

INTERNATIONAL UNION OF PURE  
AND APPLIED CHEMISTRY

MACROMOLECULAR DIVISION  
COMMISSION ON MACROMOLECULAR NOMENCLATURE\*

**STRUCTURE-BASED NOMENCLATURE  
FOR IRREGULAR SINGLE-STRAND  
ORGANIC POLYMERS**

(IUPAC Recommendations 1994)

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# **Structure-based nomenclature for irregular single-strand organic polymers (IUPAC Recommendations 1994)**

## Synopsis

There is no accepted practice for the naming of many types of irregular polymers. This document describes a structure-based nomenclature system for irregular single-strand organic polymers, i.e., single-strand organic polymers that can be described by the repetition of more than one type of constitutional unit or that comprise constitutional units not all connected identically with respect to directional sense. The new system names irregular polymers for which the source-based system is inadequate, e.g., polymers that have undergone partial chemical modification, homopolymers having both head-to-tail and head-to-head arrangements of monomeric units, and polymers derived from a single monomer that can provide more than one kind of monomeric unit. In addition, it provides a structure-based alternative to source-based nomenclature for copolymers. Irregular polymers, oligomers, or blocks are named by placing the prefix "poly" before the structure-based names of the constitutional units; the latter are collectively enclosed in parentheses, with the names of the component constitutional units separated by oblique strokes. Block copolymers are named by using dashes for the bonding of blocks with each other and with junction units. With graft and star polymers, the grafts or the arms, respectively, are considered to be substituents to the main chain, and the structure is named in the same way as a regular or irregular polymer.

## Introduction

Previous reports from this Commission have presented structure-based systems for naming regular single-strand organic polymers (Refs. 1,2). These are polymers whose molecules can be described by only a single type of constitutional repeating unit in a single sequential arrangement (Ref. 3). A source-based system for naming copolymers, which are mostly irregular, has also been published (Ref. 4).

This document describes a structure-based nomenclature system for irregular single-strand organic polymers, i. e., single-strand organic polymers that can be described by the repetition of more than one type of constitutional unit or that comprise constitutional units not all connected indentially with respect to directional sense. The new system names irregular polymers for which the source-based system is inadequate (e. g., polymers that have undergone partial chemical modification, homopolymers having both head-to-tail and head-to-head arrangements of monomeric units, and polymers derived from a single monomer that can provide more than one kind of monomeric unit) and in addition it offers a structure-based alternative to source-based nomenclature for copolymers (Ref. 4).

## Basic Principles

Irregular polymers or blocks are named by placing the prefix "poly" before the structure-based names of the constitutional units, collectively enclosed in parentheses or brackets, with the individual constitutional units separated by oblique strokes. A typical name derived from this new system is

poly(A/B),

which represents an irregular polymer consisting of the constitutional units A and B.

Block copolymers in which the sequential arrangement of regular blocks is known are named by using dashes for the bonding of blocks with each other and with junction units:

poly(A)—X<sub>A</sub>—poly(B)—X<sub>B</sub>—poly(C)—X<sub>C</sub>—...

where A,B,C,... are the names of constitutional units and X<sub>A</sub>,X<sub>B</sub>,X<sub>C</sub>... are the names of junction units.

The procedure for structure-based naming of irregular single-strand polymers is as follows:

1. Write the structure of the polymer chain based on available information.

2. Select and orient the minimum number of constitutional units necessary to represent the polymer structure (Ref. 1); where there is a choice, selection is based on the seniority rules of Ref. 1\*. Structures are written to be read from left to right.
3. To be certain that the selected constitutional units are the correct ones, combine their individual structures in all possible ways to form a polymer chain. Incorrect constitutional units will give chain segments that do not correspond to the polymer structure or description as written.
4. Name the constitutional units according to the rules of organic (Refs. 5 and 6) and structure-based polymer (Ref. 1) nomenclatures\*\*.
5. Write the name of the polymer as described in the following rules.

Note: The fact that specific structural information, such as the location of substituents, is missing can be conveyed in the polymer name through the symbols ?-, x-, or ( $n_1$  or  $n_2$ ), where  $n_1$  and  $n_2$  are possible number locants.

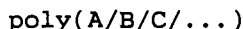
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\* The seniority of constitutional units is heterocyclic rings > hetero atoms in a chain > carbocyclic rings > acyclic carbon chains. Unsaturation is senior to saturation. Within these groups, seniority runs in the sequence: rings with nitrogen > rings with other hetero atoms > ring systems with the largest number of rings > the largest ring > a ring system having the greatest number of hetero atoms > a ring system containing the greatest variety of hetero atoms > a ring system having the greatest number of hetero atoms highest in the order given in the following list. Among hetero atoms, the order of seniority is O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Hg with other atoms placed in the order according to their positions in the periodic table. The seniority in carbocyclic ring systems follows the order: the largest number of rings > the largest ring > the lowest locant numbers for points of attachment. Other things being equal, seniority is based on substituents in the following order: the acyclic chain with the largest number of substituents > the chain having substituents with lowest locants > the alphabetical order of substituents. Further details and examples are given in Ref. 1.

\*\* Rules of organic nomenclature are under continuous development. In this document, many of the changes recommended in the latest (Ref. 6) organic rules have been incorporated, and in some cases, the resulting names differ from those in Ref. 1. Ref. 6 does provide for flexibility, and it allows the use of many trivial names; where the older names are retained, it is because of common usage.

### Rules for Naming Irregular Polymers

Rule 1. Polymers with an irregular arrangement of constitutional units are named



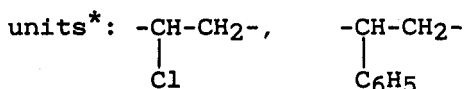
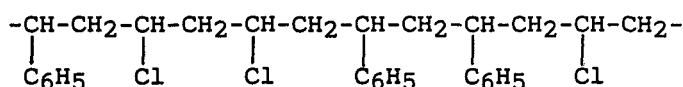
where A, B, C, ... are the structure-based names of the appropriate constitutional units, separated by oblique strokes. The preferred order for the citation of constitutional units is alphabetical.

Note 1: The oblique strokes specify that the sequential arrangement of the constitutional units is unknown.

Note 2: The constitutional unit can also be a regular or irregular block.

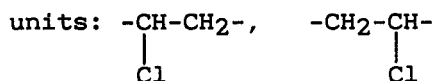
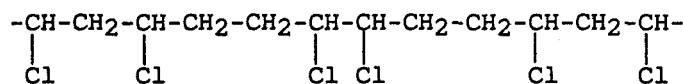
#### Examples

- 1.1 A statistical copolymer consisting of units derived from 1-phenylethene and 1-chloroethene joined head-to-tail:



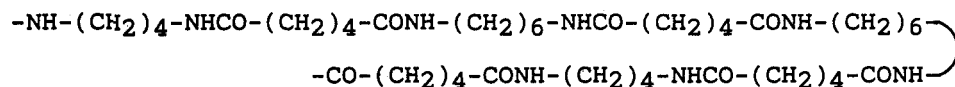
name: poly(1-chloroethylene/1-phenylethylene).

- 1.2 An irregular polymer derived from 1-chloroethene, the units of which are linked both head-to-tail and head-to-head:



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

- 1.3 A polyamide derived from adipoyl dichloride and a mixture of hexane-1,6-diamine and butane-1,4-diamine:



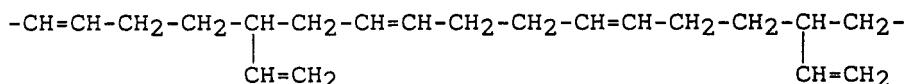
\* The term "units" in the examples refers to constitutional units.

units:  $-\text{NH}-(\text{CH}_2)_4-\text{NHCO}-(\text{CH}_2)_4-\text{CO}-$ ,  
 $-\text{NH}-(\text{CH}_2)_6-\text{NHCO}-(\text{CH}_2)_4-\text{CO}-$

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

Note: The constitutional units are selected on the basis of seniority of their constituent parts, and they are cited alphabetically.

- 1.4 A polymer consisting of units derived from the 1,4 and 1,2 polymerization of buta-1,3-diene:

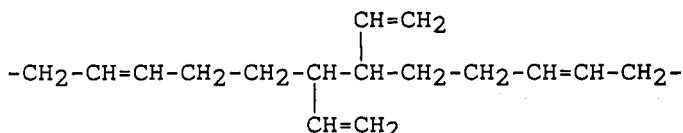


units:  $-\text{CH}=\text{CH}-\text{CH}_2-\text{CH}_2-$ ,  $-\underset{\text{CH}=\text{CH}_2}{\text{CH}}-\text{CH}_2-$

name: poly(but-1-ene-1,4-diyl/1-vinylethylene).

Note: The choice of the constitutional units is dictated by the seniority rules of Ref. 1, i. e., but-1-ene-1,4-diyl is senior to but-2-ene-1,4-diyl.

- 1.5 A polymer consisting of units derived from 1,4 polymerization and both head-to-head and head-to-tail 1,2 polymerization of buta-1,3-diene:

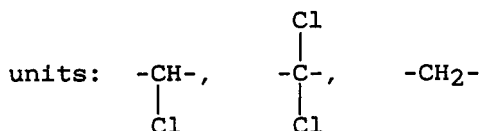
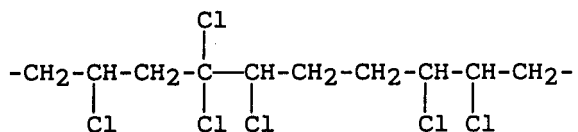


units:  $-\text{CH}_2-\text{CH}=\text{CH}-\text{CH}_2-$ ,  $-\underset{\text{CH}=\text{CH}_2}{\text{CH}}-\text{CH}_2-$ ,  $-\text{CH}_2-\overset{\text{CH}=\text{CH}_2}{\text{CH}}-$

name: poly(but-2-ene-1,4-diyl/1-vinylethylene/2-vinylethylene).

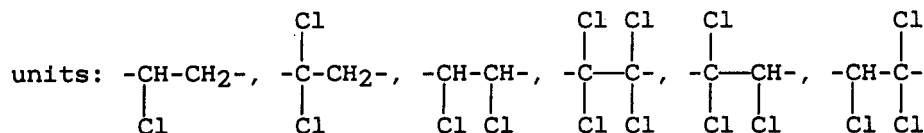
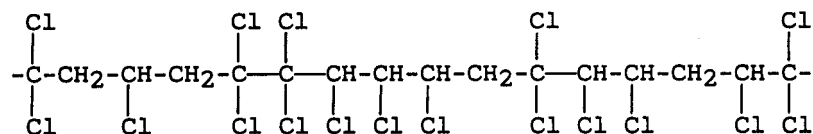
Note: But-1-ene-1,4-diyl would not be selected as a constitutional unit to represent the structure given above because its use would also require the use of the units of but-2-ene-1,4-diyl, vinylmethylene, and methylene, thus violating the principle of minimizing the number of constitutional units. In addition, the combination of the selected units, like methylene, generates chain segments that do not correspond to the polymer structure as written, such as propane-1,3-diyl.

## 1.6 A chlorinated poly(methylene):



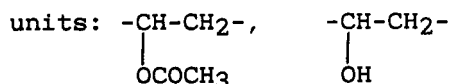
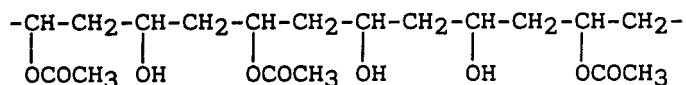
name: poly(chloromethylene/dichloromethylene/methylene).

## 1.7 A chlorinated poly(1-chloroethylene); any methylene units are necessarily separated by an odd number of carbon atoms:



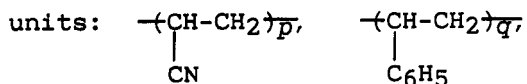
name: poly(1-chloroethylene/1,1-dichloroethylene/1,2-dichloroethylene/tetrachloroethylene/1,1,2-trichloroethylene/1,2,2-trichloroethylene)

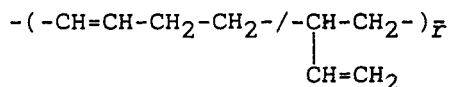
## 1.8 A partially hydrolyzed head-to-tail poly(1-acetoxyethylene):



name: poly(1-acetoxyethylene/1-hydroxyethylene)

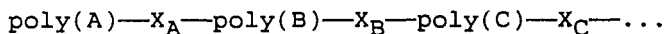
## 1.9 A polymer that consists of an irregular sequence of blocks of poly(1-cyanoethylene), poly(1-phenylethylene), and the irregular block corresponding to example 1.4:



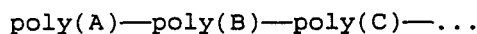


name: poly[poly(but-1-ene-1,4-diyl/1-vinylethylene)/poly(1-cyanoethylene)/poly(1-phenylethylene)].

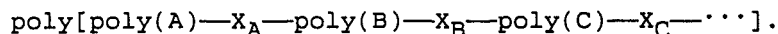
**Rule 2.** Irregular polymers with regular or irregular blocks and junction units in a specific sequential arrangement are named by linking the names of the blocks and junction units with dashes:



where A, B, C, ... are the structure-based names of the appropriate constitutional units and  $X_A$ ,  $X_B$ ,  $X_C$  ... are the structure-based names of the junction units. The order of citation of the block names corresponds to the order of the blocks in the chain as written from left to right (Ref. 4). If there are no junction units, or they are not known, the polymer is named



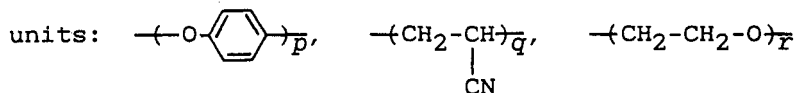
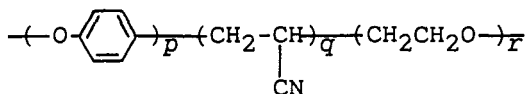
A polymer consisting of repeated specific sequences is named



Note: Since the Rules for seniority distinguishing between blocks have not been defined, use of seniority rules of Ref. 1 for blocks is regarded as one possibility. An alternative is shown in the Notes to Ex 2.1.

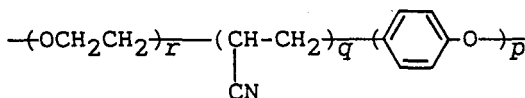
#### Examples

2.1 A triblock copolymer consisting of a sequence of three blocks joined directly or through unspecified junction units:



name: poly(oxy-1,4-phenylene)-poly(2-cyanoethylene)-poly(ethyleneoxy)

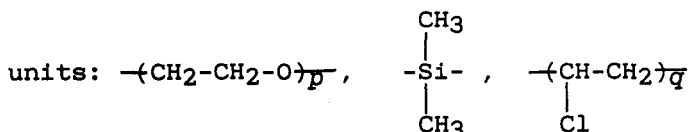
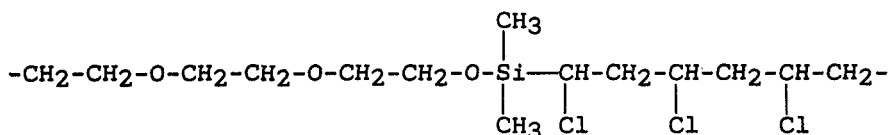
Note: A second possibility is





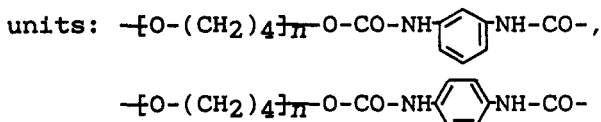
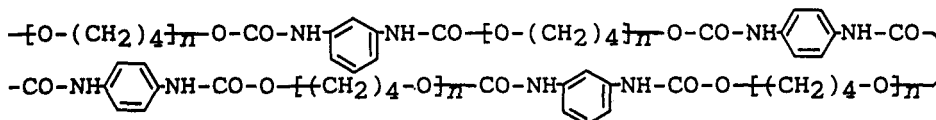
name: poly(oxyethylene)—poly(1-cyanoethylene)—  
poly(1,4-phenyleneoxy)

- 2.2 A diblock copolymer in which the blocks are joined by a specific junction unit, as in the polymer:



name: poly(ethyleneoxy)—dimethylsilanediyl—poly(1-chloroethylene).

- 2.3 A segmented polyurethane consisting of poly(oxybutane-1,4-diyl) blocks joined through junction units derived from 1,3- and 1,4-phenylene diisocyanate and arranged alternately:



name: poly[poly(oxybutane-1,4-diyl)—oxycarbonylimino-1,3-phenyleneiminocarbonyl—poly(oxybutane-1,4-diyl)—oxycarbonylimino-1,4-phenyleneiminocarbonyl]

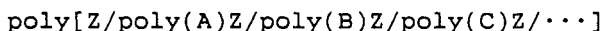
**Rule 3.** Irregular polymers in which polymer or oligomer chains are attached to the main chain (as in graft copolymers) are named as follows. The attached polymer or oligomer chains are considered to be substituents to the main chain and named in the same way as regular polymers (Ref. 1) or irregular polymers (cf. Rules 1 and 2) but without the suffix -yl. The atom in the attached chains nearest to the point of attachment to the main chain is given the locant 1.

**Note 1:** A graft copolymer with poly(A) blocks grafted to the main chain of a regular polymer consisting of constitutional units Z is named



where poly(A) is the substituent on constitutional unit Z.

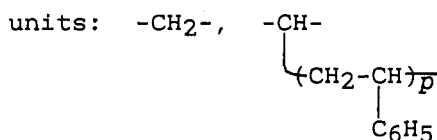
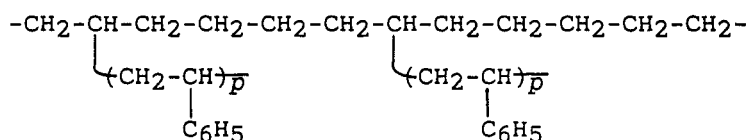
Note 2: A graft copolymer having several kinds of grafts attached to the main chain of a regular polymer consisting of constitutional units Z is named



where poly(A), poly(B), poly(C), ... are substituents on the constitutional unit Z.

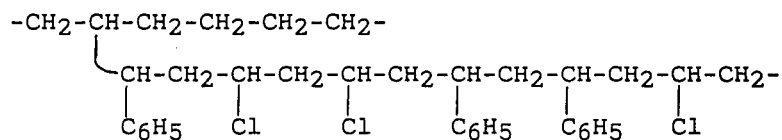
### Examples

3.1 A graft copolymer with many of one type of graft unit:



name: poly[methylene/poly(2-phenylethylene)methylene].

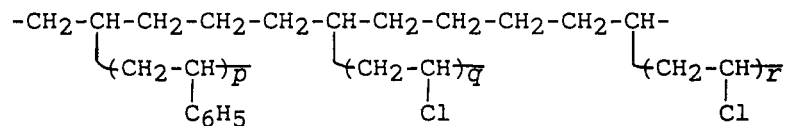
3.2 A graft copolymer with many of one type of graft unit, itself a copolymer consisting of two kinds of constitutional units, 1-chloroethylene and 1-phenylethylene:

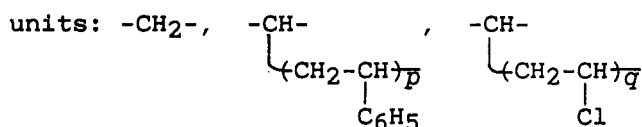


name: poly[methylene/poly(1-chloroethylene/1-phenylethylene)methylene]

Note: The graft is the copolymer specified in Ex. 1.1.

3.3 A graft copolymer with two types of graft units:

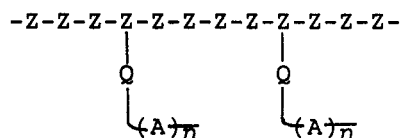




name: poly[methylene/poly(2-chloroethylene)methylene/  
poly(2-phenylethylene)methylene]

**Rule 4.** Irregular polymers in which polymer or oligomer chains are attached to the main chain through a constitutional unit (linking unit) different from the constitutional unit of the side chain are named as follows. The polymer or oligomer side chains are considered to be substituents to the linking unit and named as in Rule 3. The side chain together with the linking unit, taken as a whole, is considered to be a substituent to the main chain. In forming the name, the atom in the linking unit nearest to the point of attachment to the main chain is given the locant 1.

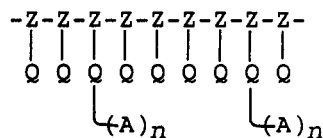
Note 1: A graft copolymer having the structure



i.e., with poly(A) blocks attached through linking unit Q to a regular polymer consisting of constitutional units -Z-, is named

poly{Z/[poly(A)Q]Z}.

Note 2: A graft copolymer having the structure

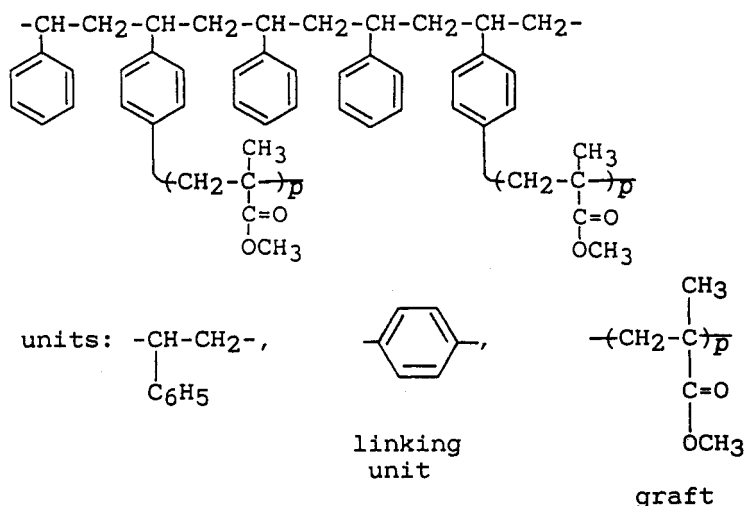


i. e., with poly(A) blocks attached to substituent Q in a regular polymer consisting of constitutional units -(Q)Z-, is named

poly{(Q)Z/[poly(A)Q]Z}.

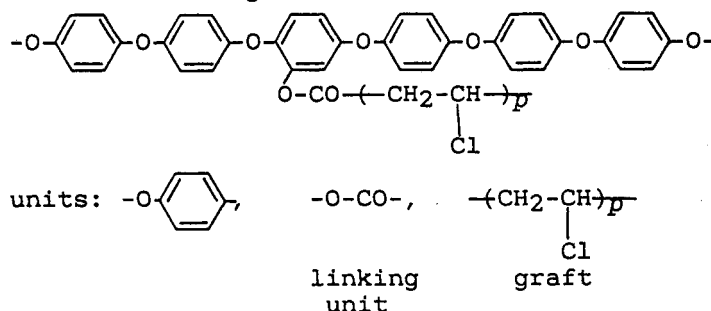
### Examples

4.1 A poly(1-phenylethylene) with poly[2-(methoxycarbonyl)-2-methylethylene] grafts on some of the phenyl groups:



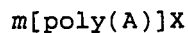
name: poly(1-phenylethylene/1-(4-poly[2-(methoxycarbonyl)-2-methylethylene]phenyl)ethylene).

- 4.2 A poly(oxyphenylene) with a poly(2-chloroethylene) block grafted through a carbonyloxy group to the 2-position in some of the rings:



name: poly{oxy-1,4-phenylene/oxy-2-[poly(2-chloroethylene)-carbonyloxy]-1,4-phenylene}

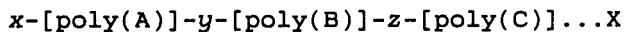
**Rule 5.** In irregular polymers in which a central unit is substituted with three or more blocks, i.e., star polymers, the blocks are treated as substituents to a single central unit. A star polymer having identical blocks as its arms is named



where  $m$  represents a Greek multiplicative prefix (tris, tetrakis...) denoting the number of poly(A) substituents on the central unit X. If the number of arms is undefined, the star polymer is named



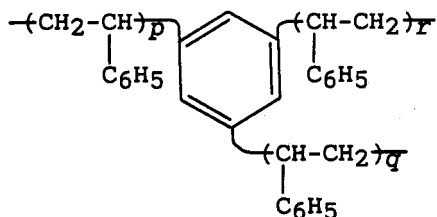
A star polymer having different blocks as its arms is named



where  $x, y, z\dots$  are locants for positions on the central unit  $X$ . The atom in the blocks nearest to the central unit is given the locant 1.

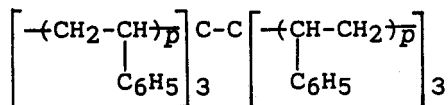
### Examples

- 5.1 A three-armed star polymer in which poly(1-phenylethylene) blocks are linked to a benzene ring at specified positions:



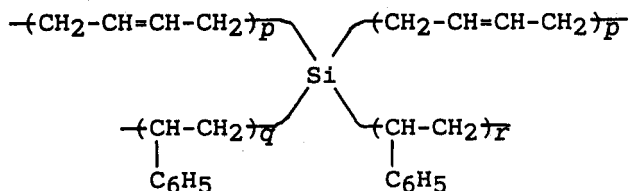
name: 1,3,5-tris[poly(1-phenylethylene)]benzene.

- 5.2 A six-armed star polymer consisting of ethane substituted with poly(1-phenylethylene) blocks:



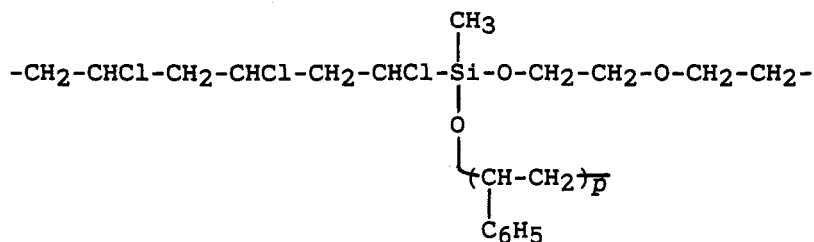
name: hexakis[poly(1-phenylethylene)]ethane.

- 5.3 A four-armed star polymer consisting of silane substituted with different polymer blocks:



name: bis[poly(but-2-ene-1,4-diyl)][poly(1-phenylethylene)][poly(2-phenylethylene)]silane.

- 5.4 A three-armed star polymer consisting of silane substituted with poly(1-chloroethylene), poly(oxyethylene) and poly(1-phenylethylene) blocks, the latter of which is linked to the central unit through oxygen as a linking unit.



name: [poly(1-chloroethylene)][poly(oxyethylene)][poly(1-phenylethylene)oxy]methylsilane.

**Rule 6.** Names of end-groups are prefixed to the name of the polymer and denoted by the Greek letters  $\alpha$  and  $\omega$ . When bonding of the end groups to specific constitutional units is unknown, the irregular polymer is named



where R and R' are the names of the end groups. To specify bonding between end groups and constitutional units, the end group is combined with the attached constitutional unit prior to naming.

#### Examples

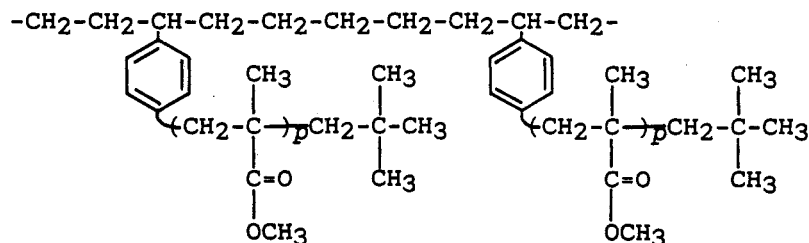
6.1 The copolymer described in Ex.1.1 with specified end groups:

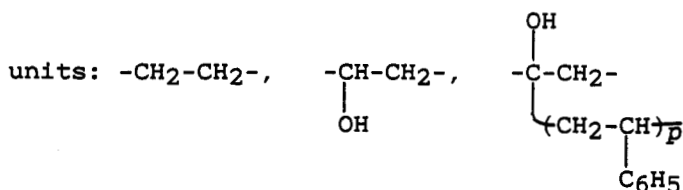
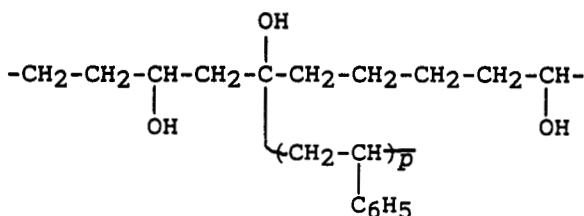
name:  $\alpha$ -chloro- $\omega$ -(trichloromethyl)-poly(1-chloroethylene/1-phenylethylene).

6.2 The copolymer described in 6.1 in which the trichloromethyl group is connected to the 2-position of a 1-phenylethylene unit and the chlorine to the 1-position of a 1-chloroethylene unit:

name:  $\alpha$ -(2,2-dichloroethyl)- $\omega$ -(3,3,3-trichloro-1-phenylpropyl)-poly(1-chloroethylene/1-phenylethylene)

6.3 The graft copolymer in which the grafts have specified end groups:



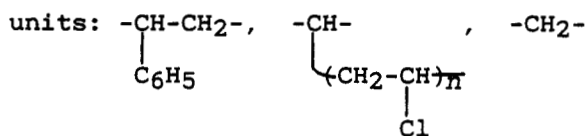
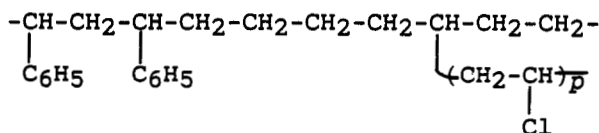


name: poly{ethylene/1-hydroxyethylene/1-hydroxy-1-[poly(2-phenylethylene)]ethylene}.

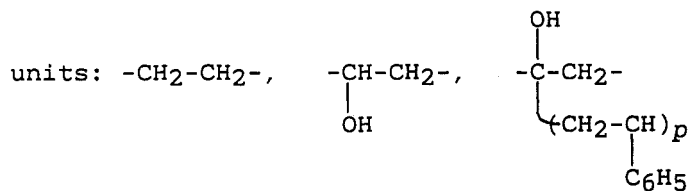
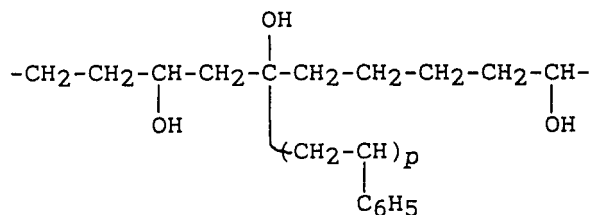
Note: If the grafting point is not known, the graft copolymer is named

poly{ethylene/1-hydroxyethylene/x-[poly(2-phenylethylene)]-ethylene/x-[poly(2-phenylethylene)]-1-hydroxyethylene}.

- 8.3 A diblock copolymer consisting of a block of poly(methylene) grafted with poly(1-chloroethylene) and a block of poly(1-phenylethylene), the structure of which is:



name: poly(1-phenylethylene)—poly[methylene/poly(2-chloroethylene)methylene].

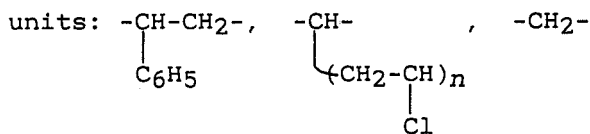
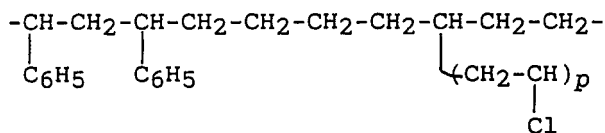


name: poly{ethylene/1-hydroxyethylene/1-hydroxy-1-[poly(2-phenylethylene)]ethylene}.

Note: If the grafting point is not known, the graft copolymer is named

poly{ethylene/1-hydroxyethylene/x-[poly(2-phenylethylene)]-ethylene/x-[poly(2-phenylethylene)]-1-hydroxyethylene}.

8.3 A diblock copolymer consisting of a block of poly(methylene) grafted with poly(1-chloroethylene) and a block of poly(1-phenylethylene), the structure of which is:



name: poly(1-phenylethylene)-poly[methylene/poly(2-chloroethylene)methylene].



## References

1. IUPAC. Commission on Macromolecular Nomenclature, "Nomenclature of regular single-strand organic polymers (rules approved 1975)", Pure Appl. Chem. 48, 373-385 (1976). Reprinted as Chapter 5 in "Compendium of Macromolecular Nomenclature" (The Purple Book), Blackwell Scientific Publications, Oxford (1991).
2. IUPAC. Commission on Macromolecular Nomenclature and Commission on Nomenclature of Inorganic Chemistry, "Nomenclature for regular single-strand and quasi single-strand inorganic and coordination polymers (rules approved 1984)", Pure Appl. Chem. 57, 149-168 (1985). Reprinted as Chapter 6 in "Compendium".
3. IUPAC. Commission on Macromolecular Nomenclature, "Basic definitions of terms relating to polymers (rules approved 1974)", Pure Appl. Chem. 40, 479-491 (1974). Reprinted as Chapter 1 in "Compendium".
4. IUPAC. Commission on Macromolecular Nomenclature, "Source-based nomenclature for copolymers (rules approved 1985)", Pure Appl. Chem. 57, 1427-1440 (1985). Reprinted as Chapter 7 in "Compendium".
5. IUPAC. Commission on Nomenclature of Organic Chemistry, "Nomenclature of organic chemistry (1979 edition)", Pergamon Press, Oxford.
6. IUPAC. Commission on Nomenclature of Organic Chemistry, "A guide to IUPAC nomenclature of organic chemistry (rules approved 1992)", in press.

## ERRATUM

The April 1994 issue of *Pure and Applied Chemistry* (Volume 66, No. 4) included the IUPAC Recommendation 'Structure-based nomenclature for irregular single-strand organic polymers' prepared by a Working Group consisting of R. B. Fox, N. M. Bikales, K. Hatada and J. Kahovec. Unfortunately, pages 887 and 888 were printed incorrectly. The full article is therefore reproduced in its entirety on the following pages, which should be used to replace those in the faulty printed copies.

Blackwell Scientific Publications apologizes to the authors and to the readers for this error.

INTERNATIONAL UNION OF PURE  
AND APPLIED CHEMISTRY

MACROMOLECULAR DIVISION  
COMMISSION ON MACROMOLECULAR NOMENCLATURE\*

**STRUCTURE-BASED NOMENCLATURE  
FOR IRREGULAR SINGLE-STRAND  
ORGANIC POLYMERS**

(IUPAC Recommendations 1994)

*Prepared by a Working Group consisting of*

R. B. FOX (USA); N. M. BIKALES (USA); K. HATADA (Japan) and J. KAHOVEC (Czech Republic)

\*Membership of the Commission during the preparation of this report (1985–93) was as follows:

*Titular Members:* G. Allegra (Italy, to 1989); R. E. Bareiss (FRG, to 1993); N. M. Bikales (USA, *Secretary* to 1987); K. Hatada (Japan, Associate Member from 1987, Titular Member from 1989); A. D. Jenkins (UK, to 1985, Associate Member to 1987); J. Kahovec (Czech Republic, Associate Member from 1987, Titular Member from 1991); P. Kratochvil (Czech Republic, *Chairman* to 1991); E. Maréchal (France, Associate Member from 1991, Titular Member from 1993); W. V. Metanowski (USA, Associate Member from 1987, Titular Member from 1991); I. Mita (Japan, to 1989, Associate Member to 1991); C. Noël (France, to 1993); I. M. Papisov (Russia, to 1987, Associate Member to 1991); V. P. Shibaev (Russia, from 1987); R. F. T. Stepto (UK, Associate Member from 1987, Titular Member from 1989, *Chairman* from 1991); U. W. Suter (Switzerland, to 1991, Associate Member to 1993); W. J. Work (USA, Associate Member from 1985, *Secretary* from 1987).

*Associate Members contributing to this report:* J. V. Aleman (Spain, from 1987); M. Baron (Argentina, National Representative from 1987, Associate Member from 1991); Jung-Il Jin (Korea, National Representative from 1991, Associate Member from 1993); R. H. Marchessault (Canada, to 1987); K. Matyjaszewski (USA, from 1991); S. Penczek (Poland, from 1993); L. Shi (PR China, from 1987); P. Sigwalt (France, to 1987); S. K. Tripathy (USA, to 1991).

*Others contributing to this report:* K. L. Loening (USA, National Representative to 1987); N. Platé (Russia, National Representative to 1991, from 1993); A. Sirigu (Italy, National Representative from 1991).

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# **Structure-based nomenclature for irregular single-strand organic polymers (IUPAC Recommendations 1994)**

## Synopsis

There is no accepted practice for the naming of many types of irregular polymers. This document describes a structure-based nomenclature system for irregular single-strand organic polymers, i.e., single-strand organic polymers that can be described by the repetition of more than one type of constitutional unit or that comprise constitutional units not all connected identically with respect to directional sense. The new system names irregular polymers for which the source-based system is inadequate, e.g., polymers that have undergone partial chemical modification, homopolymers having both head-to-tail and head-to-head arrangements of monomeric units, and polymers derived from a single monomer that can provide more than one kind of monomeric unit. In addition, it provides a structure-based alternative to source-based nomenclature for copolymers. Irregular polymers, oligomers, or blocks are named by placing the prefix "poly" before the structure-based names of the constitutional units; the latter are collectively enclosed in parentheses, with the names of the component constitutional units separated by oblique strokes. Block copolymers are named by using dashes for the bonding of blocks with each other and with junction units. With graft and star polymers, the grafts or the arms, respectively, are considered to be substituents to the main chain, and the structure is named in the same way as a regular or irregular polymer.

## Introduction

Previous reports from this Commission have presented structure-based systems for naming regular single-strand organic polymers (Refs. 1,2). These are polymers whose molecules can be described by only a single type of constitutional repeating unit in a single sequential arrangement (Ref. 3). A source-based system for naming copolymers, which are mostly irregular, has also been published (Ref. 4).

This document describes a structure-based nomenclature system for irregular single-strand organic polymers, i. e., single-strand organic polymers that can be described by the repetition of more than one type of constitutional unit or that comprise constitutional units not all connected indentially with respect to directional sense. The new system names irregular polymers for which the source-based system is inadequate (e. g., polymers that have undergone partial chemical modification, homopolymers having both head-to-tail and head-to-head arrangements of monomeric units, and polymers derived from a single monomer that can provide more than one kind of monomeric unit) and in addition it offers a structure-based alternative to source-based nomenclature for copolymers (Ref. 4).

## Basic Principles

Irregular polymers or blocks are named by placing the prefix "poly" before the structure-based names of the constitutional units, collectively enclosed in parentheses or brackets, with the individual constitutional units separated by oblique strokes. A typical name derived from this new system is

poly(A/B),

which represents an irregular polymer consisting of the constitutional units A and B.

Block copolymers in which the sequential arrangement of regular blocks is known are named by using dashes for the bonding of blocks with each other and with junction units:

poly(A)—X<sub>A</sub>—poly(B)—X<sub>B</sub>—poly(C)—X<sub>C</sub>—...

where A,B,C,... are the names of constitutional units and X<sub>A</sub>,X<sub>B</sub>,X<sub>C</sub>... are the names of junction units.

The procedure for structure-based naming of irregular single-strand polymers is as follows:

1. Write the structure of the polymer chain based on available information.

2. Select and orient the minimum number of constitutional units necessary to represent the polymer structure (Ref. 1); where there is a choice, selection is based on the seniority rules of Ref. 1\*. Structures are written to be read from left to right.
3. To be certain that the selected constitutional units are the correct ones, combine their individual structures in all possible ways to form a polymer chain. Incorrect constitutional units will give chain segments that do not correspond to the polymer structure or description as written.
4. Name the constitutional units according to the rules of organic (Refs. 5 and 6) and structure-based polymer (Ref. 1) nomenclatures\*\*.
5. Write the name of the polymer as described in the following rules.

Note: The fact that specific structural information, such as the location of substituents, is missing can be conveyed in the polymer name through the symbols ?-, x-, or ( $n_1$  or  $n_2$ ), where  $n_1$  and  $n_2$  are possible number locants.

---

\* The seniority of constitutional units is heterocyclic rings > hetero atoms in a chain > carbocyclic rings > acyclic carbon chains. Unsaturation is senior to saturation. Within these groups, seniority runs in the sequence: rings with nitrogen > rings with other hetero atoms > ring systems with the largest number of rings > the largest ring > a ring system having the greatest number of hetero atoms > a ring system containing the greatest variety of hetero atoms > a ring system having the greatest number of hetero atoms highest in the order given in the following list. Among hetero atoms, the order of seniority is O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Hg with other atoms placed in the order according to their positions in the periodic table. The seniority in carbocyclic ring systems follows the order: the largest number of rings > the largest ring > the lowest locant numbers for points of attachment. Other things being equal, seniority is based on substituents in the following order: the acyclic chain with the largest number of substituents > the chain having substituents with lowest locants > the alphabetical order of substituents. Further details and examples are given in Ref. 1.

\*\* Rules of organic nomenclature are under continuous development. In this document, many of the changes recommended in the latest (Ref. 6) organic rules have been incorporated, and in some cases, the resulting names differ from those in Ref. 1. Ref. 6 does provide for flexibility, and it allows the use of many trivial names; where the older names are retained, it is because of common usage.

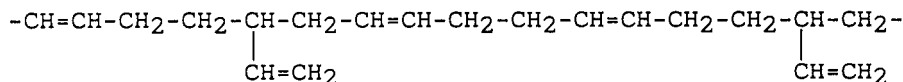


units:  $-\text{NH}-(\text{CH}_2)_4-\text{NHCO}-(\text{CH}_2)_4-\text{CO}-$ ,  
 $-\text{NH}-(\text{CH}_2)_6-\text{NHCO}-(\text{CH}_2)_4-\text{CO}-$

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

Note: The constitutional units are selected on the basis of seniority of their constituent parts, and they are cited alphabetically.

1.4 A polymer consisting of units derived from the 1,4 and 1,2 polymerization of buta-1,3-diene:

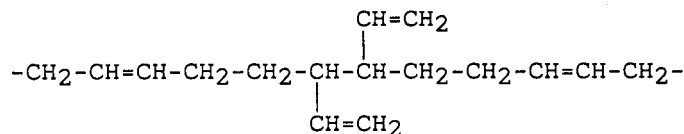


units:  $-\text{CH}=\text{CH}-\text{CH}_2-\text{CH}_2-$ ,  $-\underset{\text{CH}=\text{CH}_2}{\text{CH}}-\text{CH}_2-$

name: poly(but-1-ene-1,4-diyl/1-vinylethylene).

Note: The choice of the constitutional units is dictated by the seniority rules of Ref. 1, i. e., but-1-ene-1,4-diyl is senior to but-2-ene-1,4-diyl.

1.5 A polymer consisting of units derived from 1,4 polymerization and both head-to-head and head-to-tail 1,2 polymerization of buta-1,3-diene:



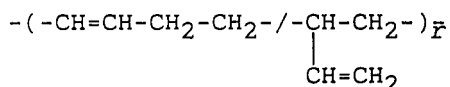
units:  $-\text{CH}_2-\text{CH}=\text{CH}-\text{CH}_2-$ ,  $-\underset{\text{CH}=\text{CH}_2}{\text{CH}}-\text{CH}_2-$ ,  $-\text{CH}_2-\overset{\text{CH}=\text{CH}_2}{\text{CH}}-$

name: poly(but-2-ene-1,4-diyl/1-vinylethylene/2-vinylethylene).

Note: But-1-ene-1,4-diyl would not be selected as a constitutional unit to represent the structure given above because its use would also require the use of the units of but-2-ene-1,4-diyl, vinylmethylene, and methylene, thus violating the principle of minimizing the number of constitutional units. In addition, the combination of the selected units, like methylene, generates chain segments that do not correspond to the polymer structure as written, such as propane-1,3-diyl.

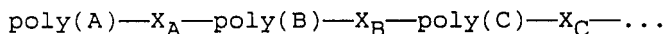




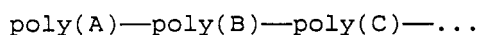


name: poly[poly(but-1-ene-1,4-diyl/1-vinylethylene)/poly(1-cyanoethylene)/poly(1-phenylethylene)].

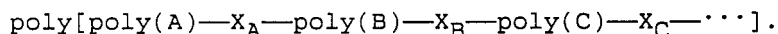
**Rule 2.** Irregular polymers with regular or irregular blocks and junction units in a specific sequential arrangement are named by linking the names of the blocks and junction units with dashes:



where A, B, C, ... are the structure-based names of the appropriate constitutional units and  $X_A$ ,  $X_B$ ,  $X_C$ , ... are the structure-based names of the junction units. The order of citation of the block names corresponds to the order of the blocks in the chain as written from left to right (Ref. 4). If there are no junction units, or they are not known, the polymer is named



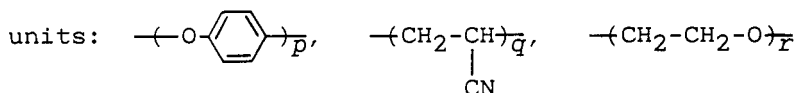
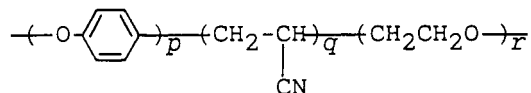
A polymer consisting of repeated specific sequences is named



**Note:** Since the Rules for seniority distinguishing between blocks have not been defined, use of seniority rules of Ref. 1 for blocks is regarded as one possibility. An alternatives is shown in the Notes to Ex 2.1.

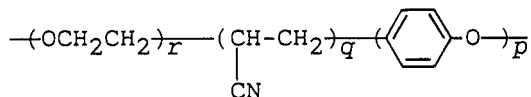
### Examples

2.1 A triblock copolymer consisting of a sequence of three blocks joined directly or through unspecified junction units:



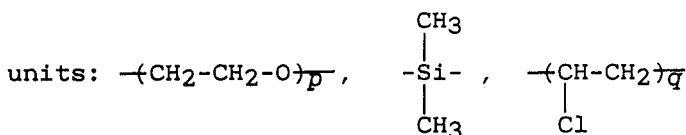
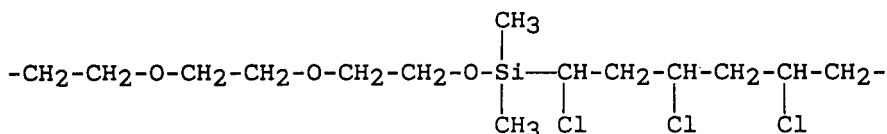
name: poly(oxy-1,4-phenylene)—poly(2-cyanoethylene)—poly(ethyleneoxy)

**Note:** A second possibility is



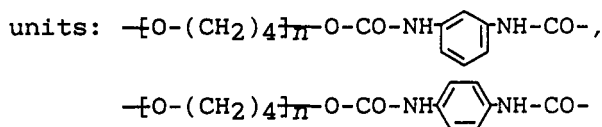
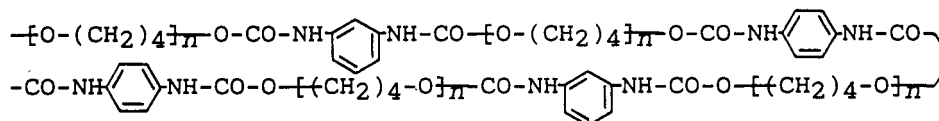
name: poly(oxyethylene)—poly(1-cyanoethylene)—  
poly(1,4-phenyleneoxy)

- 2.2 A diblock copolymer in which the blocks are joined by a specific junction unit, as in the polymer:



name: poly(ethyleneoxy)—dimethylsilanediyl—poly(1-chloroethylene).

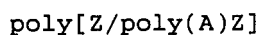
- 2.3 A segmented polyurethane consisting of poly(oxybutane-1,4-diyl) blocks joined through junction units derived from 1,3- and 1,4-phenylene diisocyanate and arranged alternately:



name: poly[poly(oxybutane-1,4-diyl)—oxycarbonylimino-1,3-phenyleneiminocarbonyl—poly(oxybutane-1,4-diyl)—oxycarbonylimino-1,4-phenyleneiminocarbonyl]

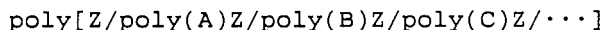
**Rule 3.** Irregular polymers in which polymer or oligomer chains are attached to the main chain (as in graft copolymers) are named as follows. The attached polymer or oligomer chains are considered to be substituents to the main chain and named in the same way as regular polymers (Ref. 1) or irregular polymers (cf. Rules 1 and 2) but without the suffix -yl. The atom in the attached chains nearest to the point of attachment to the main chain is given the locant 1.

Note 1: A graft copolymer with poly(A) blocks grafted to the main chain of a regular polymer consisting of constitutional units Z is named



where poly(A) is the substituent on constitutional unit Z.

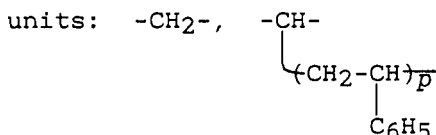
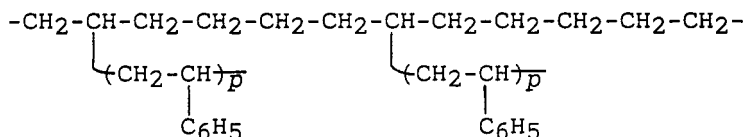
Note 2: A graft copolymer having several kinds of grafts attached to the main chain of a regular polymer consisting of constitutional units Z is named



where poly(A), poly(B), poly(C), ... are substituents on the constitutional unit Z.

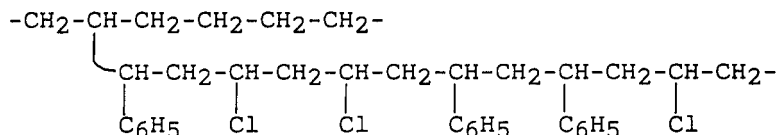
### Examples

3.1 A graft copolymer with many of one type of graft unit:



name: poly[methylene/poly(2-phenylethylene)methylene].

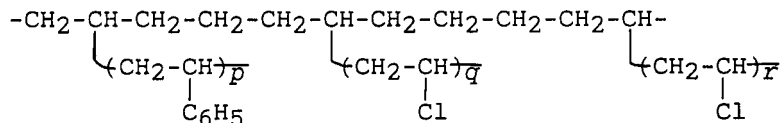
3.2 A graft copolymer with many of one type of graft unit, itself a copolymer consisting of two kinds of constitutional units, 1-chloroethylene and 1-phenylethylene:



name: poly[methylene/poly(1-chloroethylene/1-phenylethylene)methylene]

Note: The graft is the copolymer specified in Ex. 1.1.

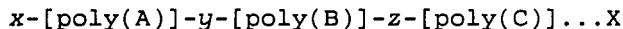
3.3 A graft copolymer with two types of graft units:







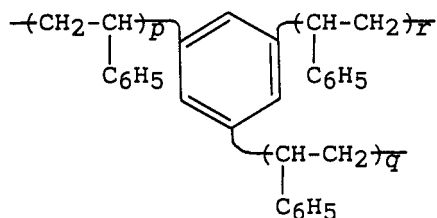
A star polymer having different blocks as its arms is named



where  $x$ ,  $y$ ,  $z\dots$  are locants for positions on the central unit  $X$ . The atom in the blocks nearest to the central unit is given the locant 1.

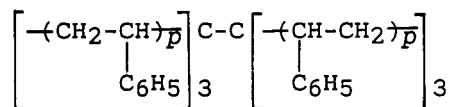
### Examples

- 5.1 A three-armed star polymer in which poly(1-phenylethylene) blocks are linked to a benzene ring at specified positions:



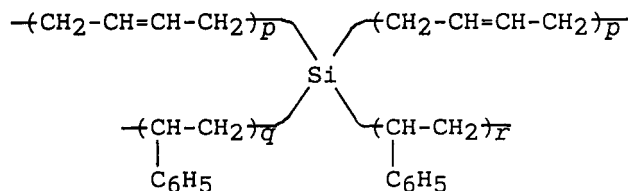
name: 1,3,5-tris[poly(1-phenylethylene)]benzene.

- 5.2 A six-armed star polymer consisting of ethane substituted with poly(1-phenylethylene) blocks:



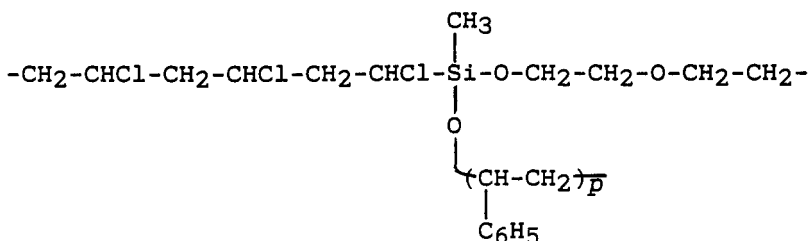
name: hexakis[poly(1-phenylethylene)]ethane.

- 5.3 A four-armed star polymer consisting of silane substituted with different polymer blocks:



name: bis[poly(but-2-ene-1,4-diyl)][poly(1-phenylethylene)][poly(2-phenylethylene)]silane.

- 5.4 A three-armed star polymer consisting of silane substituted with poly(1-chloroethylene), poly(oxyethylene) and poly(1-phenylethylene) blocks, the latter of which is linked to the central unit through oxygen as a linking unit.



name: [poly(1-chloroethylene)][poly(oxyethylene)][poly(1-phenylethylene)oxy]methylsilane.

**Rule 6.** Names of end-groups are prefixed to the name of the polymer and denoted by the Greek letters  $\alpha$  and  $\omega$ . When bonding of the end groups to specific constitutional units is unknown, the irregular polymer is named



where R and R' are the names of the end groups. To specify bonding between end groups and constitutional units, the end group is combined with the attached constitutional unit prior to naming.

#### Examples

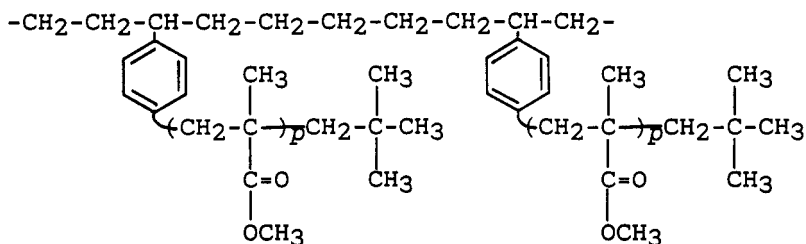
6.1 The copolymer described in Ex.1.1 with specified end groups:

name:  $\alpha$ -chloro- $\omega$ -(trichloromethyl)-poly(1-chloroethylene/1-phenylethylene).

6.2 The copolymer described in 6.1 in which the trichloromethyl group is connected to the 2-position of a 1-phenylethylene unit and the chlorine to the 1-position of a 1-chloroethylene unit:

name:  $\alpha$ -(2,2-dichloroethyl)- $\omega$ -(3,3,3-trichloro-1-phenylpropyl)-poly(1-chloroethylene/1-phenylethylene)

6.3 The graft copolymer in which the grafts have specified end groups:





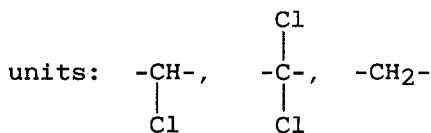
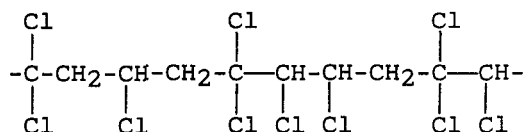
name: poly[ethylene/1-(4-{ $\omega$ -neopentyl-poly[2-(methoxy-carbonyl)-2-methylethylene]}phenyl)ethylene].

Note: The free end of the polymeric substituent is considered to be the  $\omega$ -position, the other end being linked to the parent structure.

**Rule 7.** Specification with regard to mass fractions, mole fractions, and molar masses, is handled as in source-based copolymer nomenclature (Ref. 4).

#### Example

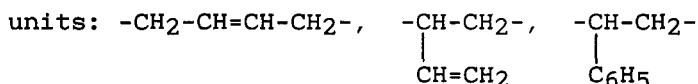
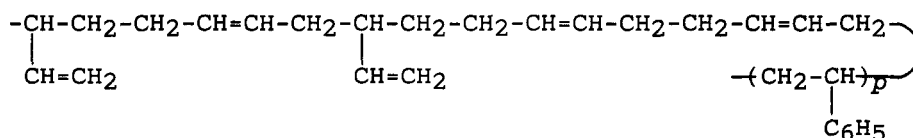
7.1 Chlorinated poly(1-chloroethylene) with a mass fraction of chlorine of 0.65:



name: poly(chloromethylene/dichloromethylene/methylene)  
(65 mass % Cl).

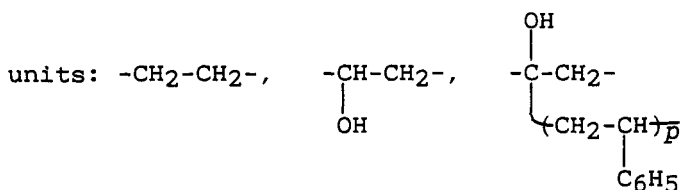
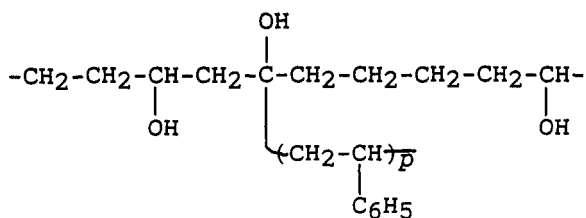
#### Additional Examples

8.1 A diblock copolymer consisting of a block derived from the 1,4 and 1,2 polymerization of buta-1,3-diene and a block of poly(1-phenylethylene):



name: poly(but-2-ene-1,4-diyl/1-vinylethylene)—poly(1-phenylethylene).

8.2 Poly(ethylene/1-hydroxyethylene) grafted with poly(1-phenylethylene) at hydroxymethylene units:

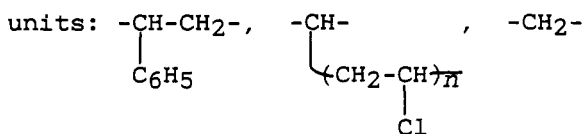
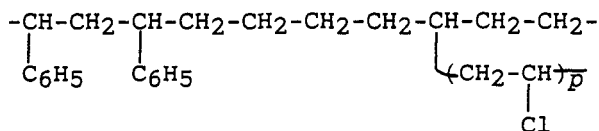


name: poly{ethylene/1-hydroxyethylene/1-hydroxy-1-[poly(2-phenylethylene)]ethylene}.

Note: If the grafting point is not known, the graft copolymer is named

poly{ethylene/1-hydroxyethylene/x-[poly(2-phenylethylene)]-ethylene/x-[poly(2-phenylethylene)]-1-hydroxyethylene}.

- 8.3 A diblock copolymer consisting of a block of poly(methylene) grafted with poly(1-chloroethylene) and a block of poly(1-phenylethylene), the structure of which is:



name: poly(1-phenylethylene)—poly[methylene/poly(2-chloroethylene)methylene].

## References

1. IUPAC. Commission on Macromolecular Nomenclature, "Nomenclature of regular single-strand organic polymers (rules approved 1975)", Pure Appl. Chem. 48, 373-385 (1976). Reprinted as Chapter 5 in "Compendium of Macromolecular Nomenclature" (The Purple Book), Blackwell Scientific Publications, Oxford (1991).
2. IUPAC. Commission on Macromolecular Nomenclature and Commission on Nomenclature of Inorganic Chemistry, "Nomenclature for regular single-strand and quasi single-strand inorganic and coordination polymers (rules approved 1984)", Pure Appl. Chem. 57, 149-168 (1985). Reprinted as Chapter 6 in "Compendium".
3. IUPAC. Commission on Macromolecular Nomenclature, "Basic definitions of terms relating to polymers (rules approved 1974)", Pure Appl. Chem. 40, 479-491 (1974). Reprinted as Chapter 1 in "Compendium".
4. IUPAC. Commission on Macromolecular Nomenclature, "Source-based nomenclature for copolymers (rules approved 1985)", Pure Appl. Chem. 57, 1427-1440 (1985). Reprinted as Chapter 7 in "Compendium".
5. IUPAC. Commission on Nomenclature of Organic Chemistry, "Nomenclature of organic chemistry (1979 edition)", Pergamon Press, Oxford.
6. IUPAC. Commission on Nomenclature of Organic Chemistry, "A guide to IUPAC nomenclature of organic chemistry (rules approved 1992)", in press.

## ERRATA

### 1. *Pure & Appl. Chem.*, Vol. 66, No. 4, pp. 873–889, 1994

The April issue of *Pure and Applied Chemistry* (Volume 66, No. 4) included the IUPAC Recommendation 'Structure-based nomenclature for irregular single-strand organic polymers' prepared by a Working Group consisting of R. B. Fox, N. M. Bikales, K. Hatada and J. Kahovec. Unfortunately, pages 887 and 888 were printed incorrectly. The full article was therefore reproduced correctly in a loose insert which came with the September issue (Volume 66 No. 9). These pages should be substituted for those originally produced when the Volume is bound.

### 2. *Pure & Appl. Chem.*, Vol. 66, No. 6, pp. 1267–1286, 1994

The June issue of *Pure and Applied Chemistry* (Volume 66, No. 6) included the articles 'Theoretical basis of non-equilibrium near atmospheric pressure plasma chemistry' by A. A. Fridman and V. D. Rosanov, and 'Modelling of dielectric barrier discharge chemistry' by B. Eliasson, W. Egli and U. Kogelschatz. Unfortunately, the front pages of these two papers were transposed during production so that the body of both papers was printed out of position within the issue, and given the wrong page numbers and running headlines.

Both articles were reproduced in their entirety in a loose insert that came with the August issue (Volume 66, No. 8), along with a revised contents list. These should be substituted for the original items when the volume is bound.

### 3. *Pure & Appl. Chem.*, Vol. 61, pp. 2075–2085, 1989

Article entitled 'New basis sets in quantum mechanics of molecules. Hermite-Gaussian function' by Z. B. Maksić, K. Kovačević, M. Primorac.

(i) Page 2075, insert the following additional author to the three above:

T. Živković

(ii) Page 2079, line 9 from bottom:

for SM = 100 (1 - Δ) (in %)

read SM = 100 (1 - ½Δ) (in %)