COMPONENT POLYAMIDE: Nylon-6
CAS structure: -[-NH-CO-$(CH_2)_5$-]$_n$-

CAS 8CI polymer name: poly[imino(1-oxohexamethylene)]
CAS 9CI polymer name: poly[imino(1-oxo-1,6-hexanediyl)]

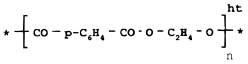
IUPAC structure: -[-NH-CO-$(CH_2)_5$-]$_n$-
IUPAC polymer name: poly[imino(1-oxohexamethylene)]

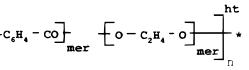
MDL structure: *-[-NH-CO-$(CH_2)_5$-]$_n$-*

SCION structure: (H_2N-$(CH_2)_5$-COOH)x
SCION polymer name: POLYAMIDE-HEXANOIC ACID, 6-AMINO-

(3) 2-COMPONENT POLYESTER: poly(ethylene terephthalate)
CAS structure: -[-O-C_2H_4-O-CO-p-C_6H_4-CO-]$_n$-
CAS 8CI polymer name: poly(oxyethyleneoxyterephthaloyl)
CAS 9CI polymer name: poly(oxy-1,2-ethanediyloxycarbonyl-1,4-phenylenecarbonyl)
(the source-based representation is also registered)

IUPAC structure: -[-O-C_2H_4-O-CO-p-C_6H_4-CO-]$_n$-
IUPAC polymer name: poly(oxyethyleneoxyterephthaloyl)

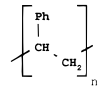
MDL structure: 

or 

For definition of a mer, see Glossary of Acronyms and Terms (Table 2).

SCION structure: (HO-CH_2-CH_2-OH . HOOC-p-C_6H_4-COOH)$_x$
SCION polymer name: POLYESTER-ETHYLENE GLYCOL/TEREPHTHALIC ACID

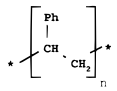
(4) ETHYLENIC POLYMER: polystyrene

CAS structure: 

CAS polymer name: poly(1-phenylethylene)
(the source-based representation is also registered)

IUPAC structure: 

IUPAC polymer names: poly(1-phenylethylene); polystyrene

MDL structure: 

MDL polymer name: poly(1-phenylethylene)

SCION structure: (Ph-CH=CH_2)$_x$
SCION polymer name: POLY-STYRENE

(5) POLYETHER: poly(oxyethylene)
CAS structure: -[-O-CH_2-CH_2-]$_n$-
CAS 8CI polymer name: poly(oxyethylene)
CAS 9CI polymer name: poly(oxy-1,2-ethanediyl)

IUPAC structure: -[-O-CH_2-CH_2-]$_n$-
IUPAC polymer names: poly(oxyethylene); poly(ethylene oxide)

MDL structure: *-[-O-CH_2-CH_2-]$_n$-*

SCION structure: -[-O-CH_2-CH_2-]$_n$-
SCION polymer name: POLY-OXYETHYLENE

IUPAC's statement[15a] that source-based registration cannot reflect whether a monomer such as 1,3-butadiene that is capable of polymerizing by 1,2-addition, 1,4-addition, or both needs qualification. If the entire record for the polymer in a particular database comprises the structure alone, the statement is true. If the entire record includes the polymer name, the statement is untrue; a simple modification to the accompanying polymer name clarifies the situation. The three polymer names given below are virtually self-explanatory (the slash could be used to indicate an "either/or" situation).

POLY-1,3-BUTADIENE(1,2)

POLY-1,3-BUTADIENE(1,4)

POLY-1,3-BUTADIENE(1,2/1,4)

Similarly, MDL terminology designations such as hh, ht, or eu can be used to modify polymer names; compare POLY-STYRENE with POLY-STYRENE(ht).

Source-based registration of PMC and ASM homopolymers is described in detail elsewhere.[16]

4.6. Summary of CAS, IUPAC, MDL, and SCION Graphic Representations of Selected Homopolymer Types. Table 7 summarizes and compares graphic representations used or recommended by CAS, IUPAC, MDL, and SCION for some condensation, ethylenic, and ether homopolymers.

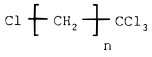
4.7. End Groups. There are differences in the treatment of end groups by the four different systems.

4.7.1. CAS.[12a,19] **4.7.1.1. Structure-Based Method.** Known end groups are specified by means of appropriate radical names, and their positions of attachment are indicated by Greek letters α and *ω*; the α end group is the end group attached to the left end of the SRU after the structure has been defined according to the rules, and it is cited first, regardless of alphabetic order. Ester and ether end groups of polyalkylene glycols (polyglycols) are indexed according to a further set of rules. Monoderivatives are cited in the α position, with *ω*-hydroxy at the other end. For polyglycols with two dissimilar ester or ether end groups, the two end

groups are alphabetized. Polyglycols with one ester end group and one ether end group have the acyl group assigned to the α end and the ether group to the *ω* end, regardless of alphabetization. When multiplying radicals are used, they are given α locants. Because CAS inverts names, a typical nomenclature style for linear, single-strand polymers is: poly(XXX), α-YYY-*ω*-ZZZ-. A 1968 ACS publication cites uninverted names,[19] but this document was for primary publications of other sources.[18]

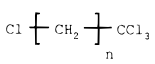
Examples are given below of representations of SRU polymers with end groups. Example 4.7.1.1.1 shows the ACS style;[19] examples 4.7.1.1.2 through 4.7.1.1.4 show the CAS style.

Example 4.7.1.1.1.

SRU: 

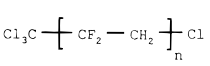
Polymer name: α-chloro-*ω*-(trichloromethyl)poly(methylene)
Online molecular formula display style: none

Example 4.7.1.1.2. (hypothetical example)



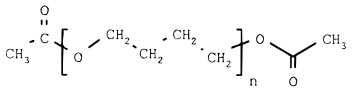
Polymer name: poly(methylene), α-chloro-*ω*-(trichloromethyl)-
Online molecular formula display style: (CH2)nCCl4

Example 4.7.1.1.3. (hypothetical example)

SRU: 

Polymer name: poly(1,1-difluoro-1,2-ethanediyl), α-(trichloromethyl)-*ω*-chloro-
Online molecular formula display style: (CH2F2)nCCl4

Example 4.7.1.1.4. CAS RN: 26248-69-1

SRU: 

Polymer name: poly(oxy-1,4-butanediyl), α-acetyl-*ω*-(acetyloxy)-
Online molecular formula display style: (C4H8O)nC4H6O3

Note on examples 4.7.1.1.2 through 4.7.1.1.4: The online appearance of names containing Greek letters such as α and *ω* depend upon whether the terminal is text-type or graphics-type. Text-type displays show α as .alpha., *ω* as .omega., etc. The online text has no subscript characters; thus, $(CH_2)_n$-CCl_4 appears as (CH2)nCCl4. Examples captured online with a text-type terminal were changed so that .alpha. reads α, etc.

There are minor differences in the formatting of names between CAS printed-copy versions and online versions—see example 4.7.1.1.5.

Example 4.7.1.1.5.
• Printed name (in CA Chemical Substance Index):
Poly(oxy-1,2-ethanediyl)
----, α-(carboxymethyl)-*ω*-(carboxymethoxy)-
dipotassium salt

Key features: multiple lines; no commas at ends of lines

• Online name:
Poly(oxy-1,2-ethanediyl), α-(carboxymethyl)-*ω*-(carboxymethoxy)-, dipotassium salt

Key features: continuous text; commas between heading parent, substituent(s) (when present), and name modification segments

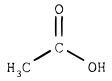
4.7.1.2. Source-Based Method. CAS has published nothing specific on how end groups of source-based homopolymers are named. In May 1995, enhancements added to File Registry include structures for polyethers and polyesters that were previously accessible only by name.[26] Example 4.7.1.2.1 shows a source-based representation for poly(tetrahydrofuran) diacetate.

Example 4.7.1.2.1. "Poly-THF, diacetate"

REGISTRY COPYRIGHT 1995 ACS
RN 71714-39-1 REGISTRY
CN Furan, tetrahydro-, homopolymer, diacetate (9CI) (CA INDEX NAME)
OTHER NAMES:
CN THF homopolymer diacetate
DR 72270-49-6
MF (C4H8 O)x. 2 C2 H4 O2
PCT Polyether, Polyether formed
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
DES 8:GD,ESTER

CM 1

CRN 64-19-7
CMF C_2 H_4 O_2



CM 2

CRN 24979-97-3
CMF $(C_4$ H_8 $O)_x$
CCI PMS

CM 3

CRN 109-99-9
CMF C_4 H_8 O

:

The nomenclature follows that for other polymer esters and polymer ethers as described in the Index Guide, Appendix IV.[12a] Note that polymers posttreated to form these two classes of polymer derivatives are the only ones that are registered and can be found in the Registry File (other than salts and molecular addition compounds).

The "GD" in the 8:GD,ESTER descriptor stands for "general derivative". It is used both for polymer derivatives (esters and ethers) and for nonpolymer esters with an

unknown number of ester groups. It allows distinction between ester and ether derivatives (derivatives that actually have covalent bonds not represented by the registration format). It also allows distinction between these two classes of substances and other dot-disconnect derivatives such as the "compound with" registrations.[20]

Notice the inconsistency between the name, which says "diacetate", and the MF and structure of the first component (CM 1), which show acetic acid registered as a component.

This source-based registration is *in addition to* the structure-based representation RN 26248-69-1 shown as example 4.7.1.1.4. On the basis of the evidence of examples 4.7.1.1.4 and 4.7.1.2.1, therefore, it is clear that it is advisable to search for such substances in File Registry as both structure-based *and* source-based polymers, especially because there is no online cross-referencing between the two polymer records. However, for some polymers, e.g. "poly(tetramethylene ether glycol)" there is a cross-reference in the Index Guide: under "Poly(oxy-1,4-butanediol), α-hydro-ω-hydroxy-", there is a cross-reference to "Furan, tetrahydro-, homopolymer"; similarly, under "Furan, tetrahydro-, homopolymer" there is a cross-reference to "Poly(oxy-1,4-butanediol), α-hydro-ω-hydroxy-". The mismatch between name ("acetate") and MF (for acetic acid, not acetate anion) shown in example 4.7.1.2.1 may cause search problems.

In File Registry, cross-referencing has been applied to both the structure-based and the source-based representations for poly(ethylene terephthalate) in the following manner: the structure-based polymer record includes the registry number (RN) for the source-based polymer from ethylene glycol and terephthalic acid in the AR (alternate RN) field; conversely, the source-based polymer record includes the RN for the SRU (structure-based polymer) in the PR (preferred RN) field. Extension to other polymers of this cross-referencing technique, by either the AR/PR method or introduction of an XREF [cross-referenced RN(s)] field, would be welcome.

4.7.2. IUPAC. 4.7.2.1. Structure-Based Method. For structure-based polymers, the end group attached to the left side of the SRU is designated as the α group, and the other end group is identified by ω. A typical IUPAC nomenclature style for linear, single-strand polymers is: α-YYY-ω-ZZZpoly(XXX).

Two examples are given below of IUPAC representation of SRU polymers with end groups.[13,15]

Example 4.7.2.1.1.

SRU: $H-[-O-CH_2-CH_2-]_n-OH$

Polymer name: α-hydro-ω-hydroxypoly(oxyethylene)

Synonym: poly(ethylene glycol)

Example 4.7.2.1.2.

SRU: $CCl_3-[-p-C_6H_4-CH_2-]_n-Cl$

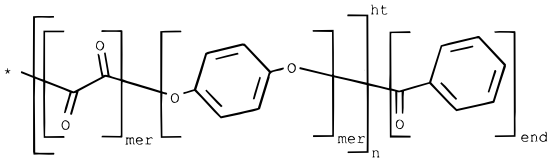
Polymer name: α-(trichloromethyl)-ω-chloropoly(1,4-phenylenemethylene)

Other IUPAC polymer end group examples are published elsewhere.[27a]

4.7.2.2. Source-Based Method. Since IUPAC does not discuss source-based homopolymers (see section 4.1.2), there can be no discussion of their end groups.

4.7.3. MDL. 4.7.3.1. Structure-Based Method. The MACCS-II substance module provides a way to create custom Sgroup types and custom polymer Sgroups.[2] The desired structure is drawn and a generic Sgroup that consists of the atoms of interest is defined. By use of the CUSTOM Sgroup data field, the generic Sgroup is labeled with a custom Sgroup type, such as END (end-group). The structure can then be registered in the database. Example 4.7.3.1.1 shows how the benzoyl end group can be attached to the polyester formed between oxalic acid and hydroquinone.

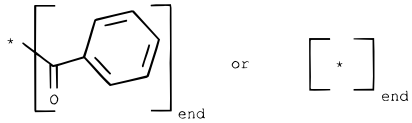
Example 4.7.3.1.1.



To search for a polymer that contains a custom polymer Sgroup type, the query structure is drawn and defined as a generic Sgroup type, and the generic Sgroup is labeled with the required custom Sgroup type using the CUSTOM Sgroup data field.

Queries for custom end groups can be, for example, as shown in example 4.7.3.1.2.

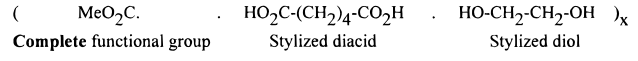
Example 4.7.3.1.2.



4.7.3.2. Source-Based Method. MDL does not discuss end groups on graphic representations of source-based homopolymers.

4.7.4. SCION. Beginning in 1990, previous end-group indexing methods were superseded by the indexing of end groups at the polymer level. This differs from other systems in that the *complete functional group*, as perceived by a chemist, is indexed. The complete functional group means, for example, *methoxycarbonyl* not methoxy in a carboxylic acid ended polyester that has been esterified with methanol—see example 4.7.4.1.

Example 4.7.4.1. End groups on the esterified polyester from adipic acid and ethylene glycol



Polymer name: POLYESTER-ADIPIC ACID/ETHYLENE GLYCOL, END GROUP

METHOXYCARBONYL (not METHOXY)

An end group is defined as a grouping of atoms that terminates a polymer backbone and is different from the main body of the polymer. The method is described in detail elsewhere.[16]

Table 8. Comparison of Names of End Groups of Some Oxyethylene Homopolymers by CAS, IUPAC, and SCION (Note: MDL offers no systematic nomenclature, and is therefore not represented in this table)

Polymer: $H-[-O-CH_2-CH_2-]_n-OH$

CAS 9CI polymer name: poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-
IUPAC polymer name: α-hydro-ω-hydroxypoly(oxyethylene)
SCION polymer name: POLY-OXYETHYLENE, END GROUP HYDROXY

Polymer: $CH_3-CH_2-CO-[-O-CH_2-CH_2-]_n-OH$

CAS 9CI polymer name: poly(oxy-1,2-ethanediyl), α-(1-oxopropyl)-ω-hydroxy-
IUPAC polymer name: α-propionyl-ω-hydroxypoly(oxyethylene)
SCION polymer name: POLY-OXYETHYLENE, END GROUP HYDROXY, END GROUP PROPIONYLOXY (not propionyl)

Polymer: $CH_3-[-O-CH_2-CH_2-]_n-OH$

CAS 9CI polymer name: poly(oxy-1,2-ethanediyl), α-methyl-ω-hydroxy-
IUPAC polymer name: α-methyl-ω-hydroxypoly(oxyethylene)
SCION polymer name: POLY-OXYETHYLENE, END GROUP HYDROXY, END GROUP METHOXY (not methyl)

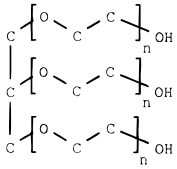
Polymer: $CH_3-CO-[-O-CH_2-CH_2-]_n-O-CO-Ph$

CAS 9CI polymer name: poly(oxy-1,2-ethanediyl), α-acetyl-ω-(benzoyloxy)-
IUPAC polymer name: α-acetyl-ω-(benzoyloxy)poly(oxyethylene)
SCION polymer name: POLY-OXYETHYLENE, END GROUP ACETYLOXY*, END GROUP BENZOYLOXY (* not acetyl)

Polymer: $CH_3-CH_2-[-O-CH_2-CH_2-]_n-O-CH_3$

CAS 9CI polymer name: poly(oxy-1,2-ethanediyl), α-ethyl-ω-methoxy-
IUPAC polymer name: α-ethyl-ω-methoxypoly(oxyethylene)
SCION polymer name: POLY-OXYETHYLENE, END GROUP ETHOXY*, END GROUP METHOXY (* not ethyl)

POLYMER: (Note 1)



CAS 9CI polymer name: poly(oxy-1,2-ethanediyl), α,α′,α″-1,2,3-propanetriyltris[ω-hydroxy-
IUPAC polymer name: α,α′,α″-1,2,3-propanetriyltris[ω-hydroxypoly(oxyethylene)]
SCION polymer name: POLY-OXYETHYLENE, END GROUP HYDROXY, END GROUP 1,2,3-PROPANETRIYLTRIOXY (not 1,2,3-propanetriyl)

[a] This polymer is classified in SCION as a homopolymer because there is only one polymeric species; for comparison, therefore, the corresponding CAS and IUPAC names are supplied regardless of whether these systems classify it as a homopolymer.

4.7.4.1. Structure-Based Method. The following example shows the representation in SCION of an SRU homopolymer with end groups:

Structure: $H-[-O-CH_2-CH_2-]_n-OH$

Polymer name: POLY-OXYETHYLENE, END GROUP HYDROXY

Synonym: poly(ethylene glycol)

Graphic representation:

$$(-[-O-CH_2-CH_2-]_n- \,.\, HO.)_x$$

The "hydro" end group concept at the left-hand end of polymers like POLY-OXYETHYLENE was abandoned in favor of more realistic expressions of the chemical nature of the end groups—in this case, a hydroxy group on each end. The key point is to avoid splitting functional groups. In SCION, the OH group is searchable as a separate chemical fragment; this is not possible in CAS's File Registry. This is discussed in more detail elsewhere.[16]

Table 8 summarizes treatment of oxyethylene homopolymer end groups by CAS, IUPAC, MDL, and SCION.

4.7.4.2. Source-Based Method. The complete end group is named. The end group fragments are stored as components of the polymer structure. Two examples illustrate the method.

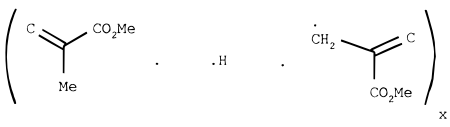
Example 4.7.4.2.1. The polyamide from p-aminobenzoyl chloride is esterified at the carbonyl chloride end with methanol, and then acetylated at the amine end with acetyl chloride

Structure: $(H_2N\text{-}p\text{-}C_6H_4\text{-}CO_2H \;.\; CO_2CH_3 \;.\; .NH\text{-}CO\text{-}CH_3)_x$

Polymer name: POLYAMIDE-BENZOIC ACID, P-AMINO-, END GROUP ACETAMIDO, END GROUP METHOXYCARBONYL (not POLYAMIDE-BENZOIC ACID, P-AMINO-, END GROUP ACETYL, END GROUP METHOXY)

Example 4.7.4.2.2. Methyl methacrylate (MMA) homopolymer is prepared by a special process that results in a hydrogen end group and a 2-(methoxycarbonyl)allyl end group

Structure:



Polymer name: POLY-METHACRYLIC ACID, METHYL ESTER, END GROUP HYDRO, END GROUP 2-(METHOXYCARBONYL)ALLYL
Text descriptors: POLY-HOMO; END GROUP POLYMERIZABLE CC

Note on example 4.7.4.2.2: The important points are that (1) the hydro and 2-(methoxycarbonyl)allyl end groups are searchable as components, and (2) the final homopolymer

is a macromonomer with a polymerizable end group that contains a carbon-carbon multiple bond.

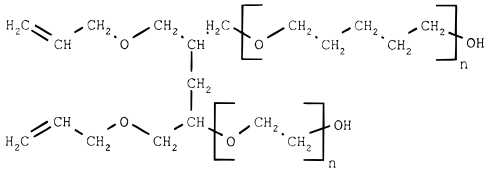
5. NOMENCLATURE AND GRAPHIC REPRESENTATION OF "REGULAR", SINGLE-STRAND, ORGANIC COPOLYMERS

This section includes copolymers containing two or more SRUs or comonomers as components. The word "regular" in the heading is used here to mean "ordinary", random, or statistical copolymers with no non-polymeric "spacer groups" (also called "junction units") or other special attributes. Polymers with special attributes, e.g., alternating, block, comb, graft, periodic, etc. are discussed in section 6.

5.1. CAS Nomenclature and Structural Representation. 5.1.1. Structure-Based Method. CAS does not generally index copolymers of *unterminated* SRUs by the structure-based method. Formats such as poly(oxyethylene)/poly(oxytetramethylene) or poly[(oxyethylene)/(oxytetramethylene)] are not used. Instead a source-based representation is used—see section 5.1.2. However, as shown in example 5.1.1.1, there are some cases of polymer registration that contain more than one SRU within the complete structure.

Example 5.1.1.1. Example of multiple SRUs within a structure

REGISTRY COPYRIGHT 1995 ACS
RN 141028-46-8 REGISTRY
CN Poly(oxy-1,4-butanediyl), α-[4-hydroxy-5-(2-propenyloxy)-2-[(2-propenyloxy)methyl]pentyl]-*ω*-hydroxy-, monoether with α-hydro-*ω*-hydroxypoly(oxy-1,2-ethanediyl) (9CI) (CA INDEX NAME)
MF (C4 H8 O)n (C2 H4 O)n C12 H22 O4
CI COM
SR CA
:



Linear polymers containing SRUs within SRUs are not assigned structure-based names; instead they are indexed at the monomer names only.[12a] CAS does not use a format that includes an SRU within an SRU. Thus, the polyester from isophthalic acid and poly(oxyethylene) is registered as the source-based polymer [57447-52-4] and *not* as shown as example 5.1.1.2.

Example 5.1.1.2. Theoretical "SRU-within-an-SRU" format for polymer from isophthalic acid and poly(oxyethylene) (*not* used by CAS)

$$-[-[-O-CH_2-CH_2-]_n-O-CO-m-C_6H_4-CO-]_n-$$

5.1.2. Source-Based Method. CAS currently names copolymers containing two component monomers as follows. The preferred index name is determined by the usual rules for selection of a heading parent.[12c] An expression such as "polymer with ..." is inserted between the heading parent and the other monomer name(s). A stereoparent is preferred over a nonstereoparent; e.g., *d*-glucose, polymer with butanedioic acid.[12c]

The "complementary" name, i.e., the name with the components reversed, is added as a systematic synonym. Thus, for a copolymer of A and B (where A is the preferred parent), the CA index name is "A, polymer with B"; "B, polymer with A" is added as a systematic synonym. Only the heading parent name is inverted, e.g., benzenamine, 4-ethenyl-, polymer with ethenylbenzene—see example 5.1.2.1.

Example 5.1.2.1. p-Vinylaniline/styrene copolymer

REGISTRY COPYRIGHT 1995 ACS
RN 27987-76-4 REGISTRY
CN Benzenamine, 4-ethenyl-, polymer with ethenylbenzene (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzene, ethenyl-, polymer with 4-ethenylbenzenamine (9CI)
CN Aniline, p-vinyl-, polymer with styrene (8CI)
:
MF (C8 H9 N . C8 H8)x
CI PMS, COM
PCT Polystyrene
:

For condensation polymers such as polyamides, polyesters, etc., older indexes, e.g., 8CI, sometimes used an expression such as "polyamide with", "polyester with", etc., to indicate the polymer class. These may be found in either the index name or the systematic synonyms. This was applied inconsistently in the 8CI and the practice was abandoned in the 9CI. This is shown in example 5.1.2.2, which also shows that this is not the CAS preferred format for this particular two-component condensation polymer—the presence of the PR (preferred registry number) indicates that for this polymer the preferred CAS Registry Number is [25038-59-9], which contains the SRU-format record.

Example 5.1.2.2. Illustration of use of "polyester with" in 8CI name

REGISTRY COPYRIGHT 1995 ACS
RN 9003-68-3 REGISTRY
CN 1,4-Benzenedicarboxylic acid, polymer with 1,2-ethanediol (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethylene glycol, polyester with terephthalic acid (8CI)
:
PR 25038-59-9
DR 9009-28-3
MF (C8 H6 O4 . C2 H6 O2)x
CI PMS, COM
PCT Polyester, Polyester formed
:

For copolymers containing more than two comonomers, the CAS format is modified to include all the monomers; in addition to the index name, enough systematic synonyms are created to ensure that for every monomer there is a name that begins "AAA, polymer with...", where AAA is one of the monomers in the polymer. Thus, for a quaterpolymer, there are four names—one index name and three systematic synonyms. For the case where A is the preferred parent,

the CA index name is "A, polymer with B, C and D"; systematic synonyms are "B, polymer with A, C and D"; "C, polymer with A, B and D"; and "D, polymer with A, B and C". Other synonyms based on trivial or common names may also be added.

As in the case of two-component polymers, some 8CI index names for polymers containing three or more monomers used an expression that indicated the class, such as "polyamide with" or "polyester with", but this was applied inconsistently during the 8CI and abandoned in the 9CI.

Thus, the 8CI index name for the three-component polyester containing ethylene glycol, dimethyl terephthalate, and isophthalic acid contains the expression "polyester with", whereas the three-component polyester containing 1,4-butanediol, sebacic acid, and terephthalic acid does not—see examples 5.1.2.3 and 5.1.2.4.

Example 5.1.2.3. Example of terpolymer containing the 8CI name expression "polyester with"

REGISTRY COPYRIGHT 1995 ACS
RN 26006-30-4 REGISTRY
CN 1,3-Benzenedicarboxylic acid, polymer with dimethyl 1,4-benzenedicarboxylate and 1,2-ethanediol (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
:
CN Ethylene glycol, polyester with dimethyl terephthalate and isophthalic acid (8CI)
:
MF (C10 H10 O4 . C8 H6 O4 . C2 H6 O2)x
CI PMS
PCT Polyester, Polyester formed
:

Example 5.1.2.4. Example of terpolymer containing the 8CI name expression "polymer with", not "polyester with"

REGISTRY COPYRIGHT 1995 ACS
RN 28205-74-5 REGISTRY
CN 1,4-Benzenedicarboxylic acid, polymer with 1,4-butanediol and decanedioic acid (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,4-Butanediol, polymer with sebacic acid and terephthalic acid (8CI)
MF (C10 H18 O4 . C8 H6 O4 . C4 H10 O2)x
CI PMS
PCT Polyester, Polyester formed
:

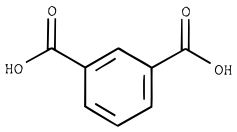
Polymers of mixed classes, e.g., polyamide/polyester or polyester/polyether, are named using the expression "polymer with" in both the 8CI and 9CI. This is illustrated in examples 5.1.2.5 and 5.1.2.6.

Example 5.1.2.5. Source-based registration of a polyether/polyester

REGISTRY COPYRIGHT 1995 ACS
RN 28850-52-4 REGISTRY
CN Isophthalic acid, polymer with ethylene oxide (8CI) (CA INDEX NAME)
MF (C8 H6 O4 . C2 H4 O)x
CI PMS
PCT Polyester, Polyester formed, Polyether, Polyether formed
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

CM 1

CRN 121-91-5
CMF C_8 H_6 O_4



CM 2

CRN 75-21-8
CMF C_2 H_4 O

Note on example 5.1.2.5: There is no firm indication that this polymer is, in fact, a polyether; if single ethylene oxide units alternate with isophthaloyl units, with no oligomerization of ethylene oxide, then the polymer is, in effect, poly(ethylene isophthalate) [26948-62-9], and the polymer class terms (PCTs) "Polyether" and "Polyether formed" are incorrectly assigned. This is an example of where the PCTs, which are assigned algorithmically based *solely* upon structure, may be incorrect; it is known that they are not 100% accurate.[20]

Example 5.1.2.6. Example of polyamide/polyester registration

REGISTRY COPYRIGHT 1995 ACS
RN 25767-67-3 REGISTRY
CN 1,4-Benzenedicarboxylic acid, polymer with 1,2-ethanediol and 1,6-hexanediamine (9CI) (CA INDEX NAME)-
OTHER CA INDEX NAMES:
:
CN Ethylene glycol, polymer with 1,6-hexanediamine and terephthalic acid (8CI)
:
MF (C8 H6 O4 . C6 H16 N2 . C2 H6 O2)x
CI PMS
PCT Polyamide, Polyamide formed, Polyester, Polyester formed
:

Although structure-based representations of homopolymers are common in File Registry, e.g., poly(oxyethylene), with the exception of those cited in section 5.1.1, this style of registration is not extended to their copolymers. Thus, the copolymer of poly(oxyethylene) and poly(oxytetramethylene) is indexed as a source-based polymer—see example 5.1.2.7.

Example 5.1.2.7. "Poly(oxyethylene)/poly(oxytetramethylene)" copolymer

REGISTRY COPYRIGHT 1995 ACS
RN 27637-03-2 REGISTRY
CN Furan, tetrahydro-, polymer with oxirane (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethylene oxide, polymer with tetrahydrofuran (8CI)

CN Furan, tetrahydro-, polymer with ethylene oxide (8CI)
CN Oxirane, polymer with tetrahydrofuran (9CI)
:
DR 88161-31-3, 72514-58-0
MF (C4 H8 O . C2 H4 O)x
CI PMS, COM
PCT Polyether, Polyether formed
:

CM 1

CRN 109-99-9
CMF C_4 H_8 O

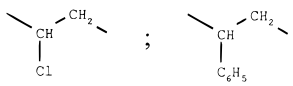
CM 2

CRN 75-21-8
CMF C_2 H_4 O

CAS does not use the words such as "random" or "statistical" to describe random or statistical copolymers; copolymers without special attributes such as "block" are assumed to be random.

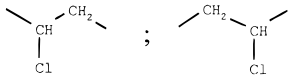
5.2. IUPAC Nomenclature and Structure Representation. 5.2.1. Structure-Based Method. Recommendations on the naming of structure-based copolymers have been published.[15b,c,27b] IUPAC calls these copolymers "irregular polymers" and suggests that they be named poly(A/B/C...), where A, B, C, ... are the structure-based names of the appropriate SRUs. The preferred order for citation of SRUs is alphabetical. The slashes indicate that the sequential arrangement of the SRUs is unknown.

Example 5.2.1.1. Statistical head-to-tail polymer derived from styrene and vinyl chloride

Units: 

Polymer name: poly(1-chloroethylene/1-phenylethylene)

Example 5.2.1.2. Irregular head-to-head and/or head-to-tail polymer derived from 1-chloroethene

Units: 

Polymer name: poly(1-chloroethylene/2-chloroethylene)

Example 5.2.1.3. A polyamide derived from adipoyl chloride and a mixture of 1,4-butanediamine and 1,6-hexanediamine

Units: $-NH-(-CH_2-)_4-NHCO-(-CH_2-)_4-CO-$; $-NH-(-CH_2-)_6-NHCO-(-CH_2-)_4-CO-$

Polymer name: poly(iminobutane-1,4-diyliminoadipoyl/iminohexane-1,6-diyliminoadipoyl)

5.2.2. Source-Based Method. In its 1985 publication,[23] IUPAC states that in principle a comprehensive, structure-based system of naming copolymers would be desirable but that such a system presupposes a knowledge of the structural identity of all the constitutional units (i.e., SRUs) as well as their sequential arrangements within the polymer molecules. Since this information is rarely available, a source-based nomenclature system is needed, but structure-based nomenclature is still preferred whenever the copolymer structure is fully known and amenable to treatment by the rules for single-strand polymers.[13,28]

Table 9. IUPAC Source-Based Copolymer Classification

no	type	connective	example
(1)	unspecified	*-co-*	poly(A-*co*-B)
(2)	statistical	*-stat-*	poly(A-*stat*-B)
(3)	random	*-ran-*	poly(A-*ran*-B)
(4)	alternating	*-alt-*	poly(A-*alt*-B)
(5)	periodic	*-per-*	poly(A-*per*-B-*per*-C)
(6)	block	*-block-*	polyA-*block*-polyB
(7)	graft	*-graft-*	polyA-*graft*-polyB

IUPAC presents a nomenclature system for copolymers[23] and discusses the following classes: unspecified, statistical, random, alternating, periodic, block, and graft.

Polymers having monomers differing in constitutional or configurational features, but derived from a single monomer, are not regarded as copolymers—e.g., polybutadiene with mixed sequences of 1,2 and 1,4 units.

The IUPAC source-based nomenclature system identifies the constituent monomers and provides a description of the sequence arrangement of the different types of monomers present by means of a specific italicized connective. In the examples in Table 9, A, B, and C represent three different monomers; the citation of A, B, and C is not intended to reflect an order of seniority. As a result, more than one name is often possible.

When end groups are specified, systematic names of terminal units precede the polymer name. The prefix α or *ω* refers to the terminal unit attached to the left or right, respectively, of the structure as written.

Example 5.2.2.1. α-X-*ω*-Y-poly(A-*co*-B)

Types 1, 2, and 3 in Table 9 are discussed in more detail here. Types 4 and 5 are discussed in section 6.2.2, type 6 is discussed in section 6.3.2, and type 7 is discussed in section 6.4.2.

An unspecified sequence arrangement of monomers is represented by (A-*co*-B), and the corresponding copolymer is named poly(A-*co*-B). Thus, an unspecified copolymer of styrene and methyl methacrylate is named either poly[(methyl methacrylate)-*co*-styrene] or poly[styrene-*co*-(methyl methacrylate)].

Statistical copolymers are copolymers in which the sequential distribution of the monomers obeys known statistical laws. The term statistical copolymer is proposed to embrace a large proportion of copolymers prepared by simultaneous polymerization of two or more monomers in an admixture. Such copolymers are often described in the literature as "random copolymers", but this is almost always an improper use of the term random, and IUPAC recommends that the practice be abandoned.

Statistical copolymers are represented by poly(A-*stat*-B), poly(A-*stat*-B-*stat*-C), etc.

Example 5.2.2.2. Poly(styrene-*stat*-butadiene)

A random copolymer is a special case of a statistical copolymer, namely one in which the probability of finding a given monomer at any given site in the chain is independent

of the nature of neighboring units at that position (Bernoullian distribution). In other words, for such a copolymer, the probability of finding a sequence ...ABC... of monomers A, B, C..., i.e., P[...ABC...] is given by:

$$P[...ABC...] = P[A].P[B].P[C]... = \prod_{i = A,B,C...} P[i]$$

where P[A], P[B], P[C], etc. are the unconditional probabilities of the occurrence of various monomers.

A random sequence arrangement of monomers is represented by (A-*ran*-B), (A-*ran*-B-*ran*-C), etc.

Example 5.2.2.3. Poly[ethylene-*ran*-(vinyl acetate)]

In the area of condensation polymers,[23a] source-based representation is included for a type referred to by CAS and SCION as homopolymers but called alternating polymers by IUPAC. Thus, polymers such as poly(hexamethylene adipamide) and poly(ethylene terephthalate) can be represented by the source-based names:

poly(adipic acid-*alt*-hexamethylenediamine)

poly(ethylene glycol-*alt*-terephthalic acid)

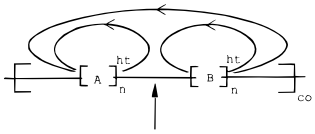
Alternate nomenclature offered[23b] for these polymers is

alt-copoly(adipic acid/hexamethylenediamine)

alt-copoly(ethylene glycol/terephthalic acid)

While it is pedantically correct to call these alternating polymers, the "alternating" concept is superfluous because, for either of these two examples, the two monomers are mers (see Table 2), and therefore cannot be in the polymer in any pattern other than alternating. Other examples of alternating polymers are given in section 6.2.2.

5.3. MDL Graphic Representation. 5.3.1. Structure-Based Method. A bond that connects two SRUs indicates that the connectivity between the SRUs is known and that the bond is permitted:[2]



Bond identifies the connectivity between the SRUs in the copolymer

In contrast, absence of this bond indicates that nothing is known about the connectivity.

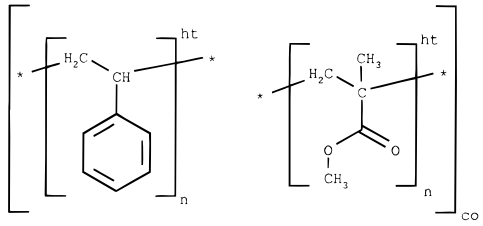
Poly(A-*co*-B) is represented by either of the two graphic formats:

$[-[-A-]_n- -[-B-]_n-]_{co}$

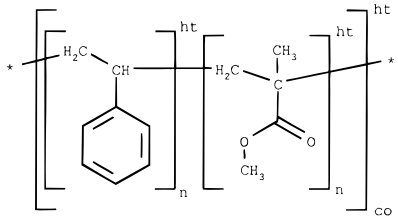
or

$[-[-A-]_n-[-B-]_n-]_{co}$

Example 5.3.1.1. Poly[styrene-co-(methyl methacrylate)]

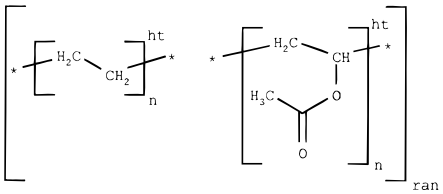


or



Poly(A-*ran*-B) is represented graphically by $[-[-A-]_n- -[-B-]_n-]_{ran}$

Example 5.3.1.2. Poly[ethylene-ran-(vinyl acetate)]

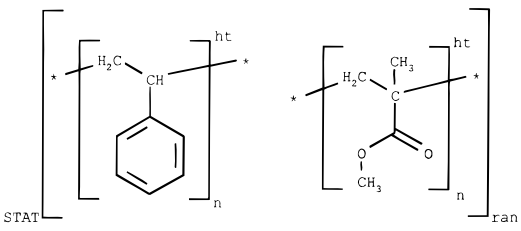


A random polymer with three or more distinct units is most simply represented as a combination of separate SRUs without connecting bonds:

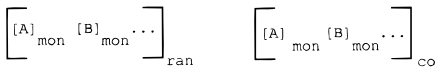
$[-[-A-]_n- -[-B-]_n- -[-C-]_n-]_{ran}$

Statistical copolymers are represented as random copolymers with repeating unit probabilities specified by attached Sgroup data.

Example 5.3.1.3. Poly[styrene-stat-(methyl methacrylate)]

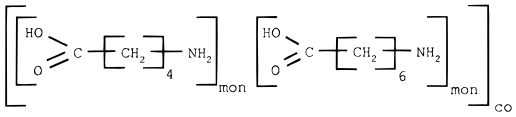


5.3.2. Source-Based Method. Random or unspecified copolymers are represented thus:



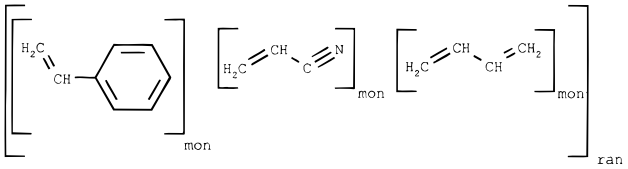
The representation shown as example 5.3.2.1 is used for a polyamide copolymer in which each SMU Sgroup represents a homopolyamide:

Example 5.3.2.1.



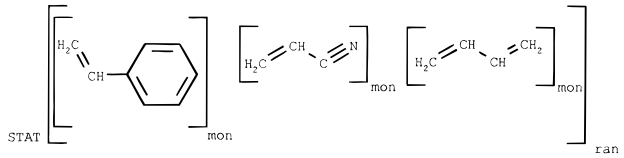
The representation shown as example 5.3.2.2 is used for a random terpolymer of acrylonitrile, butadiene, and styrene:

Example 5.3.2.2.



The representation shown as example 5.3.2.3 is used for a statistical terpolymer of acrylonitrile, butadiene, and styrene:

Example 5.3.2.3.



The STAT indicates that Sgroup data specify the statistical information.

5.4. SCION Nomenclature and Structure Representation. 5.4.1. Structure-Based Method. As shown in Table 3, SCION does not classify as SRUs many classes of polymer that are considered by CAS and IUPAC to be structure-based or SRU polymers. Therefore, discussion here is limited to those types that are classified in SCION as SRUs. Names of copolymers of polyanhydrides, polyethers, and polysulfides are used as examples here. Copolymer names are generated by alphabetizing the individual SRUs, separating them with slashes, and preceding the combination with POLY-. Thus, the copolymer of ethylene oxide and tetrahydrofuran is named

POLY-OXYETHYLENE/OXYTETRAMETHYLENE

This is the only name in the file, and systematic synonyms such as

"POLY-OXYTETRAMETHYLENE/OXYETHYLENE"

or

"OXYTETRAMETHYLENE, POLYMER WITH OXYETHYLENE"

are not used. The slash is critical; without it, the name would read: POLY-OXYETHYLENEOXYTETRAMETHYLENE which is, of course, a different polymer. The SCION record for POLY-OXYETHYLENE/OXYTETRAMETHYLENE is shown as example 5.4.1.1.

Table 10. SCION PMC-Category Polymer Classes

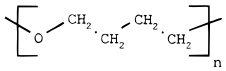
POLYAMIDE
POLYAMIDE-ESTER
POLYAMIDE-ESTER-IMIDE
POLYAMIDE-ESTER-IMIDE-URETHANE
POLYAMIDE-ESTER-URETHANE
POLYAMIDE-IMIDE
POLYAMIDE-IMIDE-URETHANE
POLYAMIDE-URETHANE
POLYESTER
POLYESTER-IMIDE
POLYESTER-IMIDE-URETHANE
POLYESTER-URETHANE
POLYIMIDE
POLYIMIDE-URETHANE
POLYURETHANE

Example 5.4.1.1. SCION representation of the copolymer OXYETHYLENE/OXYTETRAMETHYLENE

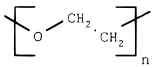
DUPONT PROPRIETARY INFORMATION

CNUM: 289002T
DUP: POLY-OXYETHYLENE/OXYTETRAMETHYLENE
MF: ((C4 H8 O)n . (C2 H4 O)n)x
CI: PMS

COM 1
CNUM 2803L
MF $(C_4\ H_8\ O)_n$
CI PMS, COM



COM 2
CNUM 3719X
MF $(C_2\ H_4\ O)n$
CI PMS, COM



Copolymers in SCION are assumed to be random unless there is information to the contrary in a source document. For polymers specifically identified as random or statistical, the random copolymer is indexed together with controlled terms at the document level; the concepts of random or statistical polymers are not registered at the polymer level.

5.4.2 Source-Based Method. Source-based polymers are divided into two broad categories:

•**Category 1:** Prescribed-monomer condensation (PMC)—condensation polymers of the classes polyamide, polyester, polyimide, polyurethane, and combinations of these, e.g., polyamide ester. In contrast with IUPAC (see section 4.1.2), one-component PMC polymers are registered by the source-based method. The 15 PMC classes are summarized in Table 10.

Regardless of the actual reactants polymerized, monomers in this category are "stylized" to their parents; thus, if terephthaloyl chloride is an actual reactant in a polymerization, terephthalic acid is the stylized monomer stored as a polymer component. Table 11 compares the actual monomers of some typical condensation polymers with their corresponding stylized parents.

Table 11. Comparison of Actual and Stylized Monomers of Some PMC Polymers

actual monomer(s) polymerized	stylized parent (polymer component)
caprolactam	hexanoic acid, 6-amino-
caprolactone	hexanoic acid, 6-hydroxy-
ethylene bis(chloroformate)	ethylene glycol
hexamethylene diisocyanate	1,6-hexanediamine[a]
lactide	lactic acid
phosgene	carbonic acid[b]
pyromellitic anhydride	1,2,4,5-benzenetetracarboxylic acid
terephthaloyl chloride	terephthalic acid

[a] Carbonic acid is omitted as a component of polyurethanes (see also footnote *a* under Table 6). Thus, the polyurethane from hexamethylene diisocyanate and ethylene glycol is named POLYURETHANE-ETHYLENE GLYCOL/1,6-HEXANEDIAMINE, not POLYURETHANE-ETHYLENE GLYCOL/ISOCYANIC ACID, HEXAMETHYLENE ESTER; the carbonic acid component is neither stored as a structural component nor cited in the polymer name (explicitly as CARBONIC or implicitly, e.g., in an isocyanate). However, a poly-**thio**urethane is named as a **polyester** with thiocarbonic acid as a stylized component. [b] Carbonic acid is named and included as a structural component in polycarbonates (which are classified in SCION as polyesters) and polyureas (which are classified in SCION as polyamides). It is also named and included as a structural component in polymers that are both polycarbonates and polyurethanes (polyester-urethanes) and both polyureas and polyurethanes (polyamide-urethanes).

Category 1 (PMC) polymer names consist of CAS 8CI monomer names (see point 5.4.2.1) alphabetized, separated by slashes, and prefaced by a prefix that indicates the PMC polymer class, e.g., POLYAMIDE. There is only one systematic polymer name, and addition of systematic, monomer-based synonyms is omitted. Synonyms such as trade names, acronyms, or trivial names are added. Examples 5.4.2.1 through 5.4.2.3 illustrate the nomenclature style. The absence of carbonic acid as a stylized component of a polyurethane (e.g., example 5.4.2.3) is explained in note *a* under Table 6.

Point 5.4.2.1: SCION does not follow the CAS policy of using the name of an exotic alcohol as the parent even when it is esterified with a common acid; see discussion in section 3.3.

Example 5.4.2.1.

POLYAMIDE-IMIDE-1,2,4-BENZENETRICARBOXYLIC ACID/M-PHENYLENEDIAMINE/P-PHENYLENEDIAMINE

Example 5.4.2.2.

POLYESTER-1,4-BUTANEDIOL/ETHYLENE GLYCOL/TEREPHTHALIC ACID

Example 5.4.2.3.

POLYURETHANE-1,4-BUTANEDIOL/HYDROQUINONE/1,6-HEXANEDIAMINE/1,3-PROPANEDIOL

Derivatives of functional groups that do *not* participate in polymerization are not stylized to the parent functional group. Example 5.4.2.4 illustrates this.

Example 5.4.2.4. Adipoyl chloride and methyl-3,5-diaminobenzoate form a polyamide

POLYAMIDE-ADIPIC ACID/BENZOIC ACID, 3,5-DIAMINO-, METHYL ESTER

•**Category 2:** Actual starting monomer (ASM)—carbon—carbon multiple bond monomers (acetylenic, acrylic, ethylenic, vinyl), and polymers with incompletely identified or unknown structures (e.g., polymers from formaldehyde, melamine, phenol, urea).

Category 2 (ASM) polymer names consist of CAS 8CI monomer names alphabetized, separated by slashes, and prefaced by POLY-. There is only one systematic name, and addition of systematic, monomer-based synonyms is usually omitted. Synonyms such as trade names, acronyms, or trivial names are added. Examples 5.4.2.5 through 5.4.2.7 illustrate the nomenclature style.

Example 5.4.2.5.

POLY-ACRYLONITRILE/METHACRYLIC ACID, METHYL ESTER
Synonyms: POLY-AN/MMA; AN/MMA POLYMER; AN/MMA COPOLYMER

Example 5.4.2.6.

POLY-ETHYLENE/1,4-HEXADIENE/PROPENE
Synonym: POLY-E/14HD/P

Example 5.4.2.7.

POLY-FORMALDEHYDE/MELAMINE
Synonyms: Melamine* 366; MELAMINE-FORMALDEHYDE POLYMER

Source-based registration of PMC and ASM polymers, including end group treatment, is described in detail elsewhere.[16]

"Mixed-class" polymers (e.g., polymers containing monomers from categories 1 and 2) are named with the category 1 (PMC) style part of the name first (polymer class and alphabetized monomers), followed by the category 2 (ASM) part of the name (alphabetized monomers); the two categories are separated by the word **with** in the polymer name—see example 5.4.2.8.

Example 5.4.2.8.

POLYESTER-ETHYLENE GLYCOL/TEREPHTHALIC ACID WITH POLY-STYRENE

5.4.3. Mixed Structure-Based/Source-Based Polymers. Polymers containing monomers and SRUs are named with the PMC monomers first (if any), then the ASM monomers (if any), and then the SRUs. The word **with** is inserted between the categories, and the prefix POLY- is repeated in front of the next group of monomers or SRUs. Examples 5.4.3.1 through 5.4.3.3 illustrate the method, which is described in more detail elsewhere.[16]

Example 5.4.3.1.

POLYAMIDE-ADIPIC ACID/1,6-HEXANEDIAMINE WITH POLY-ETHYLENE

Example 5.4.3.2.

POLYESTER-ETHYLENE GLYCOL/TEREPHTHALIC ACID WITH POLY-OXYETHYLENE

Example 5.4.3.3.

POLYAMIDE-HEXANOIC ACID, 6-AMINO- WITH POLY-ETHYLENE WITH POLY-OXYETHYLENE

Although the presence of the word **with** in these polymer names implies blockiness, they are neither named as a block polymer nor identified with the text descriptor POLY-BLOCK (see section 6.3.4 for SCION block polymers).

SUMMARY AND CONCLUSIONS

Until all four parts are published, any attempt to write a comprehensive summary and conclusions would be premature; this section is therefore postponed until the end of part 4.

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APPENDIX

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