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MACROMOLECULAR DIVISION

COMMISSION ON MACROMOLECULAR NOMENCLATURE*

GENERIC SOURCE-BASED NOMENCLATURE FOR POLYMERS

(IUPAC Recommendations 2001)

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Generic source-based nomenclature for polymers

(IUPAC Recommendations 2001)

Abstract: The commission has already published two documents on the source-based names of linear copolymers and nonlinear polymers; however, in some cases this nomenclature leads to ambiguous names. The present document proposes a generic source-based nomenclature that solves these problems and yields clearer source-based names. A generic source-based name comprises two parts:

- 1) polymer class (generic) name followed by a colon
- 2) the actual or hypothetical monomer name(s), always parenthesized in the case of a copolymer

The formula, the structure-based name, the source-based name, and the generic source-based name of the polymer are given for each example in the document. In some cases, only generic source-based give unambiguous names, for example, when a polymer has more than one name or when it is obtained through a series of intermediate structures. The rules concern mostly polymers with one or more types of functional group or heterocyclic system in the main chain, but to some extent they are also applicable to polymers with side-groups, carbon-chain polymers such as vinyl or diene polymers, spiro and cyclic polymers, and networks.

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1. INTRODUCTION

The IUPAC Commission on Macromolecular Nomenclature has published three documents [1–3] on the structure-based nomenclature for polymers that enable most polymers, except networks, to be named. The Commission has also produced two documents [4,5] on the source-based nomenclature of linear copolymers and nonlinear polymers. In general, source-based names are simpler and less rigorous than structure-based names. However, there are cases in which the simplicity of the source-based nomenclature leads to ambiguous names for polymers. For example, the condensation of a dianhydride (A) with a diamine (B) gives first a polyamide-acid, which can be cyclized to a polyimide; however, both products have the same name poly(A-*alt*-B) according to current source-based nomenclature. If the class name of the polymer “amide-acid” or “imide” is incorporated in the name, differentiation is easily accomplished. Even in cases where only a single product is formed, use of the class name (generic name) may help to clarify the structure of the polymer, especially if it is very complex.

Examples of ambiguous names exist also for homopolymers. The source-based name “polybutadiene” does not indicate whether the structure is 1,2-, 1,4-*cis*-, or 1,4-*trans*-; supplementary information is needed to distinguish between the possibilities.

It is the objective of the present document to introduce a generic nomenclature system to solve these problems, and to yield better source-based names.

Most trivial names, such as polystyrene, are source-based names. Hitherto, the Commission has not systematically recommended source-based names for homopolymers because it considered that the more rigorous structure-based names were more appropriate for scientific communications. However, since the publication of "Nomenclature of Regular Single-Strand Organic Polymers" in 1976, scientists, in both industry and academia, have continued to use trivial names. Even the Commission itself adopted (1985) a source-based nomenclature for copolymers owing to its simplicity and practicality. Based on these facts, the Commission has now decided to recommend source-based nomenclature as an alternative official nomenclature for homopolymers. In this document, the rules for generating source-based names for homopolymers are described. Consequently, source-based and structure-based names are available for most polymers.

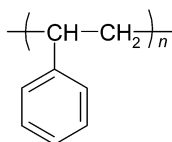
Names of the monomers in the source-based names of polymers should preferably be systematic but they may be trivial if well established by usage. Names of the organic groups, as parts of constitutional repeating units (CRU) in structure-based names, are those based on the principles of organic nomenclature and recommended by the 1993 *A Guide to IUPAC Nomenclature of Organic Compounds* [6].

2. SOURCE-BASED NOMENCLATURE FOR HOMOPOLYMERS

RULE 1

The source-based name of a homopolymer is made by combining the prefix "poly" with the name of the monomer. When the latter consists of more than one word, or any ambiguity is anticipated, the name of the monomer is parenthesized.

Example 1.1



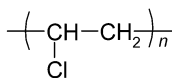
Source-based name:

polystyrene

Structure-based name:

poly(1-phenylethylene)

Example 1.2



Source-based name:

poly(vinyl chloride)

Structure-based name:

poly(1-chloroethylene)

3. GENERIC NOMENCLATURE

3.1 Fundamental principles

The basic concept for generic source-based nomenclature is very simple; just add the polymer class name to the source-based name of the polymer. Addition of the polymer class name is frequently

OPTIONAL; in some cases, the addition is necessary to avoid ambiguity or to clarify. However, the addition is undesirable if it fails to add clarification.

The system presented here can be applied to almost all homopolymers, copolymers, and others, such as networks. However, generic source-based nomenclature should not be considered as a third nomenclature system to be added to the other two systems of nomenclature; it must be considered as an auxiliary system and a simple extension of current source-based nomenclature. When the generic part of the name is eliminated from the name of a polymer, the well-established source-based name remains.

3.2 General rules

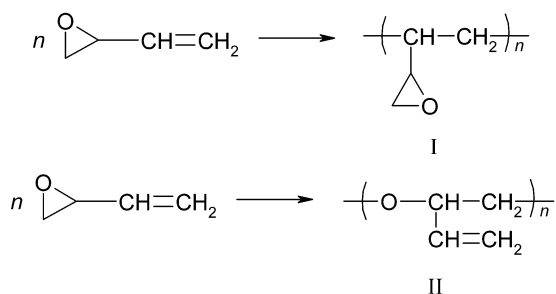
RULE 2

A generic source-based name of a polymer has two components in the following sequence: (1) a polymer class (generic) name (polyG) followed by a colon and (2) the actual or hypothetical monomer name(s) (A, B, etc.), always parenthesized in the case of a copolymer. In the case of a homopolymer, parentheses are introduced when it is necessary to improve clarity.



- Note 1** The polymer class name (generic name) describes the most appropriate type of functional group or heterocyclic ring system.
- Note 2** All the rules given in the two prior documents on source-based nomenclature [4,5] can be applied to the present nomenclature system, with the addition of the generic part of the name.
- Note 3** A polymer may have more than one name; this usually occurs when it can be prepared in more than one way.
- Note 4** If a monomer or a pair of complementary monomers can give rise to more than one polymer, or if the polymer is obtained through a series of intermediate structures, the use of generic nomenclature is essential (see examples 2.1, 2.3, and 2.4).

Example 2.1



Generic source-based name:

- I. polyalkylene:vinylloxirane
- II. polyether:vinylloxirane

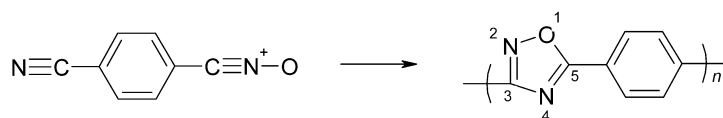
Source-based names:

- I and II have the same source-based name: poly(vinylloxirane).

Structure-based names:

- I. poly(1-oxiranylethylene)
- II. poly[(oxy(1-vinylethylene)]

Example 2.2



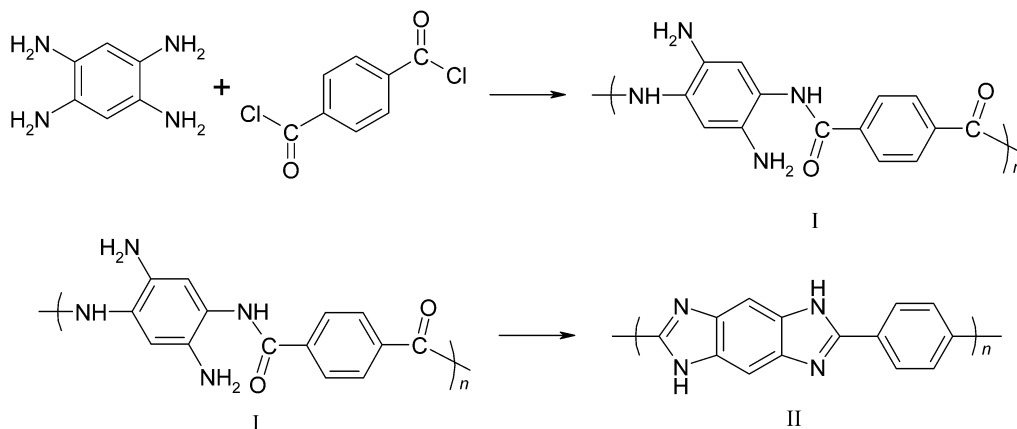
Generic source-based name:

polyoxadiazole:(4-cyanobenzonitrile *N*-oxide)

Structure-based name:

poly(1,2,4-oxadiazole-3,5-diyl-1,4-phenylene)

Example 2.3



Generic source-based name:

I. polyamide:[(terephthaloyl dichloride)-*alt*-benzene-1,2,4,5-tetramine]

II. polybenzimidazole:[(terephthaloyl dichloride)-*alt*-benzene-1,2,4,5-tetramine]

Source-based name:

I and II have the same source-based name:

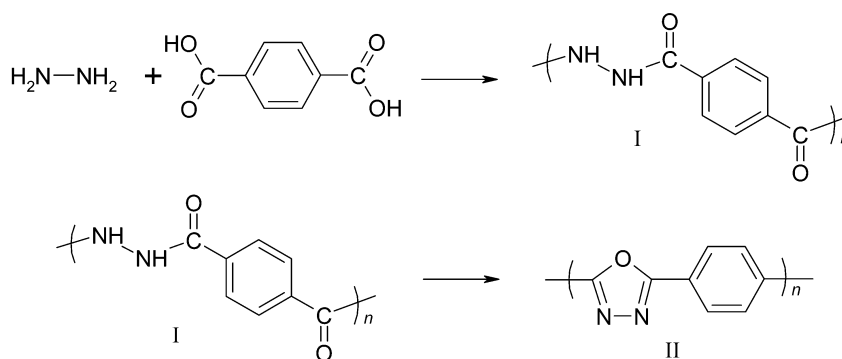
poly[(terephthaloyl dichloride)-*alt*-benzene-1,2,4,5-tetramine]

Structure-based names:

I. poly[imino (2,5-diamino-1,4-phenylene)iminoterephthaloyl]

II. poly[(1,5-dihydrobenzo[1,2-*d*:4,5-*d'*]diimidazole-2,6-diyl)-1,4-phenylene]

Example 2.4



Generic source-based names:

I. polyhydrazide:[hydrazine-*alt*-(terephthalic acid)]

II. polyoxadiazole:[hydrazine-*alt*-(terephthalic acid)]

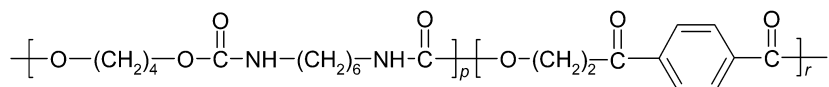
Source-based name:

I and II have the same source-based name: poly[hydrazine-*alt*-(terephthalic acid)]

Structure-based names:

- I. poly(hydrazine-1,2-diylterephthaloyl)
- II. poly(1,3,4-oxadiazole-2,5-diyl-1,4-phenylene)

Example 2.5



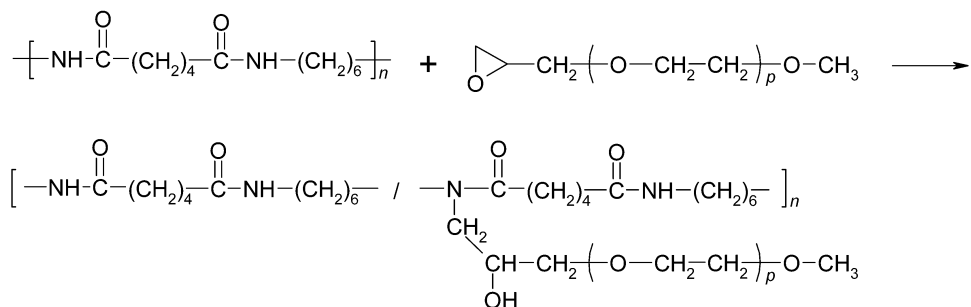
Generic source-based names:

polyurethane:[butane-1,4-diol-*alt*-(hexane-1,6-diyl diisocyanate)]-*block*-polyester:
[(ethylene glycol)-*alt*-(terephthalic acid)]

Structure-based name:

poly(oxybutane-1,4-diyloxycarbonyliminohexane-1,6-diyliminocarbonyl)-*block*-poly(oxyethyleneoxyterephthaloyl)

Example 2.6



Generic source-based name:

polyamide:[hexane-1,6-diamine-*alt*-(adipic acid)]-*graft*-polyether:(ethylene oxide)

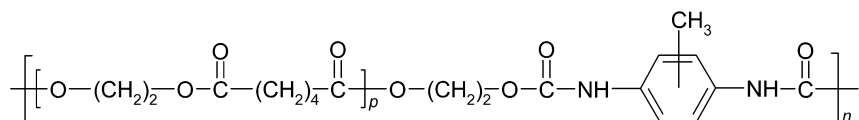
Note 5 It is assumed that this reaction is limited to only one graft for each CRU.

RULE 3

When more than one type of functional group or heterocyclic system is present in the polymer structure, names should be alphabetized; for example, poly(GG'):(A-*alt*-B).

Note 6 It is preferable, but not mandatory, to cite all generic classes.

Example 3.1



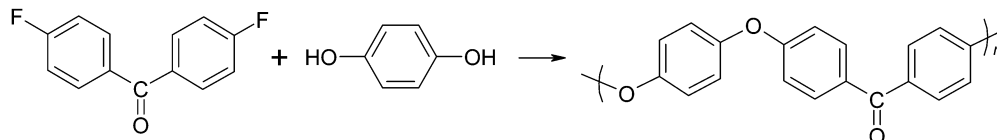
Generic source-based name:

polyesterurethane:{ α,ω -dihydroxyoligo[(ethylene glycol)-*alt*-(adipic acid)]-*alt*-(2,5-tolylene diisocyanate)}

Structure-based name:

poly{[oligo(oxyethyleneoxyadipoyl)]oxyethyleneoxycarbonylimino(x-methyl-1,4-phenylene) iminocarbonyl}

Example 3.2



Generic source-based name:

polyetherketone:(4,4'-difluorobenzophenone-*alt*-hydroquinone)

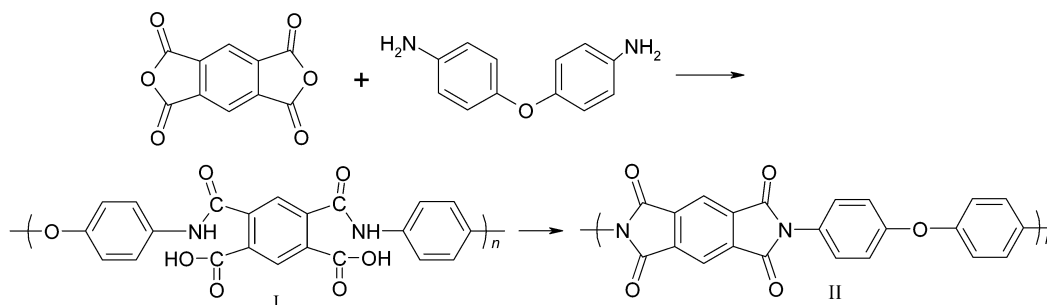
Structure-based name:

poly(oxy-1,4-phenyleneoxy-1,4-phenylenecarbonyl-1,4-phenylene)

RULE 4

Polymer class names relevant only to the main chain are specified in the name; names of side-chain functional groups may also be included after a hyphen if they are formed during the polymerization reaction.

Example 4.1



Generic source-based names:

I. poly(amide-acid):[(pyromellitic dianhydride)-*alt*-(4,4'-oxydianiline)]

(Both carboxy groups result from the polymerization reaction.)

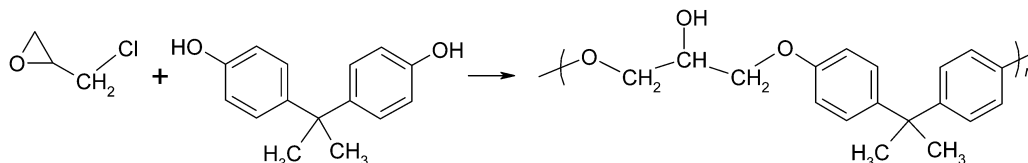
II. polyimide:[(pyromellitic dianhydride)-*alt*-(4,4'-oxydianiline)]

Structure-based names:

I. poly[oxy-1,4-phenyleneiminocarbonyl(4,6-dicarboxy-1,3-phenylene)carbonylimino-1,4-phenylene]

II. poly[(5,7-dihydro-1,3,5,7-tetraoxobenzo[1,2-*c*:4,5-*c'*]dipyrrole-2,6(1*H*,3*H*)-diyl)-1,4-phenyleneoxy-1,4-phenylene]

Example 4.2



Generic source-based names:

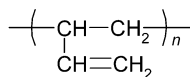
poly(ether-alcohol):(epichlorohydrin-*alt*-bisphenol A)

Structure-based name:

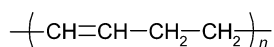
poly[oxy(2-hydroxypropane-1,3-diyl)oxy-1,4-phenylene(1-methylethane-1,1-diyl)-1,4-phenylene]

RULE 5

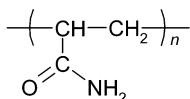
In the case of carbon-chain polymers such as vinyl polymers or diene polymers, the generic name is to be used only when different polymer structures may arise from a given monomeric system.

Example 5.1

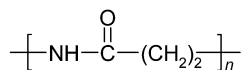
Generic source-based name:
polyalkylene:(buta-1,3-diene)
Source-based name:
poly(buta-1,3-diene)
Structure-based name:
poly(1-vinylethylene)

Example 5.2

Generic source-based name:
polyalkenylene:buta-1,3-diene
Source-based name:
poly(buta-1,3-diene)
Structure-based name:
poly(but-1-ene-1,4-diyl)

Example 5.3

Generic source-based name:
polyalkylene:acrylamide
Structure-based name:
poly[1-(aminocarbonyl)ethylene]

Example 5.4

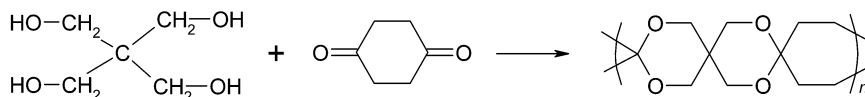
Generic source-based name:
polyamide:acrylamide
Structure-based name:
poly[imino(1-oxopropane-1,3-diyl)]

Note 7 The terms polyalkylene and polyalkenylene have been defined in ref. 7, p. 149.

4. FURTHER APPLICATIONS OF GENERIC NAMES

Generic source-based nomenclature can be extended to more complicated polymers such as spiro and cyclic polymers and networks.

Example 6.1



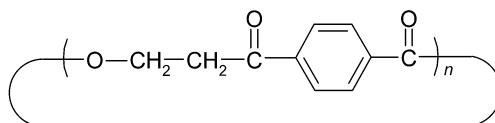
Generic source-based name:

polyspiroketal: {[2,2-bis(hydroxymethyl)propane-1,3-diol]-*alt*-cyclohexane-1,4-dione}
or polyspiroketal:(pentaerythritol-*alt*-cyclohexane-1,4-dione)

Structure-based name:

poly[2,4,8,10-tetraoxaspiro[5.5]undecane-3,3,9,9-tetrayl-9,9-bis(ethylene)]

Example 6.2

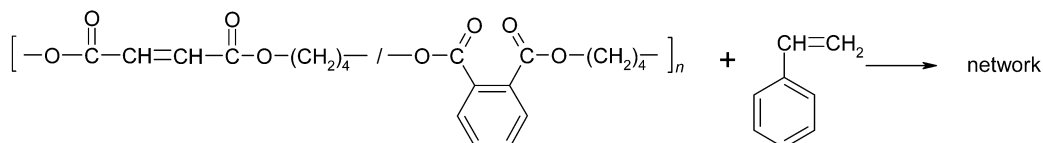


Generic source-based name:

cyclo-polyester: [(ethylene glycol)-*alt*-(terephthalic acid)]

Note 8 There is no IUPAC nomenclature for cyclic polymers.

Example 6.3



Generic source-based name:

polyester: {butane-1,4-diol-*alt*-[(maleic anhydride);(phthalic anhydride)]}-*net*-polyalkylene:
(maleic anhydride)-*co*-styrene]

5. REFERENCES

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