*Pure Appl. Chem.*, Vol. 74, No. 10, pp. 1921–1956, 2002. © 2002 IUPAC

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

MACROMOLECULAR DIVISION COMMISSION ON MACROMOLECULAR NOMENCLATURE\*

# NOMENCLATURE OF REGULAR SINGLE-STRAND ORGANIC POLYMERS

### (IUPAC Recommendations 2002)

*Prepared by a Working Group consisting of* J. KAHOVEC<sup>‡</sup>, R. B. FOX, AND K. HATADA

Prepared for publication by J. KAHOVEC

Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovsky Sq. 2, 162 06 Prague, Czech Republic

\*Membership of the Commission during the preparation of this report (1990–2000) was as follows:

*Titular Members*: R. E. Bareiss (Germany, to 1993); M. Barón (Argentina, National Representative from 1987, Associate Member from 1992, Titular Member from 1996, Secretary from 1998); K. Hatada (Japan, from 1989, Associate Member from 1997); M. Hess (Germany, Associate Member from 1996, Titular Member from 1998), Chairman from 2000); K. Horie (Japan, Associate Member from 1996, Titular Member from 1998); R. G. Jones (UK, Pool Titular Member from 1992, Titular Member from 1998); J. Kahovec (Czech Republic, Associate Member from 1992); P. Kratochvíl (Czech Republic, Chairman to 1991); E. Maréchal (France, Associate Member from 1992); C. Noël (France, to 1993); V. P. Shibaev (Russia, from 1987, Associate Member from 1992); C. Noël (France, to 1993); V. P. Shibaev (Russia, from 1987, Associate Member from 1996); R. F. T. Stepto (UK, from 1989, Chairman from 1992); U. W. Suter (Switzerland, to 1991, Associate Member to 1993); W. J. Work (USA, Secretary to 1997).

Associate Members contributing to this report: J.-I. Jin (Korea, National Representative from 1992, Associate Member from 1994); S. Penczek (Poland, from 1994); E. S. Wilks (USA, from 1998).

*Others contributing to this report*: H.-G. Elias (USA); H. Favre (Canada); A. D. Jenkins (UK); K. Thurlow (UK); J. G. Traynham (USA); T. Tsuruta (Japan).

<sup>‡</sup>Corresponding author

Republication or reproduction of this report or its storage and/or dissemination by electronic means is permitted without the need for formal IUPAC permission on condition that an acknowledgment, with full reference to the source, along with use of the copyright symbol ©, the name IUPAC, and the year of publication, are prominently visible. Publication of a translation into another language is subject to the additional condition of prior approval from the relevant IUPAC National Adhering Organization.

# Nomenclature of regular single-strand organic polymers

## (IUPAC Recommendations 2002)

*Abstract*: A structure-based nomenclature for regular single-strand organic polymers is described. In concept, a generic name for the polymer  $(ABC)_n$  is poly(ABC), in which (ABC) is a constitutional repeating unit (CRU) representing the chemical structure of the polymer chain, and A, B, and C are the subunits that comprise the CRU. To provide a unique and unambiguous name, rules are given to identify the preferred CRU and to name it using the names of A, B, and C based on current organic nomenclature. Provisions are made for naming end-groups of the polymers and the polymer substituents. In addition, the document contains a glossary of concepts and definitions, a list of common subunit names, and a variety of examples of structure-based polymer names. The document is a revision of the 1975 Rules.

#### CONTENTS

- 1. INTRODUCTION
- 2. GLOSSARY
- 3. FUNDAMENTAL PRINCIPLES
- 4. SENIORITY OF SUBUNITS (Rule 1)
  - 4.1 Heterocyclic rings and ring systems (Rules 2,3)
  - 4.2 Heteroatom chains (Rules 4–7)
  - 4.3 Carbocyclic rings and ring systems (Rules 8,9)
  - 4.4 Acyclic carbon chains (Rule 10)
- 5. SELECTION OF THE PREFERRED CONSTITUTIONAL REPEATING UNIT (CRU)
  - 5.1 Simple CRUs (Rules 11,12)
  - 5.2 Complex CRUs (Rules 13–17)
- 6. NAMING THE PREFERRED CONSTITUTIONAL REPEATING UNIT (CRU)
  - 6.1 Naming subunits (Rule 18)
  - 6.2 Naming the preferred CRU (Rule 19)
- 7. NAMING THE POLYMER (Rules 20,21)
- 8. POLYMER CHAIN AS A SUBSTITUENT (Rule 22)
- 9. EXAMPLES OF POLYMER NAMES
- 10. REFERENCES
- 11. APPENDIX
  - 11.1 List of names of common subunits
  - 11.2 Structure- and source-based names for common polymers

#### **1. INTRODUCTION**

In 1952, the Subcommission on Nomenclature of the IUPAC Commission on Macromolecules published a report [1] on the nomenclature of polymers that included a method for the systematic naming of linear organic polymers on the basis of structure. A later report [2] dealing with steric regularity utilized that system of nomenclature. When the first report was issued, the skeletal rules were adequate for most needs; indeed, most polymers could at that time be reasonably named on the basis of the real or

hypothetical substance used in producing the polymer. In the intervening years, however, the rapid growth of the polymer field had dictated a need for modification and expansion of the earlier rules. The result was a set of rules approved in 1975 [3]. The present report is an updating of the 1975 rules with special attention to developments in the nomenclature of organic chemistry since that time [4,5].

The rules in the present report are designed to name, uniquely and unambiguously, the structures of regular single-strand organic polymers whose repeating structures can be written within the framework of ordinary chemical principles. Although the stereochemistry of polymers is not considered here, examples of names with stereodescriptors are given. A detailed survey of stereochemical notation of polymers is given in a special report [6]. As with organic chemistry nomenclature, this nomenclature describes chemical structures rather than substances. It is realized that a polymeric substance ordinarily may include many structures, and that a complete description of even a single polymer molecule would include an itemization of terminal groups, branching, random impurities, degree of steric regularity, chain imperfections, etc.

Nevertheless, it is useful to think of the macromolecules of a polymer as being represented by a single structure that may itself be hypothetical. To the extent that the structure can be portrayed as a chain of regular structural repeating units (SRUs) or constitutional repeating units (CRUs) (the terms are synonymous), the structure can be named by the rules in this report; in addition, provision has been made for including end-groups in the name.

The fundamental principles and the basic rules of the structure-based nomenclature are given first, accompanied by detailed extensions and applications. An Appendix contains names of common subunits as well as a list of acceptable source-based names, along with the corresponding structure-based names, of common polymers. The Commission sees no objection to the continued use of such sourcebased names where these names are clear and unambiguous, but prefers the use of the structure-based nomenclature detailed in these rules.

The rules of structure-based nomenclature of regular single-strand polymers are of fundamental importance in polymer nomenclature. The names of other kinds of polymers such as double-strand [7] and irregular polymers [8] are based on the principles given in this Report.

After more than two decades of use, many improvements in the 1975 rules [3] have been suggested. As a result, the present new rules are proposed. The new rules do not represent any change in principles. They involve mainly rearrangement of the material, a generalization of basic rules, a clearer presentation, an avoidance of manifold repetition of the same principles at various places, and the use of graphical means for the visualization of the principles. Also, some additions are made, such as a rule on naming polymer chain substituents, and several new examples of polymers, including those with an "inorganic" backbone and those where stereodescriptors are essential.

#### 2. GLOSSARY

#### Regular polymer [9]

A polymer composed of regular macromolecules, i.e., macromolecules the structure of which essentially comprises the repetition of a single constitutional unit with all units connected identically with respect to directional sense.

#### Single-strand polymer [3,7,9,10]

A polymer, the macromolecules of which are single-strand macromolecules, i.e., macromolecules comprising constitutional units connected in such a way that adjacent constitutional units are joined to each other through two atoms, one on each constitutional unit.

#### Constitutional unit [9]

An atom or group of atoms (with pendant atoms or groups, if any) comprising a part of the essential structure of a macromolecule, an oligomer molecule, a block, or a chain.

#### Constitutional repeating unit (CRU) [9]

The smallest constitutional unit, the repetition of which constitutes a regular macromolecule, a regular oligomer molecule, a regular block, or a regular chain.

#### Main chain (backbone) [9]

That linear chain to which all other chains, long or short or both, may be regarded as being pendant.

#### End-group [9]

A constitutional unit that is an extremity of a macromolecule or oligomer molecule.

#### Subunit

The largest main-chain (backbone) segment of the CRU that can be named as a single unit under organic nomenclature rules [4,5]. This may be a ring or ring system, a heteroatom or a homogeneous heteroatom chain, or an acyclic carbon chain.

#### Path length

The path length between two subunits is the number of polymer main-chain (backbone) atoms between the two subunits. Where a ring or ring system constitutes all or part of a path between two subunits, the shortest continuous chain of atoms in the ring or ring system is selected.

#### Seniority

Priority in a set of atoms or groups of atoms according to a prescribed order.

#### Locant

A numeral or letter that identifies position in a structure.

$E^{1} - (A - B - C - D)_{n} E^{2}$	regular single-strand polymer
$\begin{array}{c} -A - B - C - D - \\ R^1 & R^2 \end{array}$	constitutional repeating unit (CRU)
-A-, -B-, -C-, -D-	subunits
$\begin{array}{c} -\mathbf{B}-, \ -\mathbf{D}-\\ \mathbf{R}^{1} & \mathbf{R}^{2} \end{array}$	substituted subunits
$\mathbf{R}^1, \mathbf{R}^2$	substituents to subunits
$E^1, E^2$	end-groups

#### **3. FUNDAMENTAL PRINCIPLES**

This nomenclature method rests upon the selection of a preferred CRU of which the polymer molecule is a multiple. Wherever possible, the CRU and subunits are named according to the IUPAC-recommended nomenclature of organic chemistry [4,5].

In this nomenclature, the steps to be followed when naming a polymer are:

- 1. Write the structure of the polymer chain. A sufficient portion of the chain should be written to show structure repetition. The portion that repeats is a CRU.
- 2. Select the preferred CRU.
- 3. Name the preferred CRU by citing, from left to right, the names of the subunits, including their substituents, if present.
- 4. Name the polymer.

#### Structure of the polymer chain

In simple cases, the CRU involves a single subunit. In more complex cases, it is often necessary to draw a large segment of the polymer chain, for example,

$$\begin{array}{c} - \underset{l}{\text{OCHCH}_2\text{OCHCH}_2\text{OCHCH}_2\text{OCHCH}_2\text{OCHCH}_2\text{OCHCH}_2\text{OCHCH}_2\text{OCHCH}_2\text{--}\\ \\ \text{Br} & \text{Br} & \text{Br} & \text{Br} & \text{Br} & \text{Br} \end{array}$$

#### Selection of the preferred CRU

There are many ways to write the CRU for most chain structures. In simple cases, these units are readily identified. In the polymer chain given above, the possible CRUs are

$$-OCHCH_2-$$
,  $-CH_2OCH-$ ,  $-OCH_2CH-$ ,  $-CH_2CHO-$ ,  $-CHOCH_2-$ ,  $-CHCH_2O-$   
Br Br Br Br Br Br Br Br Br

To allow construction of a unique name, a single CRU must be selected. The following rules have been designed to specify both seniority among subunits, i.e., the point at which to begin writing the CRU, and the direction along the chain in which to continue to the end of the CRU. The preferred CRU will be one beginning with the subunit of highest seniority (see Section 4). From this subunit, one proceeds toward the subunit next in seniority. In the preceding example, the subunit of highest seniority is an oxygen atom, and the subunit next in seniority is a substituted  $-CH_2CH_2$ - unit. The CRU is written to read from left to right. The preferred CRU will, therefore, be either

$$- \begin{array}{c} - \operatorname{OCHCH}_2 - & \\ Br & Br \end{array} \quad OCH_2 CH - \\ Br & Br \end{array}$$

Further choice in this case is based on the lowest locant for substitution, so that the preferred CRU

$$\begin{array}{ccc} -\text{OCHCH}_2- & \text{rather than} & -\text{OCH}_2\text{CH}- \\ & Br & Br \\ 1-\text{substitution} & 2-\text{substitution} \end{array}$$

#### Naming the preferred CRU

is

The name of the preferred CRU is formed by citing, in the order in which they appear in the CRU, the names of the subunits within the CRU. In the example, the oxygen atom is called oxy and the  $-CH_2CH_2$ - (preferred to  $-CH_2$ - because it is larger and can be named as a unit) is called ethylene; the latter unit substituted with one bromine atom is called 1-bromoethylene. The preferred CRU is, therefore, named oxy(1-bromoethylene).

#### Naming the polymer

The name of the polymer is simply the name of the preferred CRU enclosed in curves, square brackets, or braces and prefixed by poly. The nesting order of enclosing marks is curves, square brackets, braces, then curves, square brackets, braces, etc., i.e.,  $\{[(\{[()\}\})]\}$ . This is well illustrated in Examples 21 and 31 in Section 9.

The  $(OCHCH_2)_n$  polymer is named poly[oxy(1-bromoethylene)].

#### 4. SENIORITY OF SUBUNITS

#### Rule 1

The basic order of seniority of subunits is:

heterocyclic rings and ring systems > heteroatom chains > carbocyclic rings and ring systems > acyclic carbon chains

The order of seniority of subunits is of primary importance in the generation of polymer names. Further classification according to seniority is based on the nature of the subunits (kind or size or both) and, among identical subunits, (a) on their degree of unsaturation and (b) on their substituents (number, kind and locants). The following criteria are applied consecutively until a decision is reached.

#### 4.1 Heterocyclic rings and ring systems

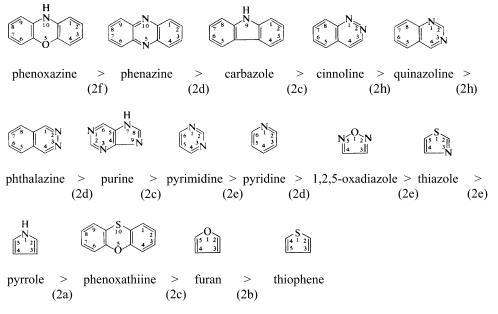
#### Rule 2

Among heterocyclic rings and ring systems, the descending order of seniority is:

- a. a ring or ring system containing nitrogen;
- b. a ring or ring system containing the heteroatom occurring earliest in the order given in Rule 4;
- c. a ring or ring system containing the greatest number of rings;
- d. a ring or ring system having the largest individual ring;
- e. a ring or ring system having the greatest number of heteroatoms;
- f. a ring or ring system containing the greatest variety of heteroatoms;
- g. the ring or ring system having the greatest number of heteroatoms highest in the order given in Rule 4;
- h. of the two rings or ring systems of the same size containing the same number and kind of heteroatoms, the senior system is that one with the lower locants for the heteroatoms.

Note: This order is a paraphrased extract of that in [11].

Examples of the application of seniority rules among different heterocyclic rings and ring systems are (appropriate rule in parentheses):



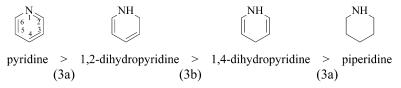
#### 1927

#### Rule 3

The order of decreasing seniority within a given heterocyclic ring or ring system is:

- a. when rings or ring systems differ only in degree of unsaturation, the senior system is the most unsaturated one;
- b. when rings or ring systems of the same degree of unsaturation differ in the positions of double bonds, the senior system is that having the lowest locants for double bonds;
- c. in heterocyclic ring assemblies, the assembly of highest seniority is that having lowest locants for the points of attachment between the rings within the assembly, consistent with the fixed numbering of the ring or ring system;
- d. a ring or ring system with the lowest locants of free valences;
- e. a ring or ring system with the largest number of substituents;
- f. a ring or ring system having substituents with the lowest locants;
- g. a ring or ring system in which the substituent first in alphabetical order has the lowest locant.

Examples of the application of seniority rules within a given heterocyclic ring or ring system are (appropriate rule in parentheses):



#### 4.2 Heteroatom chains

#### Rule 4

For the most common heteroatoms, the descending order of seniority is:

O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Hg

*Note*: Other heteroatoms may be placed within this order as indicated by their positions in the periodic table [5].

#### Rule 5

A more substituted single heteroatom is senior to a less substituted single heteroatom of the same kind.

Examples:



#### Rule 6

Within mono- or disubstituted single heteroatoms, the heteroatom carrying a substituent (substituents) earlier in the alphabet is senior.

Example:

$$-N - > -N - > -N -$$
  
 $C_2H_5 CH_3 C_6H_5$ 

#### Rule 7

The order of decreasing seniority for chains of heteroatoms of the same kind that have equal length is:

J. KAHOVEC et al.

- a. when chains differ only in degree of unsaturation, the senior chain is the most unsaturated one; *Note:* This rule applies also to single heteroatoms.
- b. when chains of the same degree of unsaturation differ in the positions of multiple bonds, the senior chain is that having the lowest locants for double bonds;
- c. the chain with the largest number of substituents;
- d. the chain having substituents with the lowest locants;
- e. the chain in which the substituent first in alphabetical order has the lowest locant.

Examples:

#### 4.3 Carbocyclic rings and ring systems

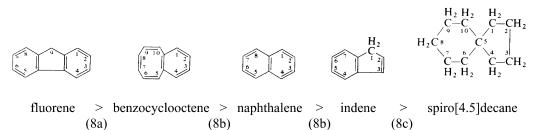
#### Rule 8

Among carbocyclic rings and ring systems, the decreasing order of seniority is:

- a. a ring system containing the greatest number of rings;
- b. the largest ring or a ring system with the largest individual ring;
- c. a ring system having the greatest number of atoms common to the rings.

Note: The criteria for further choice are found in Rule C-14.1 in [4].

Examples of the application of seniority among carbocyclic rings and ring systems are (appropriate rule in parentheses):



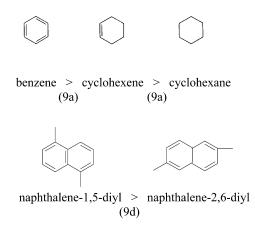
#### Rule 9

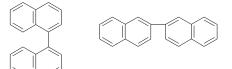
The order of decreasing seniority within a given carbocyclic ring or ring system is:

- a. when rings or ring systems differ only in degree of unsaturation, the senior system is the most unsaturated one;
- b. when rings or ring systems of the same degree of unsaturation differ in the positions of double bonds, the senior system is that having the lowest locants for double bonds;
- c. in carbocyclic ring assemblies, the assembly of highest seniority is that having lowest numbers for the points of attachment between the systems within the assembly, consistent with the fixed numbering of the ring or ring system;
- d. a ring or ring system with the lowest locants for free valences;
- e. a ring or ring system with the largest number of substituents;
- f. a ring or ring system having substituents with the lowest locants;
- g. a ring or ring system in which the substituent first in alphabetical order has the lowest locant.

© 2002 IUPAC, Pure and Applied Chemistry 74, 1921–1956

Examples of the application of seniority rules within a given carbocyclic ring or ring system are (appropriate rule in parentheses):





1,1'-binaphthalene > 2,2'-binaphthalene (9c)

#### 4.4 Acyclic carbon chains

#### Rule 10

The order of decreasing seniority of acyclic carbon chains of equal length is:

- a. when chains differ only in degree of unsaturation, the senior chain is the most unsaturated one; *Note*: This rule applies also to single carbon atoms.
- b. when chains of the same degree of unsaturation differ in the positions of multiple bonds, the senior chain is that having multiple bonds with the lowest locants;
- c. the chain with the largest number of substituents;
- d. the chain having substituents with the lowest locants;
- e. the chain in which the substituent first in alphabetical order has the lowest locant.

Examples:

$$-CH = > -CH_{2} - CH = CHCH_{2}CH_{2} - > -CH_{2}CH = CHCH_{2} - > -(CH_{2})_{4}$$

$$(10a) (10b) (10a)$$

$$-CHCH_{2}CH - > -CHCH_{2}CH - -CHCH_{2} - > -CHCH_{2} - > -CH_{2}CH - > -CH_{2}CH_{2} -$$

$$Br Cl Cl Br F CHCH_{2} - > -CHCH_{2} - > -CH_{2}CH_{2} - > -CH_{2}CH$$

(10e)

(10d)

(10c)

#### 5. SELECTION OF THE PREFERRED CONSTITUTIONAL REPEATING UNIT (CRU)

The CRU in a polymer chain may contain one or more subunits. A simple CRU is one that can be described by single subunit. A complex CRU has at least two subunits.

#### 5.1 Simple CRUs

(10e)

In selecting the preferred CRU, the steps to be followed in sequence are:

#### J. KAHOVEC et al.

- 1. write the structure of a representative portion of the polymer chain;
- 2. identify the single subunit and its substituents;
- 3. choose the direction so that the locants of free valences of the subunit are as low as possible;
- 4. choose the direction so that the locants of the substituents are as low as possible.

#### Rule 11

For acyclic and monocarbocyclic subunits, preference in lowest numbers is given to the carbon atoms through which they are attached to the main chain of the CRU. The point of attachment at the left-hand side of the subunit as written in the CRU must have locant 1.

#### Examples:

 $- \overset{l}{\overset{}_{\underset{l}{Cl}}} \overset{3}{\overset{}_{\underset{l}{CHCH_2}}} \overset{3}{\overset{}_{\underset{l}{CH2}}} -$ 1-chloropropane-1,3-diyl cyclohexane-1,4-diyl

#### Rule 12

In polycyclic hydrocarbons, bridged hydrocarbons, spiro hydrocarbons, ring assemblies, and heterocyclic systems, numbering is fixed for the ring system. The points of attachment of such subunits to the main chain of the CRU should have the lowest permissible locants consistent with the fixed numbering. The same fixed numbering is retained for either direction of progress through the group in generating the subunit name. Where there is a choice, the point of attachment at the left-hand side of the ring as written in the CRU should have the lowest permissible locant.

Examples:

naphthalene-2,6-diyl

morpholine-2,6-diyl

#### 5.2 Complex CRUs

The factors in the selection of the preferred CRU are in order:

- seniority of subunits
- path length between subunits

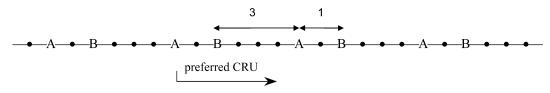
In selecting the preferred CRU, the steps to be followed in sequence are:

- 1. write the structure of a representative portion of the polymer chain;
- 2. identify subunits and substituents;
- 3. classify the subunits according to their seniority;
- 4. find the shortest path in atoms, irrespective of their nature, from the subunit of the highest seniority to the subunit of the same seniority (Rules 15,16), if present, or of the second highest seniority (Rules 13,14). Where paths of equal length are identified as shortest, the choice depends on the seniority of the remaining subunits and the number and positions of substituents;
- 5. orient the structure so that the direction from the most senior subunit to the subunit of the next highest seniority reads left to right;
- 6. identify the preferred CRU starting from the highest seniority subunit and moving in the direction determined above.

These steps are further elaborated in Rules 13-16.

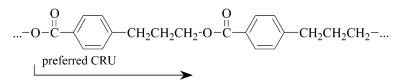
#### Rule 13

The starting point for the preferred CRU is at the subunit of highest seniority (A). Of the two paths leading from the subunit of highest seniority (A) along the main chain (backbone) to both the next subunits of second highest seniority (B), the shorter path is to be followed.



(dots represent subunits of lowest seniority)

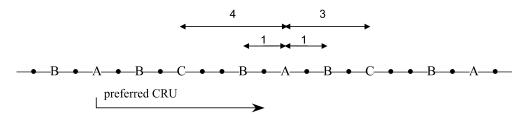
Example:



(O is senior to a benzene ring; the one-atom path from O to the benzene ring is preferred to the threeatom path)

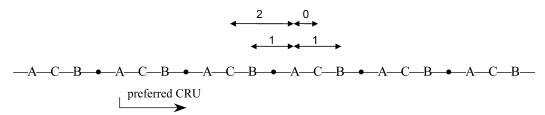
#### Rule 14

When two paths from the starting subunit (A) to both the next subunits of second highest seniority (B) are equally long, the shorter path from the starting subunit A to the subunit of third highest seniority (C) is to be followed.



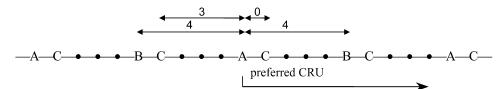
Example:

(O is senior to S, which is senior to N; the one-atom path from O to S is to be followed by the six-atom path from S to O in which N is closer to S)



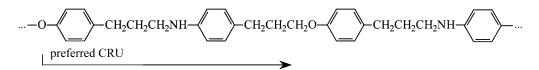
...-ONHCH<sub>2</sub>SCH<sub>2</sub>CH<sub>2</sub>ONHCH<sub>2</sub>SCH<sub>2</sub>CH<sub>2</sub>ONHCH<sub>2</sub>SCH<sub>2</sub>CH<sub>2</sub>ONHCH<sub>2</sub>SCH<sub>2</sub>CH<sub>2</sub>O-... preferred CRU

(O is senior to S, which is senior to N; of the two equal paths from O to S, the one that traverses N is preferred to that which traverses  $CH_2$ )



(C is closer to A in the preferred CRU; both B's are equally distant from A)

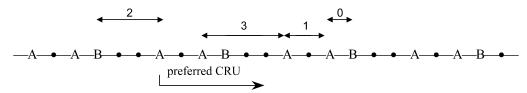
Example:



(O is senior to N, which is senior to a benzene ring; of the two equal paths from O to N, the one that traverses the benzene ring earlier is preferred)

#### Rule 15

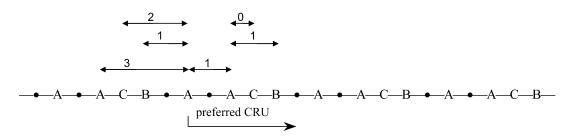
When two identical subunits of the highest seniority (A) are present in a CRU in the main chain (backbone), the shorter path between the identical subunits is to be followed. The starting point is chosen in such a way that the shorter path to the subunit of second highest seniority (B) is followed. If the paths are equal, the paths to subunits of third highest seniority (C) are considered in the sense of Rule 14.



(B is closer to both A subunits in the preferred CRU)

Example:

(O is senior to S; the one-atom path from O to O is preferred to the three-atom path from O to O; S is closer to O in the preferred CRU)



(of the two equal paths from -A - A to B, the one that traverses C is preferred to that which traverses -)

Example:

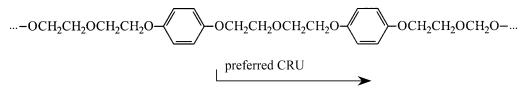
(O is senior to S, which is senior to N; the one-atom path from O to O is preferred to the five-atom path; N is closer to O in the preferred CRU)

#### Rule 16

When three or more identical subunits of the highest seniority (A) are present in a CRU in the main chain (backbone), the starting point and direction are chosen in such a way that the shortest path through all the subunits A results. If there is a choice, the CRU with the shorter path to the subunits of second or third highest seniority (B or C) is selected.

Examples:

(shortest path through all oxygens, either direction)



(shortest path through all oxygens)

(starting O and direction determined by N)

© 2002 IUPAC, Pure and Applied Chemistry 74, 1921–1956

# 1934

Rule 17

If a choice is possible between a divalent and a higher-valent CRU, the number of free valences is minimized only after all other orders of seniority have been observed.

Example:

#### 6. NAMING THE PREFERRED CONSTITUTIONAL REPEATING UNIT (CRU)

#### 6.1 Naming subunits

#### Rule 18

The subunits and substituted subunits are named by organic nomenclature rules [4,5]. Substituted subunits are parenthesized or bracketed.

*Note 1*: Alkyl-substituted acyclic carbon chain subunits are named as such, not as single-chain units to differentiate between the length of the acyclic carbon chain, which is part of the main chain (backbone), and an acyclic carbon chain substituent on that backbone. This is an exception from the rules in [5].

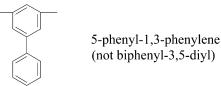
Similarly, heterocyclic or carbocyclic ring assemblies, if not in the main chain (backbone), are not named as such, but as substituted rings or ring systems.

Examples:

-CH-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>9</sub>CH<sub>3</sub>

-CHCH<sub>2</sub>CH<sub>2</sub>-

1-decylethylene (not dodecane-2,1-diyl according to ref. 5) 1-methylpropane-1,3-diyl (not butane-3,1-diyl according to ref. 5)



Note 2: A list of names of common subunits is in Appendix 11.1.

#### 6.2 Naming the preferred CRU

#### Rule 19

The name of the CRU is formed from the names of its subunits, including substituents (substituted subunits), and cited in order from left to right as they appear in the CRU.

Examples:

$$\begin{array}{ll} - \operatorname{OCH}_2\mathrm{CH}_2- & \operatorname{oxyethylene} \\ - \operatorname{OCH}_{-} & \operatorname{oxy(phenylmethylene)} \\ & \operatorname{C}_6\mathrm{H}_5 & \\ - \operatorname{OCHCH}_2- & 1-(\operatorname{methoxycarbonyl}) \\ & \operatorname{COOCH}_3 & \\ & \operatorname{COOCH}_3 & \\ & \operatorname{CH}_3 & \\ & -\operatorname{N}_{-}^{^{|}+}\mathrm{CH}_2\mathrm{CH}_2- \\ & \operatorname{CH}_3 & \operatorname{Br}_{-} & \\ \end{array} \quad (dimethyliminio) \\ \end{array}$$

#### 7. NAMING THE POLYMER

#### Rule 20

Polymers (or oligomers) are named with the prefix poly (or oligo) followed in parentheses or brackets by the name of the CRU. If the name of the repeating unit is "ABC", the corresponding polymer (or oligomer) name is

 $(ABC)_n$  poly(ABC) or oligo(ABC)

*Note*: Where it is desired to specify the chain length in an oligomer, the appropriate Greek prefix (deca, docosa, etc.) may be used.

Example:

 $-(OCH_2CH_2)_{10}$  deca(oxyethylene)

#### Rule 21

End-groups may be specified by prefixes placed ahead of the name of the polymer. The end-group designated by  $\alpha$  is that attached to the left-hand side of the CRU written as described in the preceding rules, and the other end-group is designated by  $\omega$ ; the end-groups are cited in that order. If there is a choice, the end-group with the name starting earlier in the alphabet should be cited first.

Examples:

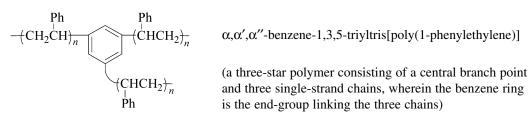
$$Cl_3C - CH_2 - CH_2 - CH_2 - CI \qquad \alpha$$
-(trichloromethyl)- $\omega$ -chloropoly(1,4-phenylenemethylene)

 $H - (OCH_2CH_2)_n OCH_3$   $\alpha$ -hydro- $\omega$ -methoxypoly(oxyethylene)

(not  $\alpha$ -methyl- $\omega$ -hydroxypoly(oxyethylene); alphabetical order of end-groups decides)

CH<sub>3</sub>O(CH<sub>2</sub>CH<sub>2</sub>O)<sub>n</sub>CO(CH<sub>2</sub>)<sub>4</sub>CO(OCH<sub>2</sub>CH<sub>2</sub>)<sub>n</sub>OCH<sub>3</sub>

 $\alpha, \alpha'$ -adipoylbis[ $\omega$ -methoxypoly(oxyethylene)]



is the end-group linking the three chains)

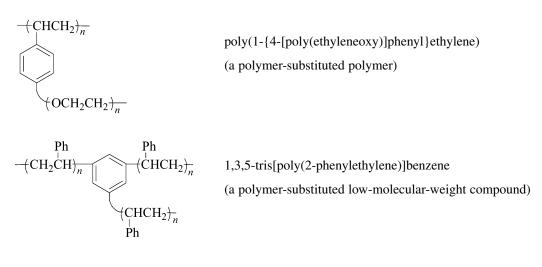
#### 8. POLYMER CHAIN AS A SUBSTITUENT

#### Rule 22

If a regular single-strand chain is linked to a constitutional unit of the main chain (backbone) of a polymer molecule or to a low-molecular-weight structure, either directly or through an intervening unit, it is considered a substituent of the constitutional unit or structure. In naming the polymeric substituent, the actual bonding relations are reflected in the name of the CRU.

Examples:

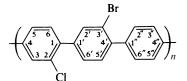
-N- (CH <sub>2</sub> CH <sub>2</sub> O) <sub>n</sub>	[poly(oxyethylene)]imino (a polymer-substituted imino subunit)
-CH- (OCH <sub>2</sub> ) <sub>n</sub>	[poly(methyleneoxy)]methylene (a polymer-substituted methylene subunit)
$\overset{-\mathrm{CH}-}{_{\mathrm{CH}_{2}-(\mathrm{OCH}_{2})_{n}}}$	{[poly(methyleneoxy)]methyl}methylene (a polymer-substituted substituted methylene subunit)



#### 9. EXAMPLES OF POLYMER NAMES

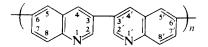
To illustrate the present rules for naming various kinds of polymers, examples of polymers are given in this section. The key steps in the naming and the corresponding rule numbers are also given.

Example 1



poly(3'-bromo-2-chloro[1,1':4',1"-terphenyl]-4,4"-diyl) (Rules 9c,9f,12)

Example 2



poly([3,3'-biquinoline]-6,6'-diyl) (Rules 3c,12)

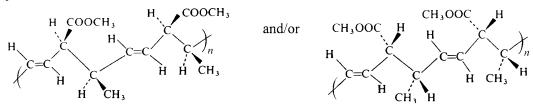
Example 3

poly([2,3'-bipyridine]-4,5'-diyl) (Rules 3c,12)

$$\overset{H}{\swarrow}C=C^{H}_{CH_{2}CH_{2}}$$

poly[(Z)-but-1-ene-1,4-diyl]
(double bond takes lowest locant; Rule 10b)

Example 5



diisotactic poly[*threo-*(*E*)-3-(methoxycarbonyl)-4-methylbut-1-ene-1,4-diyl] (double bond takes lowest locant; Rule 10b)

Example 6

$$+CH=CH + n$$

poly(ethene-1,2-diyl) (divalent CRU is preferred to  $\neq$ CH-CH $\neq_n$ , poly(ethanediylidene); Rule 17)

Example 7

$$-(CHCH_2CH_2)_n^{-2H}$$

poly[(1-<sup>2</sup>H)propane-1,3-diyl] (lowest locant for <sup>2</sup>H; Rule 10d)

Example 8

$$-(CH)_{\overline{n}}$$
  
CH<sub>3</sub>

poly(methylmethylene) (Rule 18)

Example 9

$$-(CHCH_2)_n$$
  
 $C_6H_5$ 

poly(1-phenylethylene) (Rule 10d)

 $+COCOCH_2CH_2$ 

poly(1,2-dioxobutane-1,4-diyl) (Rule 10d)

Example 11

 $-(COCH_2COCH_2CH_2CH_2)_n$ 

poly(1,3-dioxohexane-1,6-diyl) (Rule 10d)

Example 12

$$-(OCO-CO)_{\overline{n}}$$

poly(oxyoxalyl) (O is senior; Rule 1)

Example 13

 $-(\text{OCOCH}_2\text{CH}_2\text{CO})_{\overline{n}}$ 

poly(oxysuccinyl) (O is senior; Rule 1)

Example 14

$$\left(\begin{array}{ccc}1\\8\\-\\3\\4\\5\end{array}\right)_n$$

poly(naphthalene-2,7-diyl) (lower free-valence locant on the left; Rule 12)

Example 15

$$(\underbrace{\begin{smallmatrix} 0\\2&1\\3\\3\\0\end{smallmatrix}}_{q} \underbrace{\begin{smallmatrix} 0\\6\\4\\5\\0\end{smallmatrix}}_{n})$$

poly(2*H*-furo[3,2-*b*]pyran-2,6-diyl) (lower free-valence locant on the left; Rule 12)

Example 16

$$\left( \begin{array}{c} 2 & 3 \\ 1 & 2 \\ N^{1} & 6 \end{array} \right)_{n}$$

poly(pyridine-2,4-diyl) (lower free-valence locant on the left; Rule 12)

$$+$$
CHCH<sub>2</sub> $+_n$   
COO<sup>-</sup>Na<sup>+</sup>

poly(sodium 1-carboxylatoethylene) (lower locant for substituent; Rule 10d)

Example 18

poly(x-iminocyclopentane-1,2-diyl) [lower free-valence locant on the left; Rule 12; the x is required to differentiate the structure from  $+NH_{-}$ , poly(iminocyclopentane-1,2-diyl)]

Example 19

poly(pyridine-3,5-diylpiperidine-2,4-diyl) (pyridine is senior to piperidine; Rule 3a)

Example 20

$$( \underbrace{\begin{smallmatrix} \mathbf{C} \mathbf{I} \\ \mathbf{I} \\ \mathbf{I} \\ \mathbf{I} \\ \mathbf{I} \\ \mathbf{N} \\ \mathbf{N} \\ \mathbf{I} \\ \mathbf{I$$

poly[(4-chloro[3,3'-bipyridine]-5,5'-diyl)methylene] (ring assembly is senior to acyclic carbon chain; Rules 1,3c,3e,12)

#### Example 21

$$-(\text{NHCOCH})_{n}$$
  
 $S-C_6H_5$ 

poly{imino[1-oxo-2-(phenylsulfanyl)ethylene]} (heteroatom is senior to acyclic carbon chain; in the chain the substituent earlier in the alphabetical order has a lower locant; Rules 1,10e)

Example 22

$$-(O-Si)_{n}^{CH_{3}}$$

poly[oxy(methylphenylsilanediyl)] or poly(methylphenylsiloxane) (for an alternative name, see ref. [10])

© 2002 IUPAC, Pure and Applied Chemistry 74, 1921–1956

$$\underbrace{ \overset{OC_{2}H_{5}}{\overset{}{\underset{\scriptstyle -}}}}_{\overset{}{\underset{\scriptstyle -}} \overset{OC_{2}H_{5}}{\overset{}{\underset{\scriptstyle -}}}}$$

poly[nitrilo(diethoxy- $\lambda^5$ -phosphanetriyl)] or poly(diethoxyphosphazene) (N is senior to P; Rule 4; for an alternative name, see ref. [10])

Example 24



poly(piperidine-3,5-diylideneethanediylidene) (piperidine ring is senior to acyclic carbon chain; Rule 1)

Example 25

 $(-S-CO)_n$ 

poly(sulfanediylcarbonyl) (S is senior; Rule 1)

Example 26

$$\begin{array}{cccc} H_{2} H_{2} & H_{2} H_{2} \\ C-C & C-C \\ & & & \\ & &$$

poly(spiro[4.5]decane-2,8-diylmethylene) (ring system is senior to acyclic carbon chain; Rules 1,12)

Example 27

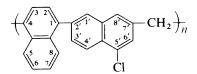
$$\begin{array}{c}
H \\
\left( 13^{4} \times 10^{-1} \text{CH}_{2} \right)_{n} \\
\left( 13^{2} \times 10^{-1} \text{N}^{-1} \text{CH}_{2} \right)_{n}
\end{array}$$

poly(4*H*-1,2,4-triazole-3,5-diylmethylene) (heterocycle is senior to acyclic carbon chain; Rules 1,12)

$$($$
  $CH_2CH_2)_n$ 

poly[(2-phenyl-1,3-phenylene)ethylene] (ring system is senior to acyclic carbon chain; Rules 1,12,18)

Example 29



poly[(5'-chloro[1,2'-binaphthalene]-4,7'-diyl)methylene] (ring system is senior to acyclic carbon chain; Rules 1,9c,12)

Example 30

$$\begin{array}{c} \overbrace{f_{0}}{1} \xrightarrow{2} \\ \overbrace{f_{0}}{1} \xrightarrow{2} \\ \overbrace{f_{0}}{4} \xrightarrow{f_{0}} \\ Br \end{array}$$

poly[(6-chlorocyclohex-1-ene-1,3-diyl)(1-bromoethylene)] (ring is senior to acyclic carbon chain; lower free-valence locant on the left; lower locant for Br in ethylene; Rules 1,9b,10d,11)

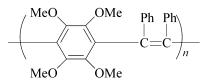
Example 31



poly(oxy{[3-(trifluoromethyl)phenyl]methylene})
(O is senior to methylene; Rule 1)

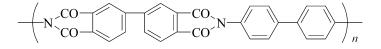
Example 32

poly(1,3-phenyleneethylene) (ring is senior to acyclic carbon chain; Rules 1,11)



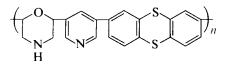
poly[(tetramethoxy-1,4-phenylene)(1,2-diphenylethene-1,2-diyl)] (ring is senior to acyclic carbon chain; Rule 1)

Example 34



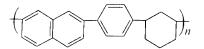
poly{(1,1',3,3'-tetraoxo[5,5'-biisoindoline]-2,2'-diyl)biphenyl-4,4'-diyl} (heterocyclic system is senior to carbocyclic system; Rules 1,3c,12)

Example 35



poly(morpholine-2,6-diylpyridine-3,5-diylthianthrene-2,8-diyl) (nitrogen heterocycles are senior to non-nitrogen heterocycle; ring with larger number of heteroatoms is senior; Rules 2a,2e,12)

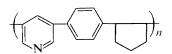
Example 36



poly(naphthalene-2,7-diyl-1,4-phenylenecyclohexane-1,3-diyl)

(two-ring system is senior to single-ring systems; benzene as least hydrogenated is senior to cyclohexane; Rules 8a,9a,11,12)

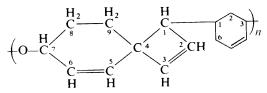
Example 37



poly(pyridine-3,5-diyl-1,4-phenylenecyclopentane-1,2-diyl) (heterocycle is senior to carbocycles; larger carbocycle is senior to smaller; Rules 1,8b,11,12)

poly(pyridine-4,2-diyl-4*H*-1,2,4-triazole-3,5-diylmethylene) (heterocycles are senior to acyclic carbon chain; larger nitrogen ring; Rules 1,2d,12)

Example 39



poly(oxyspiro[3.5]nona-2,5-diene-7,1-diylcyclohex-4-ene-1,3-diyl) (O is senior; shorter path to the senior ring system; Rules 1,8a,11,12)

Example 40

$$\left( \begin{array}{c} 4 & 3 \\ & 2 \\ 5 \\ & 5 \\ & 6 \end{array} \right) O - CH_2 - D_{\eta}$$

poly(piperidine-4,2-diyloxymethylene) (heterocycle is senior to heteroatom; shorter path between them; Rules 1,12)

Example 41

$$\underbrace{\left( \begin{array}{c} 3 \\ 1 \end{array}\right)^{2}}_{HN^{1}6} O - CH_{2} \underbrace{\right)}_{n}$$

poly(piperidine-2,4-diyloxymethylene) (heterocycle is senior to heteroatom; shorter path between them; Rules 1,12)

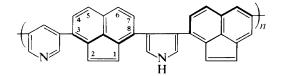
Example 42

$$($$
  $CH_2O )_n$ 

poly(pyridine-3,5-diylmethyleneoxy-1,4-phenylene) (pyridine is senior to O; shorter path between them; Rules 1,11,12)

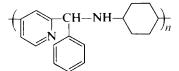
poly[imino(1-chloro-2-oxoethylene)(4-nitro-1,3-phenylene)(3-bromopropane-1,3-diyl)] (heteroatom is senior to carbocycle; shorter path between them; Rules 1,11)

Example 44



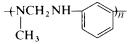
poly(pyridine-3,5-diylacenaphthylene-3,8-diylpyrrole-3,4-diylacenaphthylene-3,7-diyl) (pyridine is senior to pyrrole; shorter path between them; heavy line denotes path followed; Rules 2d,12)

Example 45



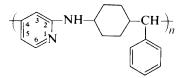
poly[pyridine-4,2-diyl(phenylmethylene)iminocyclohexane-1,4-diyl] (heterocycle is senior to heteroatom; shorter path between them; Rules 1,11,12)

Example 46



poly[(methylimino)methyleneimino-1,3-phenylene] (heteroatoms are senior to carbocycle; shorter path through both N; substituted heteroatom is senior to the same unsubstituted heteroatom; Rules 1,5,11,15)

Example 47



poly[pyridine-4,2-diyliminocyclohexane-1,4-diyl(phenylmethylene)] (heterocycle is senior to heteroatom; shorter path between them; Rules 1,11,12)

$$\underbrace{\overset{\mathsf{O}}{\overset{\mathsf{H}}{\leftarrow}}}_{\mathsf{NHCCH}_2\mathsf{SiH}_2(\mathsf{CH}_2)_3} \underbrace{\overset{\mathsf{O}}{\overset{\mathsf{H}}{\rightarrow}}}_n$$

poly[imino(1-oxoethylene)silanediylpropane-1,3-diyl] (N is senior to Si; shorter path; Rule 4)

Example 49

$$($$
  $O-(CH_2)_3)_n$ 

poly(pyridine-3,5-diylcyclohexane-1,3-diyloxypropane-1,3-diyl) (of two equal paths of three atoms between heterocycle and heteroatom, the path through carbocycle is preferred; Rules 11,12,14)

Example 50

$$\begin{array}{c} - \left( \text{SCH}_2\text{CH}_2\text{SCH}_2\text{CHCH}_2\text{CHCH}_2 \right)_n \\ \text{NH}_2 & \text{COOH} \end{array}$$

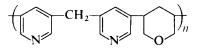
poly[sulfanediylethylenesulfanediyl(2-amino-4-carboxypentane-1,5-diyl)] (shorter path from S to S; direction determined by lower locant for the substituent earlier in the alphabetical order; Rules 10e,15)

Example 51

$$\begin{array}{c} -(\text{SCH}_2\text{CH}_2\text{SCHCH}_2\text{CH}_2\text{CH}_2\text{CH}_2)_n\\ \text{COOH} & \text{NH}_2 \end{array}$$

poly[sulfanediylethylenesulfanediyl(4-amino-1-carboxypentane-1,5-diyl)] (shorter path through both S; lowest locants for substituents; Rules 10d,15)

Example 52



poly[pyridine-3,5-diylmethylenepyridine-3,5-diyl(tetrahydropyran-3,5-diyl)] (shorter path between pyridine subunits; Rules 12,15)

Example 53

$$\frac{-(\text{SCH}_2\text{CHCH}_2\text{SCH}_2\text{CH}_2\text{CH}_2)_n}{\text{Cl}}$$

poly[sulfanediyl(2-chloropropane-1,3-diyl)sulfanediylpropane-1,3-diyl] (substituted acyclic carbon chain is senior to unsubstituted; Rules 10c,15)

$$\left( \begin{array}{c} O \\ \parallel \\ C \\ N \end{array} \right)^{-C - O - CH_2}$$

poly(pyridine-3,5-diylcarbonyloxymethylene) (heterocycle is senior to heteroatom; substituted acyclic carbon chain is senior to unsubstituted one; Rules 1,10c,12)

Example 55

poly[1,3-phenylene(1-bromoethylene)cyclohexane-1,3-diyl(2-butylethylene)] (least hydrogenated ring is senior; the direction is determined by the alphabetical order of the substituents in the carbon chain; Rules 9a,10e,11)

Example 56

$$\begin{array}{c} \text{Cl} \\ \text{-(OCCH}_2\text{NHCOCH}_2)_n \\ \text{Cl} \end{array}$$

poly[oxy(1,1-dichloroethylene)imino(1-oxoethylene)] (O is senior to N; of the two two-carbon chains the one with the larger number of substituents is senior; Rules 4,10c)

Example 57

+SCHCH<sub>2</sub>  
$$\downarrow$$
  
Cl Cl Cl

poly[sulfanediyl(1-chloroethylene)-1,3-phenylene(1-chloroethylene)] (heteroatom is senior to carbocycle; of equal chains with the same substituents that with lower locant is senior; Rules 1,10d)

Example 58

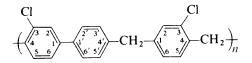
$$-($$
SCHCH<sub>2</sub>SCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CHCH<sub>2</sub>CH $-)_n$   
I Cl Br

poly[sulfanediyl(1-iodoethylene)sulfanediyl(5-bromo-3-chloropentane-1,5-diyl)] (shorter path through both S; direction determined by the lower locant of the iodo substituent; Rules 10d,15)

$$+ OCH_2N(O) = NCH_n^{-1}$$

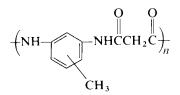
poly[oxymethylene-*ONN*-azoxy(chloromethylene)] (O is senior to N; direction in the group –N(O)=N– is indicated by the prefix *ONN*; Rules 4,7d)

Example 60



poly[(3-chlorobiphenyl-4,4'-diyl)methylene(3-chloro-1,4-phenylene)methylene] (direction determined by the lower locant for the chloro substituent in biphenyl; Rules 9c,9f,11)

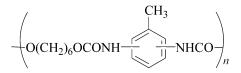
Example 61



poly[imino(x-methyl-1,3-phenylene)iminomalonyl]

(benzene is senior to acyclic carbon chain; the path from N to N through the ring can go in either direction because of the absence of a specific locant for the methyl group; Rules 1,11)

Example 62



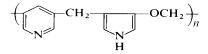
poly[oxyhexane-1,6-diyloxycarbonylimino(methylphenylene)iminocarbonyl] (path between the two oxygens through the acyclic carbon chain is shorter, since for the benzene ring with unknown positions of its attachment to other atoms the longest possible path of four carbon atoms is being considered; Rule 15)

Example 63

$$(CH_{O-CH_2}, CH_2-O_{CH_2-O}, CH-O(CH_2)_6O_{n})$$

poly(2,4,8,10-tetraoxaspiro[5.5]undecane-3,9-diyloxyhexane-1,6-diyloxy) (heterocyclic ring system is senior to heteroatoms; Rules 1,12)

© 2002 IUPAC, Pure and Applied Chemistry 74, 1921–1956



poly(pyridine-3,5-diylmethylenepyrrole-3,4-diyloxymethylene) (pyridine is senior to pyrrole; shorter path; Rules 2d,12)

Example 65

$$+OCH_2NHCS$$
  $-CH_2CH_2)_{\overline{n}}$ 

poly(oxymethyleneiminocarbonylsulfanediyl-1,3-phenyleneethylene) (O is senior to S; shorter path; Rules 4,11)

Example 66

 $-(ONHCH_2NHNHCH_2)_n$ 

poly(oxyiminomethylenehydrazine-1,2-diylmethylene) (O is senior to N; shortest path between O and N; Rule 4)

Example 67

$$\left( \begin{array}{c} CH_2 \\ NH \end{array} \right)_n CH_2 CH_2 CH_2 \\ CH_2 CH_2 \\ CH$$

poly(piperidine-4,2-diylmethylenepiperidine-4,2-diylcyclopentane-1,2-diylethylenecyclopentane-1,2-diylmethylene)

(shorter path between two identical senior heterocycles; shorter path from heterocycle to carbocycle; Rules 1,11,12,15)

Example 68

+OCH<sub>2</sub>OCH<sub>2</sub>NHCH<sub>2</sub>CH<sub>2</sub>SCH<sub>2</sub>NHCH<sub>2</sub>CH<sub>2</sub> $+_{\overline{n}}$ 

poly(oxymethyleneoxymethyleneiminoethylenesulfanediylmethyleneiminoethylene) or poly(1,3-dioxa-8-thia-5,10-diazadodecane-1,12-diyl) (O is senior to S; shorter path from O to O to N; Rules 4,15)

$$+OCH_2OCH_2OCH_2NH-CH_2NHCH_2)_n$$

poly(oxymethyleneoxymethyleneoxymethyleneimino-1,3-phenylenemethyleneiminomethylene) or poly(1,3,5-trioxa-7-azaheptane-1,7-diyl-1,3-phenylene-2-azapropane-1,3-diyl) (O is senior; the shorter path through all oxygens to the ring has been taken; Rules 4,11,16)

Example 70

$$($$
  $CH_2OCH_2NHCH_2O CH_2$   $)_n$ 

poly(pyridine-3,5-diyl-1,4-phenylenemethyleneoxymethyleneiminomethyleneoxy-1,4-phenylenemethylene)

(heterocycle is senior; shorter path from pyridine to benzene; Rules 1,11,12)

Example 71

$$+$$
SO $-$ CH $_2$  $-$ S $-$ (CH $_2$ ) $_3$  $-$ SO $_2$  $\langle$ ) $_n$ 

poly(sulfinylmethylenesulfanediylpropane-1,3-diylsulfonyl-1,4-phenylene) (shortest path between the heteroatoms; Rule 16)

Example 72

$$+ \operatorname{oc}^{O} - \operatorname{c}^{O} - \operatorname{c}^{$$

poly(oxyterephthaloylhydrazine-1,2-diylterephthaloyl) (O is senior to N; Rule 4)

Example 73

poly(nitrilo-1,4-phenylenenitriloprop-2-en-3-yl-1-ylidene-1,4-phenyleneprop-1-en-1-yl-3-ylidene)

(N is senior; shorter path between N; Rules 1,15)

+OCON=CHCH<sub>2</sub>CH=NCO $+_{n}$ 

poly(oxycarbonylnitrilopropane-1,3-diylidenenitrilocarbonyl) (O is senior to N; the direction of bonding in unsymmetrical nitrilo subunits, =N- or -N=, is indi-

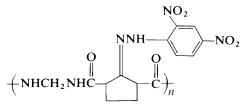
cated by the endings of the names of the adjacent subunits in the CRU; Rule 4)

Example 75

$$+\dot{O}-\dot{C}H_2-\dot{C}H_2-\dot{N}H-\dot{C}H_2-\dot{S}-\dot{C}H_2-\dot{C}H_2-\dot{N}H-\dot{D}_{\eta\eta}$$

poly(oxyethyleneiminomethylenesulfanediylethyleneiminocyclohexane-1,3-diyl) (O is senior to S; shorter path; Rules 4,11) poly(1-oxa-6-thia-4,9-diazanonane-1,9-diylcyclohexane-1,3-diyl)

Example 76



poly(iminomethyleneiminocarbonyl{2-[(2,4-dinitrophenyl)hydrazono]cyclopentane-1,3-diyl} carbonyl)

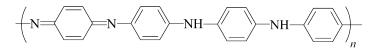
(either path through both N to ring; Rule 15)

Example 77

$$(O-CO-CO-(CH_2)_6)_n$$

poly(oxyterephthaloyloxyhexane-1,6-diyl) (O is senior to benzene; shorter path between them; Rules 1,15)

Example 78



poly(nitrilocyclohexa-2,5-diene-1,4-diylidenenitrilo-1,4-phenyleneimino-1,4-phenyleneimino-1,4-phenylene)

(-N= is most senior; Rule 7a)

$$-\left( \begin{array}{c} -CH = CH - CH_2 \right)_n$$

poly (cyclohexane-1, 4-diylmethanylylidenecyclohexane-1, 4-diylidenemethanylylidenecyclohexane-1, 4-diylmethylene)

(cyclohexane is most senior; the path to the next cyclohexane goes through a senior acyclic carbon atom –CH=; Rule 10a)

#### **10. REFERENCES**

- 1. IUPAC. "Report on nomenclature in the field of macromolecules", J. Polym. Sci. 8, 257–277 (1952).
- 2. IUPAC. "Report on nomenclature dealing with steric regularity in high polymers", *Pure Appl. Chem.* **12**, 643–656 (1966).
- IUPAC. "Nomenclature of regular single-strand organic polymers 1975", Pure Appl. Chem. 48, 373–385 (1976). Reprinted as Chapter 5 in IUPAC. Compendium of Macromolecular Nomenclature, Blackwell Scientific Publications, Oxford (1991).
- 4. IUPAC. *Nomenclature of Organic Chemistry*, Sections A, B, C, D, E, F, and H, Pergamon Press, Oxford (1979).
- 5. IUPAC. A Guide to IUPAC Nomenclature of Organic Compounds, Blackwell Scientific Publications, Oxford (1993).
- IUPAC. "Stereochemical definitions and notations relating to polymers 1980", *Pure Appl. Chem.* 53, 733–752 (1981). Reprinted as Chapter 2 in IUPAC. *Compendium of Macromolecular Nomenclature*, Blackwell Scientific Publications, Oxford (1991).
- 7. IUPAC. "Nomenclature of regular double-strand (ladder and spiro) organic polymers 1993", *Pure Appl. Chem.* **65**, 1561–1580 (1993).
- 8. IUPAC. "Structure-based nomenclature for irregular single-strand organic polymers 1993", *Pure Appl. Chem.* **66**, 873–889 (1994).
- 9. IUPAC. "Glossary of basic terms in polymer science 1996", Pure Appl. Chem. 68, 2287–2311 (1996).
- IUPAC. "Nomenclature for regular single-strand and quasi-single-strand inorganic and coordination polymers 1984", *Pure Appl. Chem.* 57, 149–168 (1985). Reprinted as Chapter 6 in IUPAC. *Compendium of Macromolecular Nomenclature*, Blackwell Scientific Publications, Oxford (1991) and as Chapter II-7 in IUPAC. *Nomenclature of Inorganic Chemistry II*, Royal Society of Chemistry, Cambridge (2001).
- 11. IUPAC. "Nomenclature of fused and bridged fused ring systems 1998", *Pure Appl. Chem.* **70**, 143–216 (1998).

#### 11. APPENDIX

#### 11.1 List of names of common subunits

(The use of subunits denoted with asterisk is not recommended [5].)

Adipoyl	-CO(CH <sub>2</sub> ) <sub>4</sub> CO-
Azo*	see Diazenediyl
Azoimino*	see Triazene-1,3-diyl
Azoxy	-N(O)=N- or -N=N(O)-
Benzoylimino	C <sub>6</sub> H <sub>5</sub> CON<

Benzylidene\* Biphenyl-3,5-diyl

Biphenyl-4,4'-diyl

Butanedioyl Butane-1,1-diyl Butane-1,4-diyl Butylidene\* But-1-ene-1,4-diyl Carbonimidoyl Carbonothioyl Carbonyl

Cyclohexane-1,1-diyl

Cyclohexane-1,4-diyl

Cyclohexylidene\* Decanedioyl Diazenediyl Dimethylmethylene Dioxy\* Diphenylmethylene Disulfanediyl Dithio\* Ethanedioyl Ethane-1,1-diyl Ethane-1,2-diyl\* Ethanediylidene Ethene-1,2-diyl Ethylene Ethylidene\* Glutaryl Hexamethylene\* Hexanedioyl Hexane-1,6-diyl Hydrazine-1,2-diyl Hydrazo\* Hydroxyimino Imino Iminio Isophthaloyl

Isopropylidene\* Malonyl Methanylylidene see Phenylmethylene see 5-Phenyl-1,3-phenylene

```
-COCH2CH2CO-
see Propylmethylene
-(CH_{2})_{4}-
see Propylmethylene
-CH=CHCH2CH2-
-C(=NH)-
-CS-
-CO-
see Cyclohexane-1,1-diyl
-CO(CH<sub>2</sub>)<sub>8</sub>CO-
-N=N-
(CH_{3})_{2}C <
see Peroxy
(C_6H_5)_2C <
-SS-
see Disulfanediyl
see Oxalyl
see Methylmethylene
see Ethylene
=CHCH=
-CH=CH-
-CH2CH2-
see Methylmethylene
-COCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CO-
see Hexane-1,6-diyl
see Adipoyl
-(CH_2)_6-
-NHNH-
see Hydrazine-1,2-diyl
HO-N<
-NH-
-NH^+-
-CO-
                 CO-
see Dimethylmethylene
-COCH2CO-
-CH=
```

#### J. KAHOVEC et al.

Methylene 1-Methylethane-1,1-diyl 1-Methylethylene Methylidenemethylene Methylidyne (–CH=) Methylmethylene Methylylidene Naphthalene-1,8-diyl	-CH <sub>2</sub> - see Dimethylmethylene -CH(CH <sub>3</sub> )CH <sub>2</sub> - CH <sub>2</sub> =C< see Methanylylidene CH <sub>3</sub> CH< see Methanylylidene
Nitrilo Oxalyl Oxy Pentamethylene Pentanedioyl Pentane-1,5-diyl Peroxy	$-N=$ $-COCO-$ $-O-$ see Pentane-1,5-diyl see Glutaryl $-(CH_2)_5-$ $-OO-$
1,4-Phenylene	
Phenylmethylene	C <sub>6</sub> H <sub>5</sub> CH<
5-Phenyl-1,3-phenylene Phthaloyl	CO- CO- CO-
Piperidine-1,4-diyl	
Propanedioyl Propane-1,3-diyl Propane-2,2-diyl Propylene* Propylmethylene Silanediyl Silylene Succinyl Sulfanediyl Sulfanediyl Sulfonyl Thio*	see Malonyl $-(CH_2)_3-$ see Dimethylmethylene See 1-Methylethylene $CH_3CH_2CH_2CH<$ $-SiH_2-$ see Silanediyl $-COCH_2CH_2CO-$ -S- -SO- $-SO_2-$ see Sulfanediyl -CO-
	\ <u></u> /

© 2002 IUPAC, Pure and Applied Chemistry 74, 1921–1956

Tetramethylene	see Butane-1,4-diyl
Thiocarbonyl*	see Carbonothioyl
Triazene-1,3-diyl	-N=N-NH-
Trimethylene*	see Propane-1,3-diyl
Vinylene*	see Ethene-1,2-diyl
Vinylidene	see Methylidenemethylene

#### 11.2 Structure- and source-based names for common polymers

The Commission recognized that a number of common polymers have semisystematic or trivial sourcebased names that are well established by usage; it is not intended that they be immediately supplanted by the structure-based names. Nevertheless, it is hoped that for scientific communication the use of semisystematic or trivial source-based names for polymers will be kept to a minimum.

For the following idealized structural representations, the semisystematic or trivial source-based names given are approved for use in scientific work; the corresponding structure-based names are given as alternative names. Equivalent names for close analogues of these polymers [e.g., other alkyl ester analogues of poly(methyl acrylate)] are also acceptable.

Structure	Source-based name (preferred given first)	Structure-based name
$-(CH_2)_n^*$	polyethene polyethylene**	poly(methylene)
$-(\operatorname{CHCH}_2)_n$ CH <sub>3</sub>	polypropene polypropylene	poly(1-methylethylene)
$\begin{array}{c} \operatorname{CH}_{1} \\ \operatorname{CCH}_{2} \\ \operatorname{CCH}_{2} \\ \operatorname{CH}_{3} \end{array}$	poly(2-methylpropene) polyisobutylene	poly(1,1-dimethylethylene)
$-(CH=CHCH_2CH_2)_n$	poly(buta-1,3-diene) polybutadiene	poly(but-1-ene-1,4-diyl)
$-(C=CHCH_2CH_2)_n$ CH <sub>3</sub>	polyisoprene	poly(1-methylbut-1-ene-1,4-diyl)
$\begin{array}{c} -(\operatorname{CHCH}_2 \rightarrow_n \\ {\operatorname{C_6H}_5} \end{array}$	polystyrene	poly(1-phenylethylene)
$+ \underbrace{\operatorname{CHCH}_2}_{\operatorname{CN}}_n$	polyacrylonitrile	poly(1-cyanoethylene)
$-(CHCH_2)_n$ OH	poly(vinyl alcohol)	poly(1-hydroxyethylene)
$+$ CHCH <sub>2</sub> $+_n$ OCOCH <sub>3</sub>	poly(vinyl acetate)	poly(1-acetoxyethylene)
$(\operatorname{CHCH}_2)_n$	poly(vinyl chloride)	poly(1-chloroethylene)
$-(CF_2CH_2)_n$ $-(CF_2)_n^*$	poly(1,1-difluoroethene) poly(vinylidene fluoride)	poly(1,1-difluoroethylene)
$-(CF_2-)_n^*$	poly(tetrafluoroethene) poly(tetrafluoroethylene)	poly(difluoromethylene)

(continues on next page)

#### J. KAHOVEC et al.

Structure	Source-based name (preferred given first)	Structure-based name
$\begin{array}{c} \hline \\ \hline \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	poly(vinyl butyral)	poly[(2-propyl-1,3-dioxane-4,6-diyl)methylene]
$(\operatorname{CHCH}_2)_n$ COOCH <sub>3</sub>	poly(methyl acrylate)	poly[1-(methoxycarbonyl)ethylene]
$\begin{array}{c} CH_3 \\ - (-CCH_2)_{\pi} \\ - (-CCH_3)_{\pi} \end{array}$	poly(methyl methacrylate)	poly[1-(methoxycarbonyl)-1-methylethylene]
$-(\text{OCH}_2)_n$	polyformaldehyde	poly(oxymethylene)
$(\operatorname{OCH}_2\operatorname{CH}_2)_{\overline{n}}$	poly(ethylene oxide)	poly(oxyethylene)
$(0 - n)^n$	poly(phenylene oxide)	poly(oxy-1,4-phenylene)
+OCH <sub>2</sub> CH <sub>2</sub> OCO	poly(ethylene terephthalate)	poly(oxyethyleneoxyterephthaloyl)
$+$ NHCO(CH <sub>2</sub> ) <sub>4</sub> CONH(CH <sub>2</sub> ) <sub>6</sub> $+_n$	poly(hexane-1,6-diyladipamide)	poly(iminoadipoyliminohexane-1,6-diyl)
$\left( \text{NHCO(CH}_2)_5 \right)_n$	poly(hexano-6-lactam) poly(e-caprolactam)	poly[imino(1-oxohexane-1,6-diyl)]
$-(-\mathrm{NHCH}_2\mathrm{CH}_2)_n$	polyaziridine poly(ethylenimine)	poly(iminoethylene)

\*The formulae  $-(CH_2CH_2)_{\eta}$  and  $-(CF_2CF_2)_{\eta}$  are more often used; they are acceptable due to the past usage and an attempt to retain some similarity to the CRU formulae of homopolymers derived from other ethene derivatives. \*\* The name "ethylene" should be used for a divalent group, " $-CH_2CH_2$ -" only and not for the monomer, " $CH_2=CH_2$ ". The

latter is "ethene" [5].