Subcommittee on Polymer Terminology (SPT)

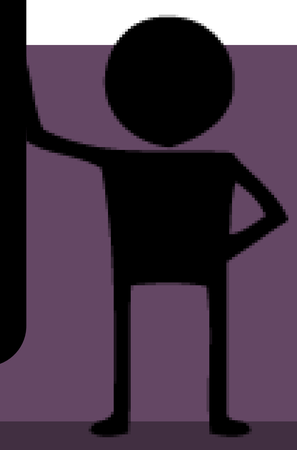
Brief Guide to Polymer Nomenclature & Terminology

Ray J. Boucher, Choon Ho Do, Rumen Duhlev, Philip Hodge, Richard G. Jones, Pavel Kratochvíl, Christine Luscombe, Christopher K. Ober, Robert F. T. Steptok, Natalie Stingelin, Michael Walter

PROJECT: 2012-048-3-400

PROJECT CHAIRS : Roger Hiorns, Jiri Vohlidal

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY



PROJECT AIM & TARGET PUBLIC

The goal of this work is to disseminate throughout the **international polymer community** a **short**, **easily assimilated**, guide to the essentials of polymer terminology.

These two-page documents are meant as basic guides that cover most of the common polymers. They can be used by **lecturers**, **students**, **authors** publishing in polymer-science journals, and indeed anyone who would like to know how polymers are named in accordance with IUPAC recommendations.

For the **complete guide** to polymer names and naming, please consult the IUPAC Purple Book, the IUPAC Compendium of Polymer Terminology and Nomenclature.

This Brief guide is not intended as a summary of **all terms**; it seeks to put the most commonly used terms into context in plain English in a manner that will be comprehensible to scientists, including those with little prior knowledge of polymers, or with little experience of the use of scientific English, or both. It includes:

- The important basic terms used in polymer science
- Careful distinctions of terms that are often misused
- Hyper-links to the relevant primary IUPAC documents

The document may reference terms in nomenclature as part of a basic introduction, but the main body of the document will deal with **terminology**, not nomenclature.

What interactive links does the Brief Guide contain?

The document carries a colour-coded hyperlinks to free IUPAC reference material; they can be used to further clarify the names and find out how to apply IUPAC rules to more complex polymers.

TEAL text links to Chemical Abstracts (CAS) website

YELLOW text links to web version of the IUPAC Gold Book

PURPLE text links to IUPAC Purple Book (Polymer Chemistry)

BLUE text links to IUPAC Blue Book (Organic Chemistry)

GREEN text links to IUPAC Green Book (Physical Chemistry)

RED text links to IUPAC Red Book (Inorganic Chemistry)

PURPLE text links also to *other* Polymer terminology documents

*Another main reference for this guide is "Principles of Chemical Nomenclature", by Jeff Leigh.

International Union of Pure and Applied Chemistry
Polymer Division
Subcommittee on Polymer Terminology

A Brief Guide to Polymer Nomenclature

Version 1.1 (2012)

R. C. Hiorns (France),* R. J. Boucher (UK), R. Duhlev (UK), K.-H. Hellwich (Germany), P. Hodge (UK), A. D. Jenkins (UK), R. G. Jones (UK), J. Kahovec (Czech Republic), G. Moad (Australia), C. K. Ober (USA), D. W. Smith (USA), R. F. T. Stepto (UK), J.-P. Vairon (France), and J. Vohlídal (Czech Republic). *E-mail: polymer.nomenclature@iupac.org; Sponsoring body: IUPAC Polymer Division, Subcommittee on Polymer Terminology.

1) Introduction

The universal adoption of an agreed nomenclature has never been more important for the description of chemical structures in publishing and on-line searching. The International Union of Pure and Applied Chemistry (IUPAC)[1a,b] and Chemical Abstracts Service (CAS)[2] make similar recommendations. The main points are shown here with hyperlinks to original documents. Further details can be found in the IUPAC Purple Book.[3]

2) Basic Concepts

The terms polymer and macromolecule do not mean the same thing. A polymer is a substance composed of macromolecules. The latter usually have a range of molar masses (unit g mol^{-1}), the distributions of which are indicated by dispersity ($Đ$). It is defined as the ratio of the mass-average molar mass (M_m) to the number-average molar mass (M_n) i.e. $Đ = M_m/M_n$.[4] Symbols for physical quantities or variables are in italic font but those representing units or labels are in roman font.

Polymer nomenclature usually applies to idealised representations; minor structural irregularities are ignored. A polymer can be named in one of two ways. Source-based nomenclature can be used when the monomer can be identified. Alternatively, more explicit structure-based nomenclature can be used when the polymer structure is proven. Where there is no confusion, some traditional names are also acceptable.

Whatever method is used, all polymer names have the prefix poly, followed by enclosing marks around the rest of the name. The marks are used in the order: {[( )]}. Locants indicate the position of structural features, e.g., poly(4-chlorostyrene). If a source-based name is one word and has no locants, then the enclosing marks are not essential, but they should be used when there might be confusion, e.g., poly(chlorostyrene) is a polymer whereas polychlorostyrene might be a small, multi-substituted molecule. End-groups are described with α- and ω-, e.g., α-chloro-ω-hydroxy-polystyrene.[3]

3) Source-Based Nomenclature[5]

3.1 Homopolymers

A homopolymer is named using the name of the real or assumed monomer (the 'source') from which it is derived, e.g., poly(methyl methacrylate). Monomers can be named using IUPAC recommendations, or well-established traditional names. Should ambiguity arise, class names can be added.[6] For example, the source-based name poly(vinyloxirane) could correspond to either of the structures shown below. To clarify, the polymer is named using the polymer class name followed by a colon and the name of the monomer, i.e., class name:monomer name. Thus on the left and right, respectively, are polyalkylene:vinyloxirane and polyether:vinyloxirane.

3.2 Copolymers[7]

The structure of a copolymer can be described using the most appropriate of the connectives shown in Table 1. These are written in italic font.

3.3 Non-linear polymers[8]

Non-linear polymers and copolymers, and polymer assemblies are named using the italicized qualifiers in Table 2. The qualifier, such as *branch,* is used as a prefix (P) when naming a (co)polymer, or as a connective (C), e.g., *comb*, between two polymer names.

Table 1 – Qualifiers for copolymers.[7]

Copolymer	Qualifier		Example
unspecified	*co*	(C)	poly(styrene-*co*-isoprene)
statistical	*stat*	(C)	poly[isoprene-*stat*-(methyl methacrylate)]
random	*ran*	(C)	poly[(methyl methacrylate)-*ran*-(butyl acrylate)]
alternating	*alt*	(C)	poly[styrene-*alt*-(maleic anhydride)]
periodic	*per*	(C)	poly[styrene-*per*-isoprene-*per*-(4-vinylpyridine)]
block	*block*	(C)	poly(buta-1,3-diene)-*block*-poly(ethene-*co*-propene)
graft[a]	*graft*	(C)	polystyrene-*graft*-poly(ethylene oxide)

[a] The first name is that of the main chain.

Table 2 – Qualifiers for non-linear (co)polymers and polymer assemblies.[5]

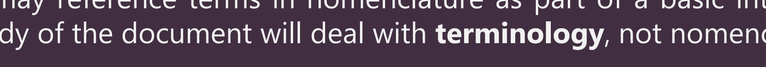
(Co)polymer	Qualifier		Example
blend	*blend*	(C)	poly(3-hexylthiophene)-*blend*-polystyrene
comb	*comb*	(C)	polystyrene-*comb*-polyisoprene
complex	*compl*	(C)	poly(2,3-dihydrothieno[3,4-*b*][1,4]dioxine)-*compl*-poly(vinylbenzenesulfonic acid)[a]
cyclic	*cyclo*	(P)	*cyclo*-polystyrene-*graft*-polyethylene
branch	*branch*	(P)	*branch*-poly[(1,4-divinylbenzene)-*stat*-styrene]
network	*net*	(C or P)	*net*-poly(phenol-*co*-formaldehyde)
interpenetrating network	*ipn*	(C)	(*net*-polystyrene)-*ipn*-[*net*-poly(methyl acrylate)]
semi-interpenetrating network	*sipn*	(C)	(*net*-polystyrene)-*sipn*-polyisoprene
star	*star*	(P)	*star*-polyisoprene

[a] In accordance with IUPAC organic nomenclature, square brackets enclose locants that refer to the numbering of the components of the fused ring.

4) Structure-Based Nomenclature

4.1 Regular single-strand organic polymers[8]

In place of the monomer name used in source-based nomenclature, structure-based nomenclature uses that of the **preferred** constitutional repeating unit (CRU). It can be determined as follows: (i) a large enough part of the polymer chain is drawn to show the structural repetition, e.g.,



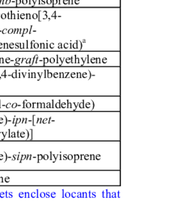
(ii) the smallest repeating portion is a CRU, so all such possibilities are identified. In this case:

(iii) the next step is to identify the subunits that make up each of these structures, i.e., the largest divalent groups that can be named using IUPAC nomenclature of organic compounds such as the examples that are listed in Table 3; (iv) using the shortest path from the most senior subunit to the next senior, the correct order of the subunits is determined using Figure 1; (v) the preferred CRU is chosen as that with the lowest possible locant(s) for substituents.

In the above example, the oxy subunits in the CRUs are heteroatom chains. From Figure 1, oxy subunits are senior to the acyclic carbon chain subunits, the largest of which are bromo-substituted -CH_2-CH_2- subunits. 1-Bromoethane-1,2-diyl is chosen in preference to 2-bromoethane-1,2-diyl as the former has a lower locant for the bromo-substituent. The preferred CRU is therefore oxy(1-bromoethane-1,2-diyl) and the polymer is thus named poly[oxy(1-bromoethane-1,2-diyl)]. Please note the enclosing marks around the subunit carrying the substituent.

Polymers that are not made up of regular repetitions of a single CRU are called irregular polymers. For these, each constitutional unit (CU) is separated by a slash, e.g., poly(but-1-ene-1,4-diyl/1-vinylethane-1,2-diyl).[9]

[1] Freely available on: (a) http://www.iupac.org/publications/pac/; (b) http://www.chem.qmul.ac.uk/iupac/
[2] http://www.cas.org/.
[3] IUPAC. The "Purple Book", RSC Publishing, (2008).
[4] IUPAC. *Pure Appl. Chem.* **81**, 351—352 (2009).
[5] IUPAC. *Pure Appl. Chem.* **69**, 2511—2521 (1997).
[6] IUPAC. *Pure Appl. Chem.* **73**, 1511—1519 (2001).
[7] IUPAC. *Pure Appl. Chem.* **57**, 1427—1440 (1985).
[8] IUPAC. *Pure Appl. Chem.* **74**, 1921—1956 (2002).
[9] IUPAC. *Pure Appl. Chem.* **66**, 873—889 (1994).

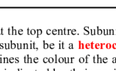


International Union of Pure and Applied Chemistry
Polymer Division
Subcommittee on Polymer Terminology

A Brief Guide to Polymer Nomenclature

Version 1.1 (2012)

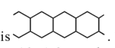
Table 3 – Representations of divalent groups in polymers.[8]

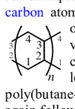
Name	Group[a]	Name	Group[a]
oxy	–O–	propylimino	
sulfanediyl	–S–	hydrazine-1,2-diyl	
sulfonyl	–SO_2–	phthaloyl	
diazenediyl	–N=N–	1,4-phenylene	
imino	–NH–	cyclohexane-1,2-diyl	
carbonyl		butane-1,4-diyl	
oxalyl		1-bromoethane-1,2-diyl	
silanediyl	–SiH_2–	1-oxopropane-1,3-diyl	
ethane-1,2-diyl	–CH_2–CH_2–	ethene-1,2-diyl	
methylene	–CH_2–	methylmethylene	

[a] To avoid ambiguity, wavy lines drawn perpendicular to the free bond, which are conventionally used to indicate free valences,[13] are usually omitted from graphical representations in a polymer context.

4.2 Regular double-strand organic polymers[10]

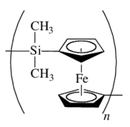
Double-strand polymers consist of uninterrupted chains of rings. In a spiro polymer, each ring has one atom in common with adjacent rings. In a ladder polymer, adjacent rings have two or more atoms in common. To identify the preferred CRU, the chain is broken so that the senior ring is retained with the maximum number of heteroatoms and the minimum number of free valences.

An example is  . The preferred CRU is an acyclic subunit of 4 carbon atoms with 4 free valences, one at each atom, as shown below. It is oriented so that the lower left atom has the lowest number. The free-valence locants are written before the suffix, and they are cited clockwise from the lower left position as: lower-left, upper-left:upper-right, lower-right. This example is thus named poly(butane-1,4:3,2-tetryal). For more complex structures, the order of seniority again follows Figure 1.



5) Nomenclature of Inorganic and Inorganic-Organic Polymers[11]

Some regular single-strand inorganic polymers can be named like organic polymers using the rules given above, e.g., $\{O\text{-}Si(CH_3)_2\}_n$ and $\{Sn(CH_3)_2\}_n$ are named poly[oxy(dimethylsilanediyl)] and poly(dimethylstannanediyl), respectively. Inorganic polymers can also be named in accordance with inorganic nomenclature, but it should be noted that the seniority of the elements is different to that in organic nomenclature. However, certain inorganic-organic polymers, for example those containing metallocene derivatives, are at present best named using organic nomenclature, e.g., the polymer on the left can be named poly[(dimethylsilanediyl)ferrocene-1,1'-diyl].



6) Traditional Names

When they fit into the general pattern of systematic nomenclature, some traditional and trivial names for polymers in common usage, such as polyethylene, polypropylene, and polystyrene, are retained.

7) Graphical Representations[12,13]

The bonds between atoms can be omitted, but dashes should be drawn for chain-ends. The seniority of the subunits does not need to be followed. For single-strand (co)polymers, a dash is drawn through the enclosing marks, e.g., poly[oxy(ethane-1,2-diyl)] shown below left. For irregular polymers, the CUs are separated by slashes, and the dashes are drawn inside the enclosing marks. End-groups are connected using additional dashes outside of the enclosing marks, e.g., α-methyl-ω-hydroxy-poly[oxirane-*co*-(methyloxirane)], shown below right.

8) CA Index Names[2]

CAS maintains a registry of substances. In the CAS system, the CRU is called a structural repeating unit (SRU). There are minor differences in the placements of locants, e.g., poly(pyridine-3,5-diylthiophene-2,5-diyl) is poly(3,5-pyridinediyl-2,5-thiophenediyl) in the CAS registry, but otherwise polymers are named using similar methods to those of IUPAC.[14,15]

Figure 1 The order of subunit seniority. The senior subunit is at the top centre. Subunits of lower seniority are found by following the arrows. The type of subunit, be it a **heterocycle**, a **heteroatom chain**, a **carbocycle**, or a **carbon chain**, determines the colour of the arrow to follow. [a] Other heteroatoms may be placed in these orders as indicated by their positions in the periodic table.[8]

[10] IUPAC. *Pure Appl. Chem.* **65**, 1561—1580 (1993).
[11] IUPAC. *Pure Appl. Chem.* **57**, 149—168 (1985).
[12] IUPAC. *Pure Appl. Chem.* **66**, 2469—2482 (1994).
[13] IUPAC. *Pure Appl. Chem.* **80**, 277—410 (2008).
[14] *Macromolecules*, **1**, 193—198 (1968).
[15] *Polym. Prepr.* **41(1)**, 6a—11a (2000).