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MACROMOLECULAR DIVISION
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SOURCE-BASED NOMENCLATURE FOR COPOLYMERS

(Recommendations 1985)

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Source-based nomenclature for copolymers

INTRODUCTION

BASIC CONCEPT

CLASSIFICATION AND DEFINITIONS OF COPOLYMERS

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Introduction

Copolymers have gained considerable importance both in scientific research and in industrial applications. A consistent and clearly-defined system for naming these polymers would, therefore, be of great utility. The nomenclature proposals presented here are intended to serve this purpose by setting forth a system for designating the types of monomeric-unit sequence arrangements in copolymer molecules.

In principle, a comprehensive structure-based system of naming copolymers would be desirable. However, such a system presupposes a knowledge of the structural identity of all the constitutional units as well as their sequential arrangements within the polymer molecules; this information is rarely available for the synthetic polymers encountered in practice. For this reason, the proposals presented in this Report embody an essentially source-based nomenclature system.

Application of this system should not discourage the use of structure-based nomenclature whenever the copolymer structure is fully known and is amenable to treatment by the rules for single-strand polymers (Ref. 1 & 2). Further, an attempt has been made to maintain consistency, as far as possible, with the abbreviated nomenclature of synthetic polypeptides published by the IUPAC-IUB Commission on Biochemical Nomenclature (Ref. 3). It is intended that the present nomenclature system supersede the previous recommendations published in 1952 (Ref. 4).

Basic concept

The nomenclature system presented here is designed for copolymers. By definition, copolymers are polymers that are derived from more than one species of monomer (Ref. 5). Various classes of copolymers are discussed, which are based on the characteristic sequence arrangements of the monomeric units within the copolymer molecules. Generally, the names of monomers are used to specify monomeric units; the latter can be named using the trivial, semi-systematic, or systematic form. The classes of copolymers are as follows:

unspecified	(Rule 1)
statistical	(Rule 2.1)
random	(Rule 2.2)
alternating	(Rule 3)
periodic	(Rule 4.1)
block	(Rule 5.1)
graft	(Rule 6.1).

In those cases where copolymer molecules can be described by only one species of constitutional unit in a single sequential arrangement, copolymers are regular polymers (Ref. 5) and can, therefore, be named on a structure basis (Ref. 1 & 2). Examples will be quoted later in the text.

Polymers having monomeric units differing in constitutional or configurational features, but derived from a single monomer, are not regarded as copolymers, in accordance with the basic definitions (Ref. 5). Examples of such polymers, which are not copolymers, are:

- (a) polybutadiene with mixed sequences of 1,2 and 1,4 units;
- (b) poly(methyloxirane), also known as poly(propylene oxide), obtained through polymerization of a mixture of the two enantiomers, R and S, and containing both R and S units.

The nomenclature system presented here can, however, also be applied to such pseudo-copolymers. Polymers having monomeric units differing in constitutional features, but derived from a homopolymer by chemical modification, can be named in the same way, e.g.,:

- (c) partially hydrolysed poly(vinyl acetate) containing both ester and alcohol units.

A closely-related alternative system of nomenclature, which may be preferred in some circumstances, is described in the Appendix.

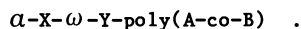
Classification and definition of copolymers

A systematic source-based nomenclature for copolymers must identify the constituent monomers and provide a description of the sequence arrangement of the different types of monomeric units present. According to the present proposals, these objectives are achieved by citing the names of the constituent monomers after the prefix "poly", and by placing between the names of each pair of monomers an italicized connective to denote the kind of arrangement by which those two types of monomeric units are related in the structure. Seven types of sequence arrangement are listed below, together with the corresponding connectives and examples, in which A, B, and C represent the names of monomers. [The citation of A, B, and C is not intended to reflect an order of seniority, unless such seniority is specified in the rules. As a result, more than one name is often possible.]

<u>type</u>	<u>connective</u>	<u>example</u>
unspecified	- <u>co</u> -	poly(A- <u>co</u> -B)
statistical	- <u>stat</u> -	poly(A- <u>stat</u> -B)
random	- <u>ran</u> -	poly(A- <u>ran</u> -B)
alternating	- <u>alt</u> -	poly(A- <u>alt</u> -B)
periodic	- <u>per</u> -	poly(A- <u>per</u> -B- <u>per</u> -C)
block	- <u>block</u> -	polyA- <u>block</u> -polyB
graft	- <u>graft</u> -	polyA- <u>graft</u> -polyB

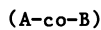
Each of these types of copolymer is considered in more detail below. When the chemical nature of the end groups is to be specified, the name of the copolymer (as described above) is preceded by the systematic names of the terminal units. The prefix α or ω refers to the terminal unit attached to the left or right, respectively, of the structure, as written.

Example:

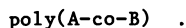


1. Copolymers with an unspecified arrangement of monomeric units

Rule 1 An unspecified sequence arrangement of monomeric units is represented by

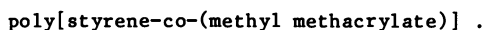


and the corresponding copolymer has the name



Example:

An unspecified copolymer of styrene and methyl methacrylate is named



2. Statistical copolymers

Statistical copolymers are copolymers in which the sequential distribution of the monomeric units obeys known statistical laws; e.g., the monomer sequence distribution may follow Markovian statistics of zeroth (Bernoullian), first, second, or a higher order. Kinetically, the elementary processes leading to the formation of a statistical sequence of monomeric units do not necessarily proceed with equal a priori probability. These processes can lead to various types of sequence distribution comprising those in which the

arrangement of monomeric units tends toward alternation, tends towards clustering of like units, or exhibits no ordering tendency at all (Ref. 6). In simple binary copolymerization, the nature of this sequence distribution can be indicated by the numerical value of a function either of the reactivity ratios or of the related run number (Ref. 6, 7).

The term statistical copolymer is proposed here to embrace a large proportion of those copolymers that are prepared by simultaneous polymerization of two or more monomers in 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 the practice should be abandoned.

Rule 2.1 A statistical sequence arrangement of monomeric units is represented by

(A-stat-B), (A-stat-B-stat-C), etc.,

where stat indicates that the statistical sequence distribution with regard to A, B, C, etc., units is considered to be known. Statistical copolymers are named

poly(A-stat-B), poly(A-stat-B-stat-C), etc.

Examples:

poly(styrene-stat-butadiene)

poly(styrene-stat-acrylonitrile-stat-butadiene) .

Random copolymers. A random copolymer is a special case of a statistical copolymer. It is a statistical copolymer in which the probability of finding a given monomeric unit at any given site in the chain is independent of the nature of the neighbouring units at that position (Bernoullian distribution). In other words, for such a copolymer, the probability of finding a sequence ...ABC... of monomeric units A, B, C..., i.e., $P[\dots ABC \dots]$, is given by

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

where $P[A]$, $P[B]$, $P[C]$, etc. are the unconditional probabilities of the occurrence of various monomeric units. As already noted above, the term "random" should not be used for statistical copolymers except in this narrow sense.

Some authors use the term "random" to denote the Bernoullian case further restricted by the condition that the monomeric units be present in exactly equal amounts (Ref. 8).

Rule 2.2 A random sequence arrangement of monomeric units is represented by

(A-ran-B), (A-ran-B-ran-C), etc.,

where ran indicates a random sequence distribution with regard to A, B, C, etc., units. Random copolymers are named

poly(A-ran-B), poly(A-ran-B-ran-C), etc.

Example:

poly[ethylene-ran-(vinyl acetate)] .

3. Alternating copolymers

An alternating copolymer is a copolymer comprising two species of monomeric units distributed in alternating sequence.

The arrangement

-ABABABAB- or (AB)_n

thus represents an alternating copolymer.

Rule 3 An alternating sequence arrangement of monomeric units is represented by

(A-alt-B)

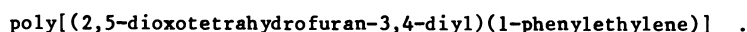
and the corresponding alternating copolymer is named

poly(A-alt-B) .

Example:

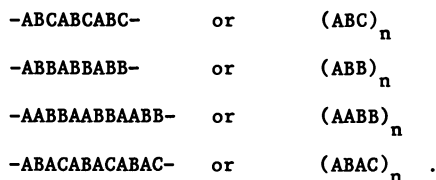


Alternating sequence arrangements can form constitutionally regular structures and may, in those cases, also be named utilizing the structure-based nomenclature for regular single-strand organic polymers. The example above would be then named

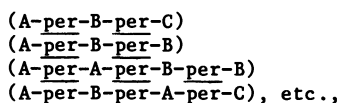


4. Other types of periodic copolymers

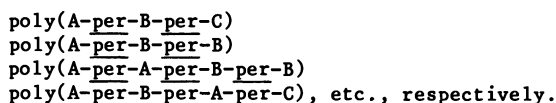
In addition to alternating polymers, other structures are known in which the monomeric units appear in an ordered sequence. Examples are:



Rule 4.1 A periodic sequence arrangement of monomeric units is represented by



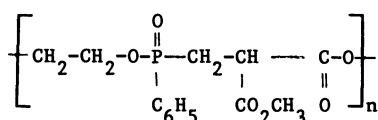
and the corresponding periodic copolymers are named



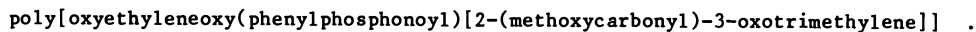
If these polymers are regular, they can also be named according to the structure-based nomenclature for regular single-strand organic polymers (Ref. 1).

Examples:

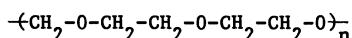
(a) The ternary monomer mixture consisting of ethylene phenylphosphonite, methyl acrylate, and carbon dioxide can yield the periodically sequenced copolymer



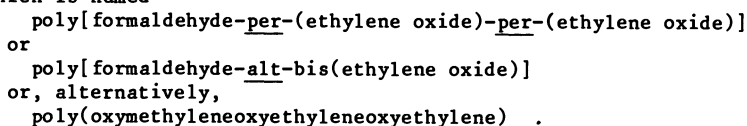
which is named poly[(ethylene phenylphosphonite)-per-(methyl acrylate)-per-(carbon dioxide)] .
The structure-based name is



(b) The binary monomer mixture consisting of formaldehyde and ethylene oxide might yield the periodically sequenced copolymer



which is named



Rule 4.2 If copolymer structures comprise several types of periodic sites, only some of which are always occupied by particular species of monomeric units (A, B...), and sites of the other types are occupied by two or more types of monomeric unit (U, V...) in irregular arrangement, the names of the monomers in the latter sites are embraced by parentheses and are separated by semicolon(s).

Examples:

(a) The copolymer with the sequence arrangement

-AUAVAVAUAVAUAVAU- is named

poly[A-alt-(U;V)] .

(b) The copolymer with the sequence arrangement

-AUBUAVBUAVBVVAUBVVAUBU- is named

poly[A-per-(U;V)-per-B-per-(U;V)] .**5. Block copolymers**

A block polymer is a polymer comprising molecules in which there is a linear arrangement of blocks, a block being defined as a portion of a polymer molecule in which the monomeric units have at least one constitutional or configurational feature absent from the adjacent portions (Ref. 5). In a block copolymer, the distinguishing feature is constitutional, i.e., each of the blocks comprises units derived from a characteristic species of monomer.

In the sequence arrangements

-AAAAAAAA-BBBBBBBBBBBB-
 -AAAAAAAA-BBBBBBBBBBBB-AAAAAAAA-
 -AABABAAABB-AAAAAAAA-BBBBBBBBBBBB-

the sequences -AAAAAAAA-, -BBBBBBBBBBB-, and -AABABAAABB- are blocks.

Rule 5.1 A block sequence arrangement is represented by A_k -block- B_m , A_k -block-(A-stat-B), etc.,

and the corresponding polymers are named

polyA-block-polyB, polyA-block-poly(A-stat-B), etc.,

respectively. If no ambiguity arises, a long dash may be used to designate block connections, as follows:

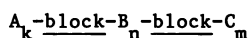
polyA—polyB.

For complex cases, use of block rather than the long dash is always encouraged. The order of citation of the block names corresponds to the order of succession of the blocks in the chain as written from left to right.

Examples:

In the following examples, the subscripts k, m, ... may be indeterminate or specific (see Rule 5.3). In each case, the first line gives a representation of the block sequence arrangement, the second the corresponding name, and the third an illustration of a specific case.

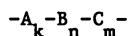
 A_k -block- B_m polyA-block-polyBpolystyrene-block-polybutadiene A_k -block- B_m -block- A_k polyA-block-polyB-block-polyApolystyrene-block-polybutadiene-block-polystyrene(A-stat-B)-block- A_k -block- B_m poly(A-stat-B)-block-polyA-block-polyBpoly(styrene-stat-butadiene)-block-polystyrene-block-polybutadiene



polyA-block-polyB-block-polyC

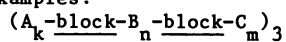
polystyrene-block-polybutadiene-block-poly(methyl methacrylate) .

Rule 5.2 Where a succession of blocks, such as

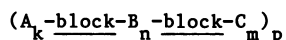


is repeated, the appropriate multiplying prefix is used.

Examples:



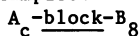
tris(polyA-block-polyB-block-polyC)



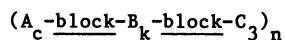
poly(polyA-block-polyB-block-polyC) .

Rule 5.3 When it is possible to specify the chain length of a block, the appropriate Greek prefix (e.g., hecta for 100) may be used rather than poly. Although short sequence lengths are not strictly embraced within the definition of "block", the same device may usefully be employed by using the general prefix "oligo" or the appropriate specific prefix (e.g., tri).

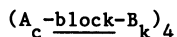
Examples:



oligoA-block-octaB



poly(oligoA-block-polyB-block-triC)



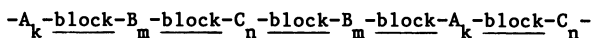
tetrakis(oligoA-block-polyB)

where c is a small integer corresponding to the degree of polymerization of the oligomeric sequence.

Rule 5.4 Those block copolymers, derived from more than two monomers, that also exhibit statistical block sequence arrangements are named according to the principles of Rule 2.1.

Example:

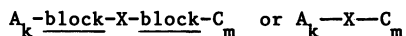
The statistical sequence arrangement



is named

poly(polyA-stat-polyB-stat-polyC) .

Rule 5.5 In the name of block copolymers with blocks connected by way of junction units, X, that are not part of the blocks, the name of the junction unit is inserted in the appropriate place. The connective, -block-, may be omitted. Thus,



is named

polyA-block-X-block-polyC or polyA-X-polyC .

The same designations can be applied to block polymers.

Examples:

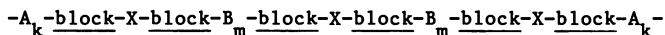
polystyrene-block-dimethylsilylene-block-polybutadiene

or

polystyrene—dimethylsilylene—polybutadiene

polystyrene-block-dimethylsilylene-block-polystyrene
or
polystyrene—dimethylsilylene—polystyrene .

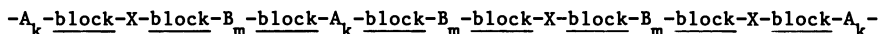
Rule 5.6 A block copolymer wherein A_k and B_m blocks, connected through junctions X, are distributed in statistical manner in the polymer molecules, as in



is named

poly[(polyA-block-X)-stat-(polyB-block-X)] .

A block copolymer wherein A_k and B_m blocks and junction units X are all distributed in statistical manner, as in



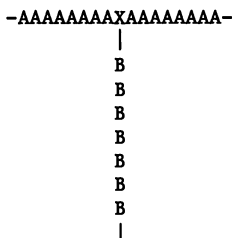
is named

poly(polyA-stat-X-stat-polyB) .

6. Graft copolymers

A graft polymer is a polymer comprising molecules with one or more species of block connected to the main chain as side chains, these side chains having constitutional or configurational features that differ from those in the main chain (Ref. 5). In a graft copolymer the distinguishing feature of the side chains is constitutional, i.e., the side chains comprise units derived from at least one species of monomer different from those which supply the units of the main chain.

Rule 6.1 The simplest case of a graft copolymer can be represented by A_k -graft- B_m or the arrangement



and the corresponding name is

polyA-graft-polyB

where the monomer named first (A in this case) is that which supplied the backbone (main chain) units, while that named second (B) is in the side chain(s).

Examples:

Each of the following examples presents in order, a representation of the graft sequence arrangement, the corresponding name, and an illustration of a specific case.

(a) A_k -graft- B_m

polyA-graft-polyB

polybutadiene-graft-polystyrene
(polystyrene grafted to polybutadiene)

(b) $(A_k\text{-}\underline{\text{block-B}}_m)$ -graft- C_n

(polyA-block-polyB)-graft-polyC

(polybutadiene-block-polystyrene)-graft-polyacrylonitrile
(polyacrylonitrile grafted to a polybutadiene - polystyrene block copolymer at unspecified sites)

(c) $(A\text{-}\underline{\text{stat}}\text{-}B)\text{-}\underline{\text{graft}}\text{-}C_n$ poly(A-stat-B)-graft-polyCpoly(butadiene-stat-styrene)-graft-polyacrylonitrile
(polyacrylonitrile grafted to a statistical butadiene - styrene copolymer at unspecified sites)(d) $A_k\text{-}\underline{\text{block}}\text{-}(B_m\text{-}\underline{\text{graft}}\text{-}C_n)$ polyA-block-(polyB-graft-polyC) or (polyB-graft-polyC)-block-polyApolybutadiene-block-(polystyrene-graft-polyacrylonitrile) or
(polystyrene-graft-polyacrylonitrile)-block-polybutadiene
(polystyrene - polybutadiene block copolymer with polyacrylonitrile grafted to the polystyrene block)(e) $[A_k\text{-}\underline{\text{graft}}\text{-}(B\text{-}\underline{\text{co}}\text{-}C)]\text{-}\underline{\text{block}}\text{-}B_m$ [polyA-graft-poly(B-co-C)]-block-polyB or polyB-block-[polyA-graft-poly(B-co-C)][polybutadiene-graft-poly(styrene-co-acrylonitrile)]-block-polystyrene or
polystyrene-block-[polybutadiene-graft-poly(styrene-co-acrylonitrile)]
(polybutadiene - polystyrene block copolymer with a styrene - acrylonitrile copolymer with an unspecified sequence arrangement of monomeric units grafted to the polybutadiene block) .**Rule 6.2** If more than one type of graft chain is attached to the backbone, semicolons are used to separate the names of the grafts or their symbolic representations.

Example:

 $A_k\text{-}\underline{\text{graft}}\text{-}(B_m;C_n)$ polyA-graft-(polyB;polyC)polybutadiene-graft-[polystyrene;poly(methyl methacrylate)]
(polystyrene and poly(methyl methacrylate) chains grafted to a polybutadiene backbone) .**Rule 6.3** Graft copolymers with known numbers of graft chains are named using numeric prefixes (mono, bis, tris, etc.).

Example:

 $A_k(\text{-}\underline{\text{graft}}\text{-}B_m)_3$ polyA-tris(-graft-polyB)polybutadiene-tris(-graft-polystyrene)
(three polystyrene grafts per polybutadiene backbone) .

If the precise site of grafting is known, it can be specified.

Example:

 $A_{10}\text{-}\underline{\text{block}}\text{-}(X\text{-}\underline{\text{graft}}\text{-}B_m)\text{-}\underline{\text{block}}\text{-}A_{15}$ decaA-block-(X-graft-polyB)-block-pentadecaAdecabutadiene-block-(methylsilanetriyl-graft-polystyrene)-block-pentadecabutadiene .

The system of naming graft copolymers is also applicable, in principle, to "star copolymers", where chains having different constitutional or configurational features are linked through a central moiety.

Examples:

(a) $A_k\text{-}\underline{\text{block}}\text{-}[X(\text{-}\underline{\text{graft}}\text{-}B_m)_2]\text{-}\underline{\text{block}}\text{-}A_k$ or $B_m\text{-}\underline{\text{block}}\text{-}[X(\text{-}\underline{\text{graft}}\text{-}A_k)_2]\text{-}\underline{\text{block}}\text{-}B_m$ polyA-block-[X-bis(-graft-polyB)]-block-polyA or
polyB-block-[X-bis(-graft-polyA)]-block-polyBpolystyrene-block-[silanetetrayl-bis(-graft-polybutadiene)]-block-polystyrene or
polybutadiene-block-[silanetetrayl-bis(-graft-polystyrene)]-block-polybutadiene
(two polystyrene and two polybutadiene chains attached to a central Si atom)

(b) A_k -block-[X-graft-($B_m; C_n$)]-block- D_p

polyA-block-[X-graft-(polyB;polyC)]-block-polyD

polystyrene-block-[silanetetrayl-graft-(polybutadiene;polyisoprene)]-block-poly(methyl methacrylate)

(a polybutadiene chain, a polyisoprene chain, a polystyrene chain, and a poly(methyl methacrylate) chain attached to the same central Si atom) .

In the absence of a seniority rule, several other names are possible.

7. *Polymers made by polycondensation or related polymerization*

The nomenclature system for copolymers is also applicable to polymers made by condensation polymerization of more than one monomeric species, or, more generally, by polymerization of more than one monomeric species where molecules of all sizes (i.e., monomers, oligomers, polymers) can react with each other. One can distinguish the case of polymers made by polycondensation of homopolymerizable monomers from that of polymers made by polycondensation of complementary ingredients that do not usually separately homopolymerize.

Rigorous application of the source-based definition of a copolymer (Ref. 5) embraces polymers such as poly(ethylene terephthalate) or poly(hexamethylene adipamide) (which are commonly regarded as homopolymers) because two ingredients are, in each case, the usual starting materials of polymerization. If polymers of this type have constitutionally regular structures and are regular polymers, the nomenclature for regular single-strand organic polymers can also be used (Ref. 1). This applies, e.g., to the polymer derived from terephthalic acid and ethylene glycol, which by source-based copolymer nomenclature would be named as

poly(ethylene glycol-alt-terephthalic acid)

if in fact the polymer has been prepared by a condensation polymerization starting with terephthalic acid and ethylene glycol. However, if the starting material is the partial ester,



the appropriate source-based name is that of a homopolymer, whereas use of the starting material bis(hydroxyethyl) terephthalate, $\text{HOCH}_2\text{CH}_2\text{OCOC}_6\text{H}_4\text{COOCH}_2\text{CH}_2\text{OH}$ (extensively employed industrially), would suggest the name

poly[bis(hydroxyethyl) terephthalate] .

Regardless of the starting materials used, the structure-based name is

poly(oxyethyleneoxyterephthaloyl) .

The trivial name poly(ethylene terephthalate) is also permitted, because it is so well established in the literature.

For all such polymers made by condensation polymerization of two complementary difunctional ingredients (or "monomers"), which can readily be visualized as reacting on a 1:1 basis to give an "implicit monomer", the homopolymerization of which would give the actual product, the single-strand structure-based nomenclature may be suitable insofar as such a polymer is regular and can be represented as possessing a single constitutional repeating unit. It is to be noted that this is applicable only to cases where the mole ratio of the ingredients is 1:1 and the ingredients are exclusively difunctional.

The introduction of a third component into the reaction system necessitates the use of copolymer nomenclature which can logically be developed from the foregoing rules, as the examples below illustrate. The copolymer derived from reaction of ethylene glycol with a mixture of terephthalic and isophthalic acids would be named:

poly[(ethylene glycol-alt-terephthalic acid)-co-(ethylene glycol-alt-isophthalic acid)] ,

poly(ethylene terephthalate-co-ethylene isophthalate), or

poly[(ethylene glycol)-alt-(terephthalic acid;isophthalic acid)] .

A copolymer formed from oligo(adipic acid-alt-1,4-butanediol) and oligo(2,4-toluenediisocyanate-co-trimethylolpropane) in the presence of trimethylolpropane is named:

poly[oligo(adipic acid-alt-1,4-butanediol)-co-oligo(2,4-toluenediisocyanate-co-trimethylolpropane)-co-trimethylolpropane].

A polymer derived from the condensation polymerization of a single actual monomer, the molecules of which terminate in two different complementary functional groups (e.g., 6-aminohexanoic acid) is, by definition, a (regular) homopolymer. When two different monomers of this type react together, the product is a copolymer that can be named in appropriate fashion. For example, if 6-aminohexanoic acid is copolycondensed with 7-aminoheptanoic acid, leading to a statistical distribution of monomeric units, the product is named:

poly[(6-aminohexanoic acid)-stat-(7-aminoheptanoic acid)].

8. Specification with regard to mass fractions, mole fractions, molar masses, and degrees of polymerization

Whereas subscripts placed immediately after the name of the monomer or the block designate the degree of polymerization or repetition, mass and mole fractions and molar masses -- which in most cases are average quantities -- may be expressed by placing corresponding figures after the complete name or symbol of the copolymer. The order of citation is the same as for the monomer species in the name or symbol of the copolymer. Unknown quantities can be designated by a, b, etc.

Although this scheme can be extended to complicated cases, it is recommended that its application be restricted to simple cases; any treatment of more complicated systems should be explained in the text.

Rule 8.1 Mass fractions, or mass percentages, for the monomeric units are placed in parentheses after the copolymer name, followed by the symbol "w", or the phrase "mass %", respectively. The order of citation in the parentheses is the same as in the name.

Examples:

(a) polybutadiene-graft-polystyrene (0.75:0.25 w) or

polybutadiene-graft-polystyrene (75:25 mass %)

(a graft copolymer containing 75 mass % polybutadiene and 25 mass % grafted polystyrene)

(b) polybutadiene-graft-poly(styrene-stat-acrylonitrile) (0.75:a:b w) or

polybutadiene-graft-poly(styrene-stat-acrylonitrile) (75:a:b mass %)

(a graft copolymer containing 75 mass % of butadiene units as backbone and unknown quantities in statistical arrangement of styrene and acrylonitrile units in the grafted chains)

Rule 8.2 Mole fractions, or mole percentages, for the monomeric units are placed in parentheses after the copolymer name, followed by the symbol "x", or the phrase "mol %", respectively. The order of citation in the parentheses is the same as in the name.

Example:

polybutadiene-graft-polystyrene (0.85:0.15 x) or

polybutadiene-graft-polystyrene (85:15 mol %)

(a graft copolymer containing 85 mol % of butadiene units and 15 mol % of styrene units)

Rule 8.3 The molar mass, relative molecular mass, or degree of polymerization may be included in the scheme of Rules 8.1 and 8.2 by adding the corresponding figures, followed by the symbol \underline{M} , \underline{M}_r , or DP, respectively.

Examples:

polybutadiene-graft-polystyrene (75:25 mass %; 90 000:30 000 \underline{M}_r)

(a graft copolymer consisting of 75 mass % of butadiene units with a relative molecular mass of 90 000 as the backbone, and 25 mass % of styrene units in grafted chains with a relative molecular mass of 30 000)

polybutadiene-graft-polystyrene (1 700:290 DP)

(a graft copolymer consisting of a polybutadiene backbone with a degree of polymerization of 1 700 to which polystyrene with a degree of polymerization of 290 is grafted) .

Appendix

Alternative nomenclature for copolymers

The nomenclature system for copolymers developed in the main text of this Report is designed to meet the requirement of providing a systematic name for any copolymer, however complex the structure; as a result, the systematic names may be undesirably long in some cases. However, many copolymers reported in the literature have relatively simple structures, which do not necessitate this elaborate system. For these simpler cases, a different, more concise nomenclature system is presented here as an alternative.

Fundamental Principles

The alternative nomenclature system is based on the following principles.

(i) A copolymer is described by the prefix "copoly" followed by citation of the names of the monomers used (source-based nomenclature). The prefix is used only once, just as the prefix "poly" is employed only once in naming regular single-strand polymers (called regular polymers hereafter) (Ref. 1) or the simple copolymers described in the main text.

Example:

copoly(styrene/butadiene) .

(ii) The specification of the type of structure in a copolymer (the connectives block, alt, etc. of the main nomenclature system) is shown by an italicized prefix preceding "copoly."

Example:

block-copoly(styrene/butadiene) .

(iii) Only the names of the monomers are included in the main part of the copolymer name; the terminal units are specified before the main name (using the prefixes α and ω), whereas the junction units between blocks are specified after the main name (using the symbol μ).

Example:

block-copoly(styrene/butadiene)- μ -dimethylsilylene .

(iv) The mass fraction, mole fraction, molar mass, or degree of polymerization of monomeric units in copolymers is specified separately in parentheses after the name.

(v) In addition to the principles stated in (i) - (iv), above, some further conventions are used for the more complex copolymers, e.g., where the structure cannot be classified in a unique fashion.

In general, no seniority rule is provided for the order of citation of the monomer names. In block or periodic copolymers, the order of citation of the names of monomers corresponds to the sequence in which the monomeric units occur in the molecules. In graft copolymers, the initially cited name is that of the backbone (main chain).

A.1. Application to simple copolymers

In the examples to be cited below, the name derived from the system elaborated in the main text of this Report is given after the alternative name proposed in this Appendix.

Rule A1.1 The name of a copolymer consists of the prefix "copoly" followed by parentheses in which the names of the monomers used are enumerated, separated by an oblique stroke, as in

copoly(A/B), copoly(A/B/C), etc.,

where A, B, and C represent the names of the monomers employed.

Example:

copoly(styrene/methyl methacrylate)	alternative name
poly(styrene- <u>co</u> -methyl methacrylate)	name from main text

Rule A1.2 The arrangement of monomeric units in a copolymer, if known, is specified by one of the following italicized prefixes: stat- (statistical), ran- (random), alt- (alternating), per- (periodic), block-, or graft- (see Classification and Definitions of Copolymers, in the main text).

Examples:

stat-copoly(styrene/butadiene)
poly(styrene-stat-butadiene)

ran-copoly(ethylene/vinyl acetate)
poly[ethylene-ran-(vinyl acetate)]

alt-copoly(styrene/maleic anhydride)
poly[styrene-alt-(maleic anhydride)]

per-copoly(ethylene phenylphosphonite/methyl acrylate/carbon dioxide)
poly[(ethylene phenylphosphonite)-per-(methyl acrylate)-per-(carbon dioxide)]

block-copoly(styrene/butadiene/methyl methacrylate)
polystyrene-block-polybutadiene-block-poly(methyl methacrylate)

graft-copoly(butadiene/styrene)
polybutadiene-graft-polystyrene .

Rule A1.3 When monomeric units of one particular kind occur in groups in a periodic copolymer, this can be indicated by a "polykis" prefix. The repetition of a set of blocks in a block copolymer for a known or unknown number of times can be represented similarly.

Examples:

per-copoly(A/B/B/B) = per-copoly(A/trisB) = alt-copoly(A/trisB)
poly(A-per-trisB)

block-copoly(A/B/C/A/B/C/A/B/C) = block-copoly[tris(A/B/C)]
tris(polyA-block-polyB-block-polyC)

per-copoly[formaldehyde/bis(ethylene oxide)]
poly[formaldehyde-per-bis(ethylene oxide)] .

Rule A1.4 When one type of site in a basically alternating or periodic copolymer can be occupied by units derived from two or more monomers (such as in the copolymers considered in Rule 4.2 of the main text), the names of the copolymers are based on the principles of the main text and the rules in this Appendix.

Examples:

per-copoly[A/B/(C;D)]
poly[A-per-B-per(C;D)]

alt-copoly[methyl methacrylate/(styrene;l-vinylnaphthalene)]
poly[methyl methacrylate-alt-(styrene;l-vinylnaphthalene)] .

The same procedure can be used to name graft copolymers with two or more different types of branch (B, C, etc.) grafted onto a backbone (A).

Examples:

graft-copoly[A/(B;C)]
polyA-graft-(polyB;polyC)

graft-copoly[butadiene/(styrene;methyl methacrylate)]
polybutadiene-graft-[polystyrene;poly(methyl methacrylate)] .

Rule A1.5 Terminal units (preceded by the prefixes α and ω) are specified before the main copolymer name, but junction units between blocks (preceded by the prefix μ) are specified after the main copolymer name. If one type of junction unit occurs in the structure more than once, the appropriate multiplying prefix (bis, tris, etc.) may be used; if more than one type of junction unit occurs in the structure, they may be designated μ_1, μ_2 , etc.

Examples:

α -butyl- ω -carboxy-block-copoly(styrene/butadiene)
 α -butyl- ω -carboxy-polystyrene-block-polybutadiene

block-copoly(styrene/butadiene)- μ -dimethylsilylene
polystyrene-block-dimethylsilylene-block-polybutadiene

block-copoly(styrene/butadiene/styrene)-bis(μ -dimethylsilylene)
polystyrene-block-dimethylsilylene-block-polybutadiene-block-dimethylsilylene-block-
polystyrene

graft-copoly(butadiene/styrene)-polykis(μ -methylsilanetriyl) .

Rule A1.6 Specification with regard to mass fractions, mole fractions, molar masses, relative molecular masses, and degrees of polymerization is treated as in the rules of Section 8 in the main text.

A2. Application to more complex copolymers

The alternative nomenclature can be extended to copolymers of some complexity. The following rules and examples deal with a few such cases. In general, the nomenclature system described in the main part of this Report will be found preferable for complex structures.

Rule A2 When a graft copolymer or block copolymer contains a constituent block which is itself a copolymer, the block is named

co(B/C)

with a descriptive prefix, if necessary (see Rule A1.2).

Examples:

block-copoly[stat-co(styrene/butadiene)/styrene/butadiene]
poly(styrene-stat-butadiene)-block-polystyrene-block-polybutadiene

block-copoly[styrene/graft-co(butadiene/acrylonitrile)]
polystyrene-block-(polybutadiene-graft-polyacrylonitrile)

graft-copoly[stat-co(butadiene/styrene)/acrylonitrile]
poly(butadiene-stat-styrene)-graft-polyacrylonitrile

block-copoly graft-co[butadiene/-stat-co(styrene/acrylonitrile)]/styrene
[polybutadiene-graft-poly(styrene-stat-acrylonitrile)]-block-polystyrene .

A3. Application to polymers made by polycondensation or related polymerization

The principles of the main text and the rules in this Appendix can be applied to polymers made by polycondensation or related polymerization.

Examples of alternative names:

copoly(6-aminohexanoic acid/7-aminoheptanoic acid)

alt-copoly(ethylene glycol/terephthalic acid)

alt-copoly[ethylene glycol/(terephthalic acid;isophthalic acid)] .

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