INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Terminology and Nomenclature: a Prerequisite or Nuisance for Polymer Science Education

Roger C. Hiorns

Chair, IUPAC Subcommittee on Polymer Terminology

CNRS, IPREM (UMR 5254), Pau, France

Polymer Education Session, Room A2

Wednesday July 9 2014 10:20 - 10:50

- my own viewpoint
- what the Subcommittee on Polymer Terminology (SPT) does
- where SPT's work can be of use
- what SPT is doing to facilitate access to recommendations

- **SPT publishes recommendations on polymer nomenclature and terminology**
- **all documents are freely available**
- **all are published with Pure and Applied Chemistry**

Are recommendations and rules a nuisance?

- No!
- Misunderstanding between different communities creates more work and hinders science and education
- Rigorous, worldwide definitions facilitate understanding, communication, scientific endeavour and education

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doi:10.1351/PAC-REC-08-05-02

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

POLYMER DIVISION
SUBCOMMITTEE ON POLYMER TERMINOLOGY*

DISPERSITY IN POLYMER SCIENCE

(IUPAC Recommendations 2009)

Prepared by a Working Group consisting of
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Dispersity in polymer science

(IUPAC Recommendations 2009)

Abstract: This recommendation defines just three terms, viz., (1) molar-mass dispersity, relative-molecular-mass dispersity, or molecular-weight dispersity; (2) degree-of-polymerization dispersity; and (3) dispersity. "Dispersity" is a new word, coined to replace the misleading, but widely used term "polydispersity index" for $\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$. The document, although brief, also has a broader significance in that it seeks to put the terminology describing dispersions of distributions of properties of polymeric (and non-polymeric) materials on an unambiguous and justifiable footing.

Keywords: dispersity; molar-mass dispersity; relative-molecular-mass dispersity; molecular-weight dispersity; degree-of-polymerization dispersity; polydispersity; polydispersity index; IUPAC Polymer Division.

INTRODUCTION

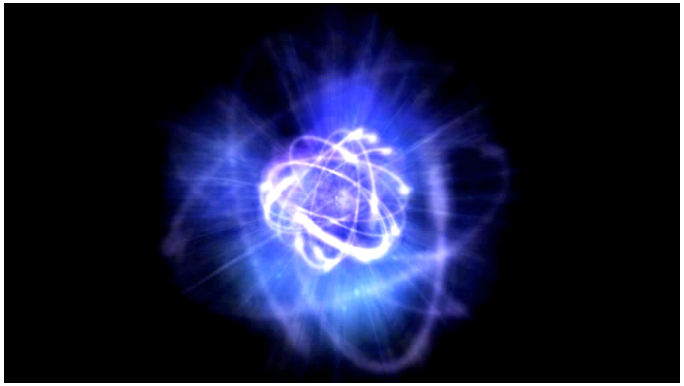
A dimensionless ratio of two average values of a property is widely used in polymer science as a characteristic of the dispersion, or spread, of the distribution of values of that property in a sample of polymer. In particular, the ratios $\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$ are quantities commonly used to characterize the dispersions of distributions of molar masses and degrees of polymerization, respectively. However, they do not have satisfactory names and the present recommendation seeks to rectify this situation.

$\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$ are both often erroneously called "polydispersity index", although they are not indices and the term "polydispersity" is not a defined quantity. In addition, a polymer sample composed of a single macromolecular species should be called a "uniform polymer" and a polymer sample composed of macromolecular species of differing molar masses a "non-uniform polymer" [1]. It is preferable if such polymer samples are *not* called "monodisperse polymer" and "polydisperse polymer", respectively [1]. "Monodisperse" is a self-contradictory term, and "polydisperse" is tautologous.

The names proposed in this recommendation for $\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$, are "molar-mass dispersity" and "degree-of-polymerization dispersity", respectively, with "relative-molecular-mass dispersity" and "molecular-weight dispersity" proposed as synonyms for molar-mass dispersity. "Dispersity" is a new word, coined to denote a measure of the dispersion of macromolecular species in a sample of polymer. The suffix "-ity" or "-ty" is described in dictionaries [2] as one used to form nouns describing quality, state of being or condition. In a scientific context, "-ity" is generally used to form nouns denoting the quality of a particular property, e.g., density, conductivity, resistivity, opacity, etc., in which the "quality" has a numerical value. Hence, "dispersity" is an appropriate word to describe a numerical attribute of the dispersion of a distribution.

The term "dispersity" is here limited to describing the dispersions of distributions of molar masses (or relative molecular masses, or molecular weights) and degrees of polymerization. With the use of suitable adjectives, it can easily be applied to distributions of other properties of samples of polymeric (and non-polymeric) materials, giving, for example, diffusion-coefficient dispersity and particle-diameter dispersity. Further applications and developments of the term will be the subject of future work. The immediate aim is to recommend satisfactory and widely acceptable names for $\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$. The general symbol $Đ$, pronounced "*D*-stroke", is introduced for dispersity to avoid confusion with the conventional use of D for diffusion coefficient.

In early stage education



even useful when making solar cells from sponges and cd cases!

IUPAC working with Wikipedia

From around 15 upwards becomes important especially through Wikipedia…

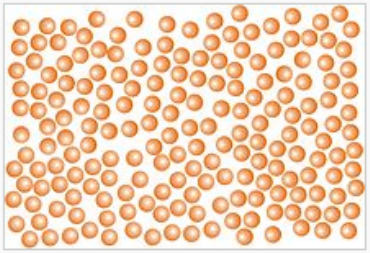
Prof. Michael Hess and colleagues found that many definitions on Wikipedia were misleading or even wrong

Dispersity

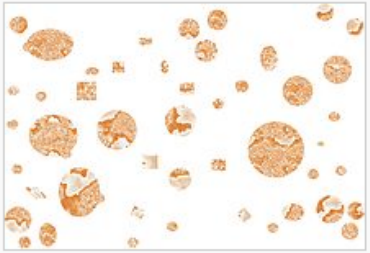
From Wikipedia, the free encyclopedia

In physical and organic chemistry, the **dispersity** is a measure of the heterogeneity of sizes of molecules or particles in a mixture. A collection of objects is called **uniform** if the objects have the same size, shape, or mass. A sample of objects that have an inconsistent size, shape and mass distribution is called **non-uniform**. The objects can be in any form of chemical dispersion, such as particles in a colloid, droplets in a cloud,[1] crystals in a rock,[2] or polymer molecules in a solvent.[3] Polymers can possess a distribution of molecular mass; particles often possess a wide distribution of size, surface area and mass; and thin films can possess a varied distribution of film thickness.[*citation needed*]

IUPAC has deprecated the use of the term *polydispersity index* having replaced it with the term *dispersity*, represented by the symbol $Đ$ (pronounced D-stroke[4]) which can refer to either molecular mass or degree of polymerization. It can be calculated using the equation $Đ_M = M_w/M_n$, where M_w is the weight-average molar mass and M_n is the number-average molar mass. It can also be calculated according to degree of polymerization, where $Đ_X = X_w/X_n$, where X_w is the weight-average degree of polymerization and X_n is the number-average degree of polymerization. In certain limiting cases where $Đ_M = Đ_X$, it is simply referred to as $Đ$. IUPAC has also deprecated the terms *monodisperse*, which is considered to be self-contradictory, and *polydisperse*, which is considered redundant, preferring the terms *uniform* and *non-uniform* instead.[4]



A uniform (monodisperse) collection



A non-uniform (polydisperse) collection

Contents [hide]

Overview [edit]

A monodisperse, or uniform, polymer is composed of molecules of the same mass.[5] Natural polymers are typically monodisperse.[6] Synthetic monodisperse polymer chains can be made by processes such as anionic polymerization, a method using an anionic catalyst to produce chains that are similar in length. This technique is also known as living polymerization. It is used commercially for the production of block copolymers. Monodisperse collections can be easily created through the use of template-based synthesis, a common method of synthesis in nanotechnology.[*citation needed*]

A polymer material is denoted by the term polydisperse, or non-uniform, if its chain lengths vary over a wide range of molecular masses. This is characteristic of man-made polymers.[1] Natural organic matter produced by the decomposition of plants and wood debris in soils (humic substances)

IUPAC definition

$Đ_M = M_w/M_n$

where M_w is the weight-average molar mass and M_n is the number-average molar mass.

Pure Appl. Chem., **2009**, 81(2), 351-353

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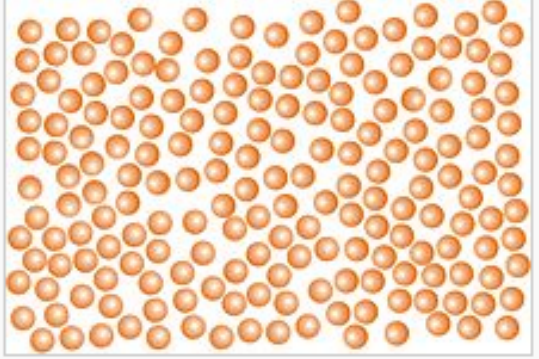
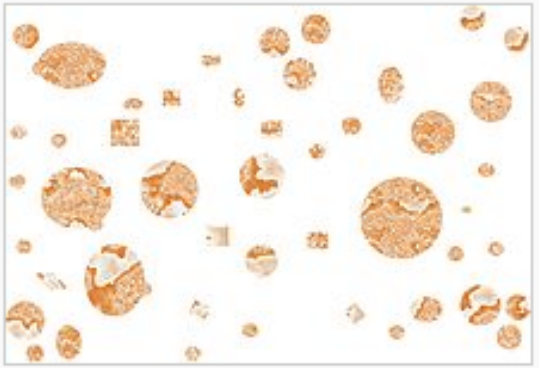


A uniform (monodisperse) collection



A non-uniform (polydisperse) collection

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IUPAC definition

$Đ_M = M_w/M_n$

where M_w is the weight-average molar mass and M_n is the number-average molar mass.

Pure Appl. Chem., **2009**, 81(2), 351-353

Three cases dealt with in Wiki

- Existing Wikipedia entries to be synchronized with IUPAC definitions
- Creation of new entries to Wikipedia basing on existing IUPAC definitions
- ‘Stubs’ in the field of polymers

modifications made

http://en.wikipedia.org/wiki/Copolymer
http://en.wikipedia.org/wiki/Adsorption
http://en.wikipedia.org/wiki/Aerogel
http://en.wikipedia.org/wiki/Anionic_addition_polymerization
http://en.wikipedia.org/wiki/List_of_synthetic_polymers
http://en.wikipedia.org/wiki/Bone_cement
https://en.wikipedia.org/wiki/Branching_(polymer_chemistry)
https://en.wikipedia.org/wiki/Carcinogen
https://en.wikipedia.org/wiki/Cationic_polymerization
https://en.wikipedia.org/wiki/Chain-growth_polymerisation
https://en.wikipedia.org/wiki/Chain_termination
http://en.wikipedia.org/wiki/Cross-link
http://en.wikipedia.org/wiki/Adhesion
http://en.wikipedia.org/wiki/Biofilm
http://en.wikipedia.org/wiki/Atom-transfer_radical-polymerization
https://en.wikipedia.org/wiki/Biodegradation
http://en.wikipedia.org/wiki/Biomineralization
http://en.wikipedia.org/wiki/Bioplastic
http://en.wikipedia.org/wiki/Colloid
http://en.wikipedia.org/wiki/Colloidal_crystal
http://en.wikipedia.org/wiki/Degree_of_polymerization

new entries

https://en.wikipedia.org/wiki/Reversible-deactivation_radical_polymerization
http://en.wikipedia.org/wiki/Degenerative_chain_transfer
http://en.wikipedia.org/wiki/Reversible-deactivation_polymerization

typical entry

Cationic polymerization

From Wikipedia, the free encyclopedia

Cationic polymerization is a type of chain growth polymerization in which a cationic initiator transfers charge to a monomer which then becomes reactive. This reactive monomer goes on to react similarly with other monomers to form a polymer.[1][2] The types of monomers necessary for cationic polymerization are limited to olefins with electron-donating substituents and heterocycles. Similar to anionic polymerization reactions, cationic polymerization reactions are very sensitive to the type of solvent used. Specifically, the ability of a solvent to form free ions will dictate the reactivity of the propagating cationic chain. Cationic polymerization is used in the production of polyisobutylene (used in inner tubes) and poly(N-vinylcarbazole) (PVK).[3]

Contents [hide]

IUPAC definition

An ionic polymerization in which the kinetic-chain carriers are cations.[4]

IUPAC working with languages

Accessing multilingual definitions

- Prof. Michael Hess, Prof. Claudio dos Santos and colleagues developed a new website
- Czech, English, French, German, Italian, Polish, Portuguese, and Spanish
- Korean, Chinese, Japanese, Thai…

http://www.iceb.ufop.br/dequi/iupac/polymerglossary/index.php

Polymer Glossary

Glossary of Basic Terms in Polymer Science

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ABOUT THE PROJECT

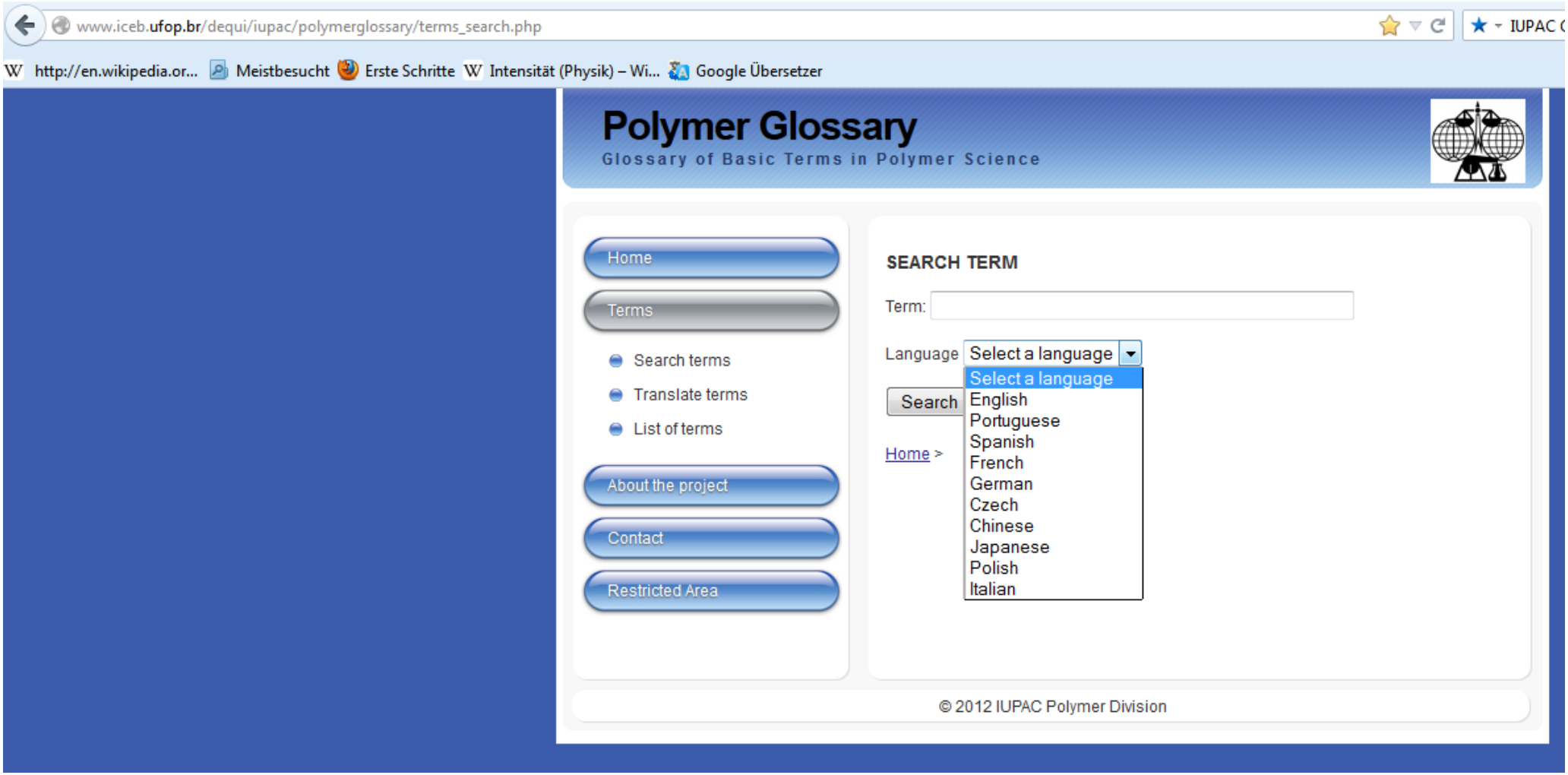
Fostering world-wide communications in all areas of Chemistry has been a long established goal of IUPAC activities since it was founded. This polymer glossary is intended as a web-based and user-friendly tool combining translations of terms of polymer science and their definitions in several languages. It is based on the "Glossary of Basic Terms in Polymer Science", which is one of the chapters of the "Compendium of Polymer Terminology and Nomenclature", known as Purple Book, published by IUPAC through the Royal Society of Chemistry.

An international team of polymer scientists are collaborating in this project and the translations are recognized by the relevant National Adhering Organization affiliated to IUPAC.

This first version includes translations in Czech, French, Spanish, Polish and Portuguese. Other translations are also going to be incorporated including non-western languages like Chinese, Japanese, Korean and Thai, to name a few.

Cláudio G. dos Santos
Project Leader

Home >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Polymer Glossary

Glossary of Basic Terms in Polymer Science

SEARCH TERM

Term: macromolecule

Language Select a language

Search

Search Results:

macromolecule

Alternative term: polymer molecule

Molecule of high relative molecular mass, the structure of which essentially comprises the multiple repetition of units derived, actually or conceptually, from molecules of low relative molecular mass.

Note 1: In many cases, especially for synthetic polymers, a molecule can be regarded as having a high relative molecular mass if the addition or removal of one or a few of the units has a negligible effect on the molecular properties. This statement fails in the case of certain properties of

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TRANSLATE TERM

Term (from english):

macromolecule

to : French

Translate

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Polymer Glossary

Glossary of Basic Terms in Polymer Science

TRANSLATE TERM

Term (from english):

to : Select a language

Translate

macromolécule

(French)

terme équivalent : molécule polymère.

Molécule de masse molaire élevée dont la structure résulte essentiellement de la répétition d'unités dérivées, de fait ou conceptuellement, de molécules de faible masse molaire.

Note 1 : Dans de nombreux cas, spécialement pour les polymères de synthèse, une molécule peut être considérée de masse molaire élevée lorsque l'adjonction ou la suppression d'une ou de quelques unité(s) a un effet négligeable sur ses propriétés. Cette assertion perd sa validité pour les macromolécules dont la structure moléculaire

Polymer Glossary

Glossary of Basic Terms in Polymer Science

REGISTERED TERMS BY CLASS (English)

Molecules and molecular structure

- atactic macromolecule
- block
- block macromolecule
- branch
- branch point
- branch unit
- branched chain
- chain
- comb macromolecule
- configurational base unit
- configurational repeating unit
- configurational sequence
- configurational unit
- constitutional repeating unit (CRU)
- constitutional sequence
- constitutional unit
- crosslink
- degree of polymerization
- double-strand chain
- double-strand macromolecule
- end-group
- graft macromolecule
- ionomer molecule
- irregular macromolecule
- isotactic macromolecule
- junction unit
- ladder chain
- ladder macromolecule
- linear chain
- linear macromolecule
- long chain
- loose end
- macrocycle
- macromolecule
- macromonomer molecule
- macromonomeric unit
- macroradical

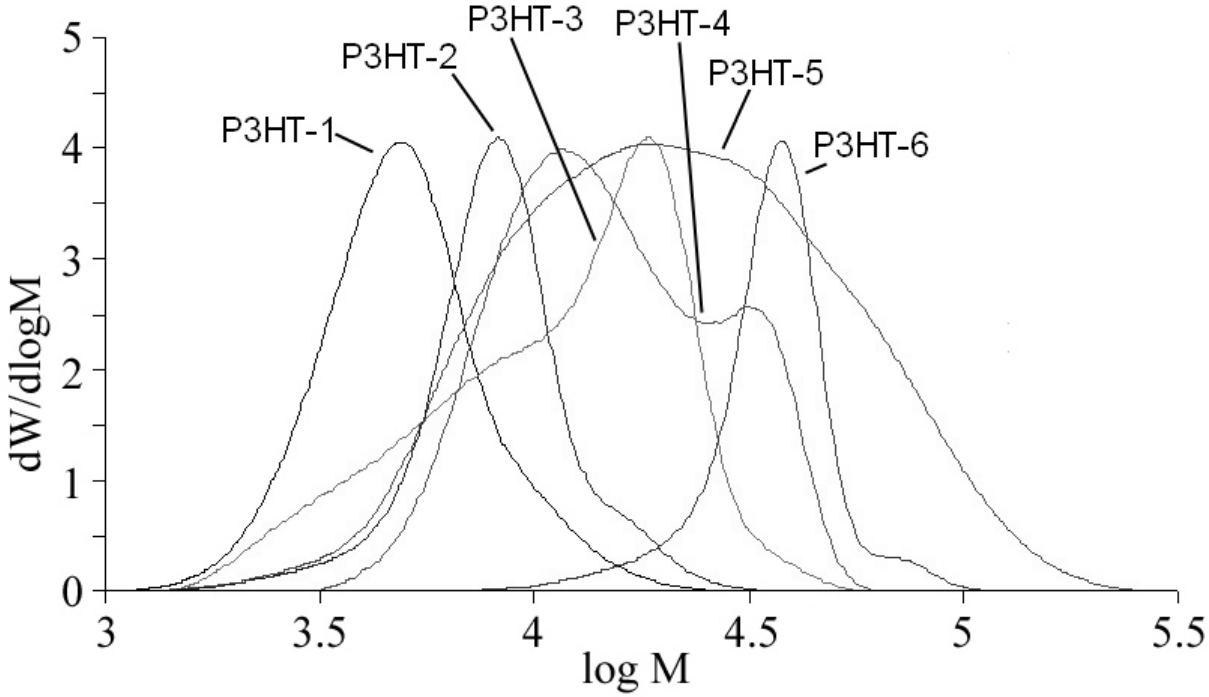
A Brief Guide to Polymer Nomenclature

Basic Terms

number average molar mass M_n
mass average molar mass M_m

SI units for M are g mol^{-1}

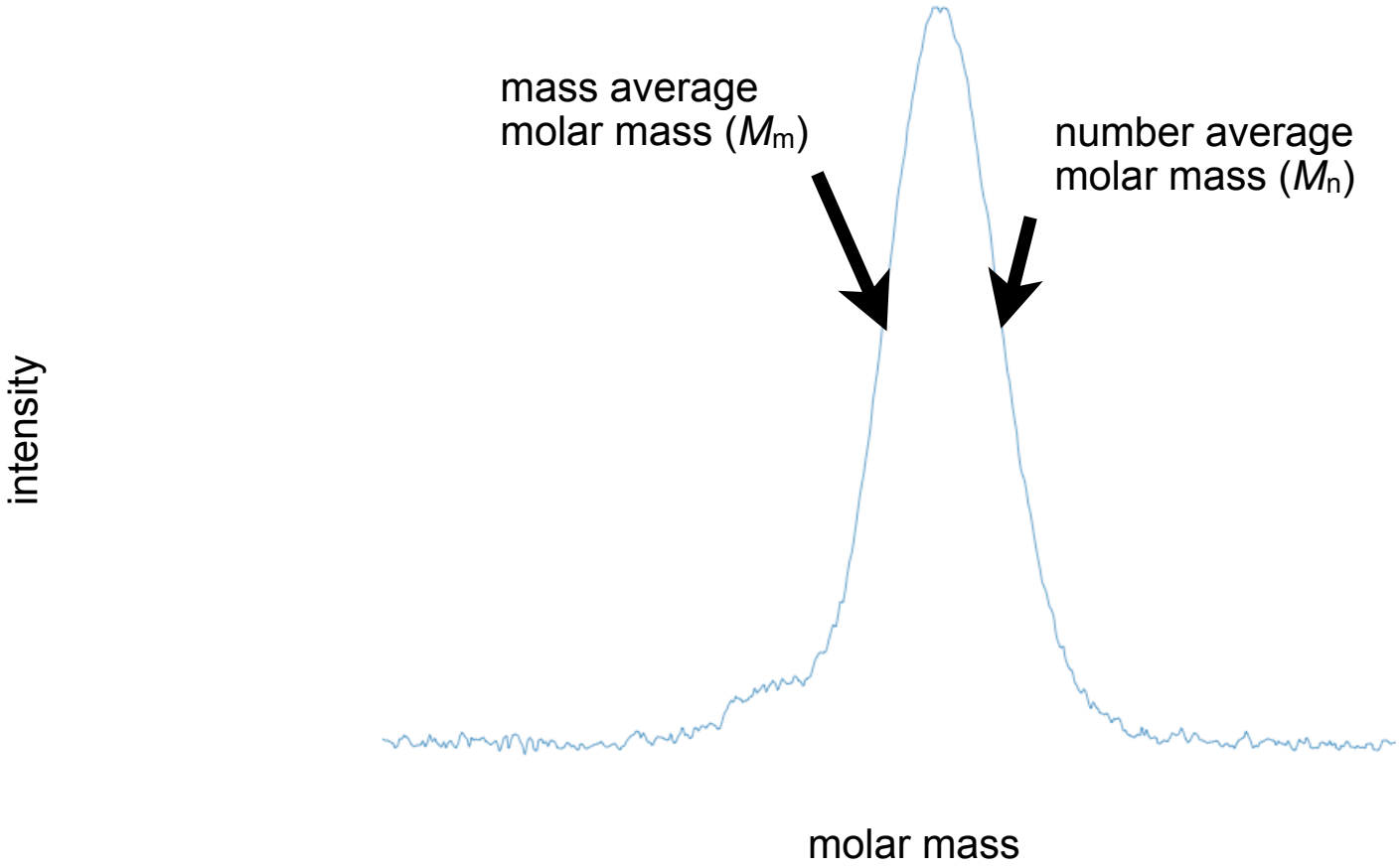
Basic Terms



the term “polydispersity index (PDI)” is discouraged

Basic Terms

dispersity is the measure of spread of molar mass



$$\text{dispersity} = Đ = M_\text{m}/M_\text{n}$$

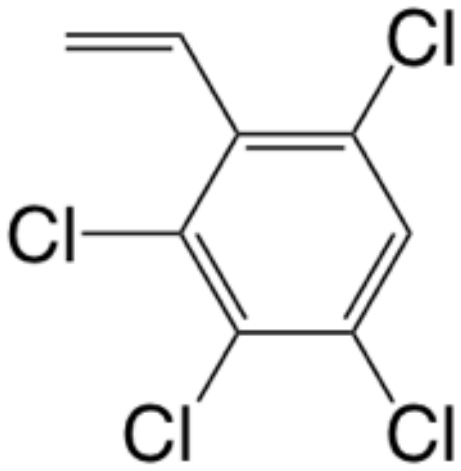
IUPAC. *Pure Appl. Chem.* **81**, 351—352 (2009).

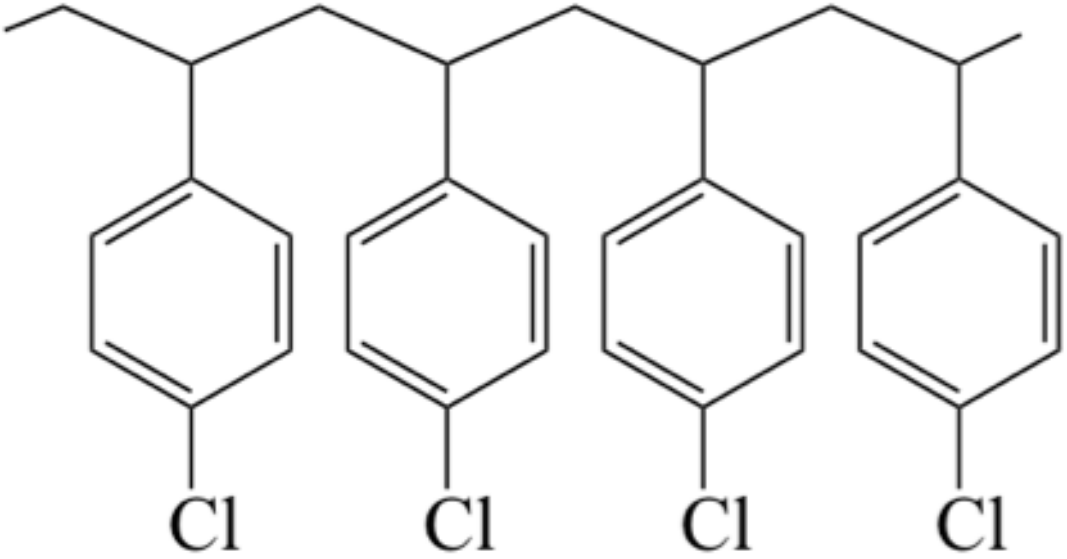
Nomenclature

each name has to be *explicit* and *different*

polychlorostyrene

?





THREE POLYMER NOMENCLATURES

source-based

structure-based

traditional

THREE POLYMER NOMENCLATURES

source-based based on a monomer

structure-based

traditional

THREE POLYMER NOMENCLATURES

source-based — based on a monomer

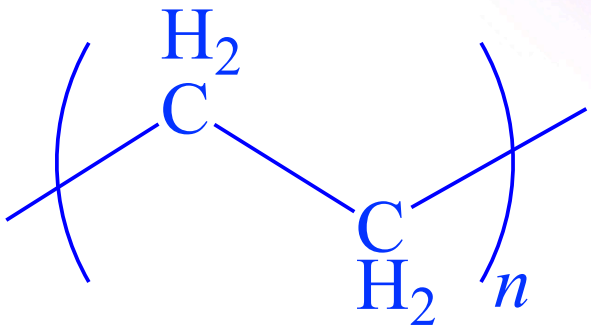
structure-based — based on a known structure

traditional

THREE POLYMER NOMENCLATURES

source-based	based on a monomer
structure-based	based on a known structure
traditional	an old, well known name

Nomenclature



source-based	based on a monomer poly(ethene)
structure-based	based on a known structure poly(ethylene) poly(ethane-1,2-diyl)
traditional	an old, well known name polyethylene

Nomenclature

source-based	based on a monomer
structure-based	based on a known structure

Nomenclature - Brief Guide

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-

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.

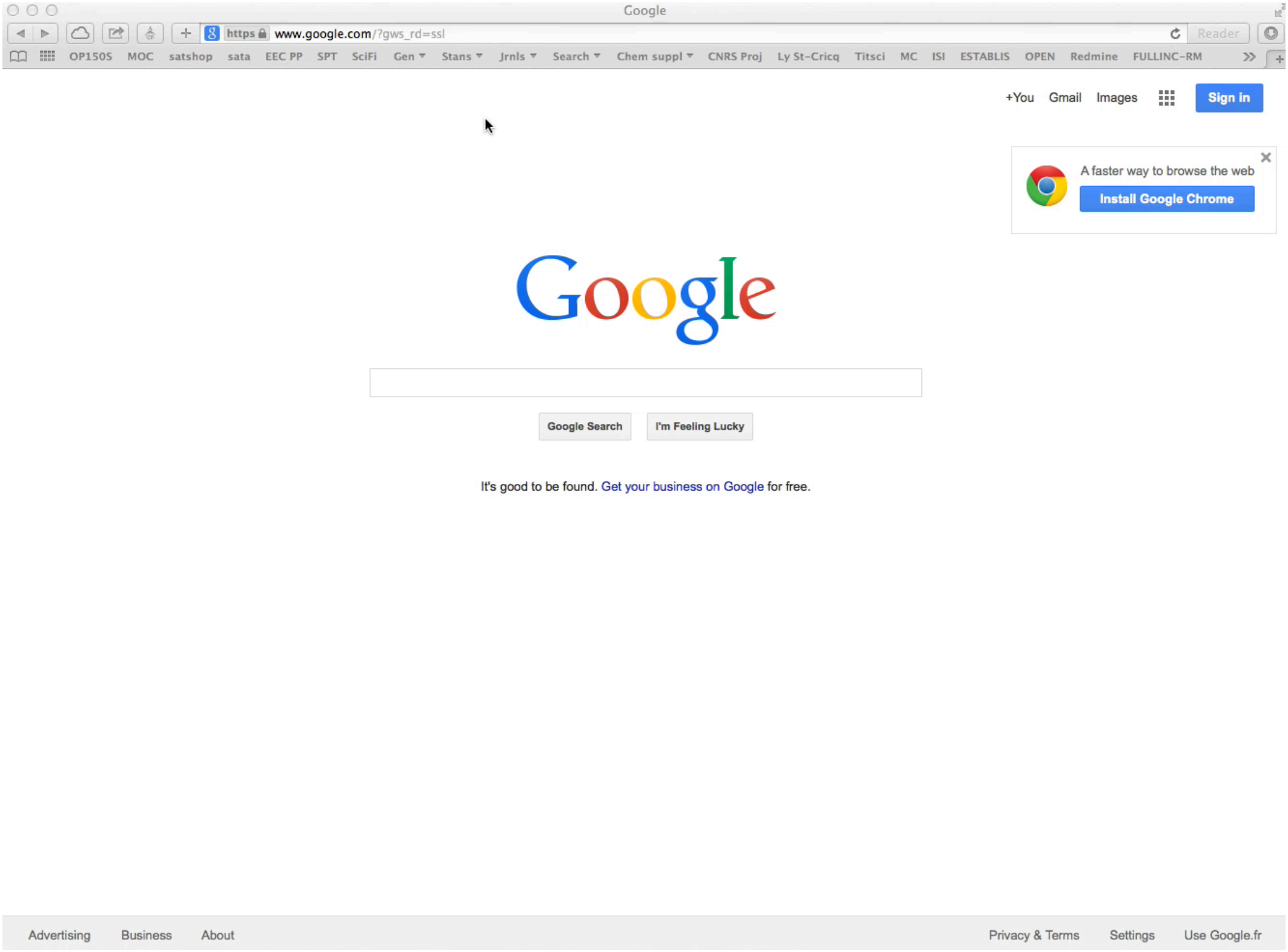
4) Structure-Based Nomenclature

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.,

$$-CH-CH_2-O-CH-CH_2-O-CH-CH_2-O-$$

- www.iupac.org/web/ins/2008-032-1-400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International Union of Pure and Applied Chemistry
Polymer Division
Subcommittee on Polymer Terminology

A Brief Guide to Polymer Nomenclature

Version 1.1 (2012)

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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)[1,2] and Chemical Abstracts Service (CAS)[3] 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_w) to the number-average molar mass (M_n) i.e. $Đ = M_w/M_n$.[4] Symbols for physical quantities or variables are in italic font but those representing units or labels are in roman font.

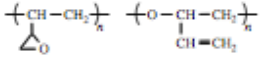
Polymer nomenclature usually applies to idealised representations; minor structural irregularities are ignored. A polymer can be named in one of two ways. Source-based nomenclature can be used when the monomer can be identified. Alternatively, more explicit structure-based nomenclature can be used when 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]

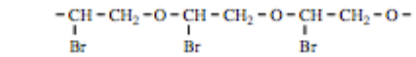
(Co)polymer	Qualifier		Example
blend	*blend*	(C)	poly(3-hexylthiophene)-*blend*-polystyrene
comb	*comb*	(C)	polystyrene-*comb*-polyisoprene
complex	*compl*	(C)	poly(2,3-dihydrothieno[3,4-*b*][1,4]dioxine)-*compl*-poly(vinylbenzenesulfonic acid)[a]
cyclic	*cyclo*	(P)	*cyclo*-polystyrene-*graft*-polyethylene
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.

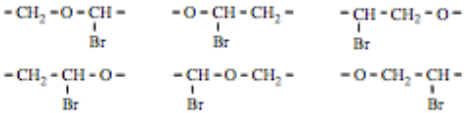
4) Structure-Based Nomenclature

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).

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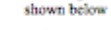
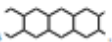
Table 3 – Representations of divalent groups in polymers.[a]

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	

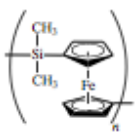
[a] To avoid ambiguity, wavy lines drawn perpendicular to the free bond, which are conventionally used to indicate free valences,[7] are usually omitted from graphical representations in a polymer context.

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-tetrayl). 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., $\{O\text{-}Si(CH_3)_2\}$, and $\{Sn(CH_3)_2\}$, 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.

[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).

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. * Other heteroatoms may be placed in these orders as indicated by their positions in the periodic table.[9]

Journal participation

Colloid and Polymer Science, **2013**, January, 1-2.
European Polymer Journal, **2013**, 73(1), iv-v.
Polymer, **2013**, 54(1), 3-4.
Polymer Degradation and Stability, **2013**, 98(1), 1-2.
Polymer Testing, **2013**, 32(1), iv-v.
Polymers for Advanced Technologies, **2013**, 24(1), i-ii.
Polymer International, **2013**, 62(1), i-ii.
Progress in Polymer Science, **2013**, 38(1), iii-iv.
Reactive and Functional Polymers, **2013**, 73(1), iv-v.
Synthetic Metals, **2013**, 1633(1), vi-vii.
Chemistry International, **2012**, November-December issue.
Pure and Applied Chemistry, **2012**, *84*, 2167-2169.

Instructions to Authors
European Polymer Journal,
Macromolecular Chemistry and Physics,
Macromolecular Rapid Communications,
Macromolecular Bioscience,
Macromolecular Theory and Simulations,
Macromolecular Materials and Engineering,
Macromolecular Reaction Engineering,
Macromolecules,
Polymer,
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Polymers for Advanced Technologies,
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Reactive and Functional Polymers
Synthetic Metals…

In Journal Editorials, Press and Society Pages
ACS Macro Letters Editorial, *Chemistry International*, *Macromolecules Editorial*, *MaterialsViews*, *Société Chimique de France*…

impact

Full Paper

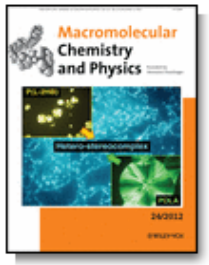
Tuning Dispersity in Diblock Copolymers Using ARGET ATRP

Andrzej Plichta, Mingjiang Zhong, Wenwen Li, Andrea M. Elsen and Krzysztof Matyjaszewski*

Article first published online: 5 NOV 2012

DOI: 10.1002/macp.201200461

Issue



Macromolecular Chemistry and Physics

Volume 213, Issue 24, pages 2659–2668, December 21, 2012

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Keywords:
activators regenerated by electron transfer; atom transfer radical polymerization; block copolymer; molecular weight distribution

Abstract

Poly(methyl acrylate)-*b*-polystyrene with controlled molecular weight distribution of each block was synthesized via activators regenerated by electron transfer atom transfer radical polymerization. Polymers with tunable dispersity, in the range of $\overline{M}_w/\overline{M}_n$ 1.32 to 2.0, were achieved by adjusting the concentration of the copper catalyst and reaction temperature, thereby controlling the rate of reversible deactivation reaction as well as the number of monomer units added during each activation cycle. Regardless of the increased dispersity, high chain-end functionality was retained and the livingness of the macroinitiators was confirmed by chain extension, resulting in diblock copolymers with controlled dispersity in each block. Liquid chromatography under critical conditions was employed to determine if any macroinitiator remained in the final product.

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these authors are using dispersity anyway…but seeing wider use of the term

University course work

http://www.tech.plym.ac.uk/sme/mats231/

MATS 231: Composite Materials and Structures for the Marine Environment

Review papers on composites technology
Subject Index to JS' web pages

ACMC

Definitive module record (DMR) for MATS231: assessment is 0% examination and **100% coursework (50:50 laboratory : in-class test)**:
a separate page gives guidance on the general requirements for each classification for an honours degree.

Recommended reading: Hull and Clyne CSHL 🕮, Bunsell and Renard CSHL 🕮, Åström CSHL 🕮, Strong CSHL 🕮

HEALTH & SAFETY
It is important that all students are aware of the Health and Safety considerations for this module. You will be required to attend the Health and Safety presentation and to sign to confirm that you have done so before you will be allowed to use the facilities in the ACMC laboratory (Brunel 007). This support material can be accessed online.

Week	Date	Topic	Powerpoint	Reading Lists
24 1	Friday 10 January 2014 09:00-11:00 Smeaton 102b	Introduction. Nomenclature and basic equations. Organic chemistry. **ESSENTIAL:** Health and safety in the laboratory.	1a 1b 1c	1a 1b 1c 1d
25 2	Tuesday 14 January 2014 11:00-14:00 Brunel 007	Demonstration of resin infusion under flexible tooling (RIFT)		
25 2	Friday 17 January 2014 09:00-11:00 Smeaton 102b	**Reinforcements**: fibres and fabrics	2a 2b	2a 2b
26 3	Tuesday 21 January 2014 11:00-14:00 Brunel 007	LABORATORY PRACTICAL: Manufacture of composite plates		
26 3	Friday 24 January 2014 09:00-11:00 Smeaton 102b	**Matrix systems:** thermoplastic polymers and thermoset (phenolic and epoxy, polyester and vinyl ester) resins	3a 3b	3a 3b 3c
27 4	Tuesday 28 January 2014 11:00-14:00 Smeaton 001	LABORATORY PRACTICAL: Flexural (modulus and strength) and interlaminanar shear strength (ILSS) testing		
27 4	Friday 31 January 2014 09:00-11:00 Smeaton 102b	**Manufacturing methods I:** **overview** Contact moulding. Vacuum-bag/AutoClave. Resin Transfer Moulding (RTM).	4a 4d 4b	4
28 5	Tuesday 04 Feb 2014 11:00-14:00 Brunel 005	LABORATORY PRACTICAL: Electron microscopy of fractured specimens		
28 5	Friday 07 February 2014 09:00-11:00 Smeaton 102b	**Manufacturing methods II:** Resin Infusion. **Characterisation:** **overview** anisotropy. E, G, v and K. Strength and failure mechanisms.	4c 5a 5b	5a 5b 5c
29 6	Friday 14 February 2014 09:00-11:00 Smeaton 102b	**Durability:** creep, fatigue and impact. osmosis and blistering, cavitation erosion, galvanic corrosion. **Manufacturing methods III:** Filament winding and pultrusion.	5c 6 4e	6
30 7	Friday 21 February 2014 09:00-11:00 Smeaton 102b	**Quality:** Product Liability. CE marking. Recreational Craft Directive (RCD). Classification societies.	7	7
31 8	**Tuesday 25 February 2014 15:00 Smeaton Admin**	**DEADLINE for the submission of coursework reports**		
31 8	Friday 28 February 2014 09:00-11:00 Smeaton 102b	**Case studies:** offshore structures, naval vessels, yacht hulls, canoes, sailcloth.	8	8
32 9	Friday 07 March 2014 09:00-11:00 Smeaton	doi> **Disposal** of marine composites at end-of-life	9	N/A

Resources

- **Careers**
  - Careers for composites graduates
  - Composites companies in Devon and Cornwall
  - UK and Irish universities
- **Case studies**
  - Composite bridges in Europe
  - Composites in marine applications
- **Coursework**
  - Academic dishonesty (including cheating and plagiarism)
  - Appendix A: resin infusion procedure
  - Appendix B: CRAG test methods for flexure and ILSS
  - Appendix C: Electron microscopy
  - Characterisation of composites (overview)
  - Citing references in your reports
  - Composite manufacturing processes (overview)
  - Equipment available at Plymouth
  - General requirements for honours degrees
  - **Health and Safety (essential!)**
  - ILS reading list for researchers
  - JS' guidance on the requirements and rules for coursework
  - Late coursework and extenuating circumstances
  - Poster design tips (Centre for Learning Technology)
  - **Risk assessment**
  - Suppliers of materials and equipment
- **Definitions**
  - Abbreviations and acronyms
  - Common tradenames for polymers
  - CompositesOne glossary of terms
  - Glossary of fibre/textile terms
  - Glossary of manufacturing terms
  - Glossary of non-destructive testing terms
- **Grey literature**
  - FreeFullPDF (full-text journal library)
  - National Technical Information Service (NTIS USA)
  - Open Access Library
  - OpenGrey SIGLE (System for Information on Open Grey Literature in Europe)
  - Prior Art Database at IP.com
  - Thesis list for composites (to circa 1994)
- **More Links for composite materials and structures**
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  - Chemistry (Chem.Answers.com)
  - ChemSpider free chemical structure database (and for iDevices)
  - CORE materials open educational resources (Search & Browse)
  - Engineering Fundamentals (efunda): Composite Materials
  - IUPAC brief guide to polymer nomenclature
  - **Kaye and Laby** Tables of Physical and Chemical Constants (on-line at NPL)

Kharlampieva Research Group

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Polystyrene

Key Concepts

- Polystyrene is also known as poly(ethenylbenzene), poly(phenylethene), poly(1-phenylethene), poly(1-phenylethane-1,2-diyl) [1].
- Polystyrene can be produced in an addition polymerisation reaction.

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[1] The IUPAC name for linear-chain polymers is made by placing the prefix poly before the name of the constitutional repeating unit in parentheses. However, the name of the repeating unit could be based on its source, poly(ethenylbenzene), or, on the structure of the polymer, poly(1-phenylethane-1,2-diyl). Luckily, some well-established common names, like polystyrene, are still acceptable. Refer to the IUPAC webiste for a guide to polymer nomenclature (A Brief Guide to Polymer Nomenclature (2012 pdf).

[2] Dow Chemical invented the Styrofoam process in 1941.

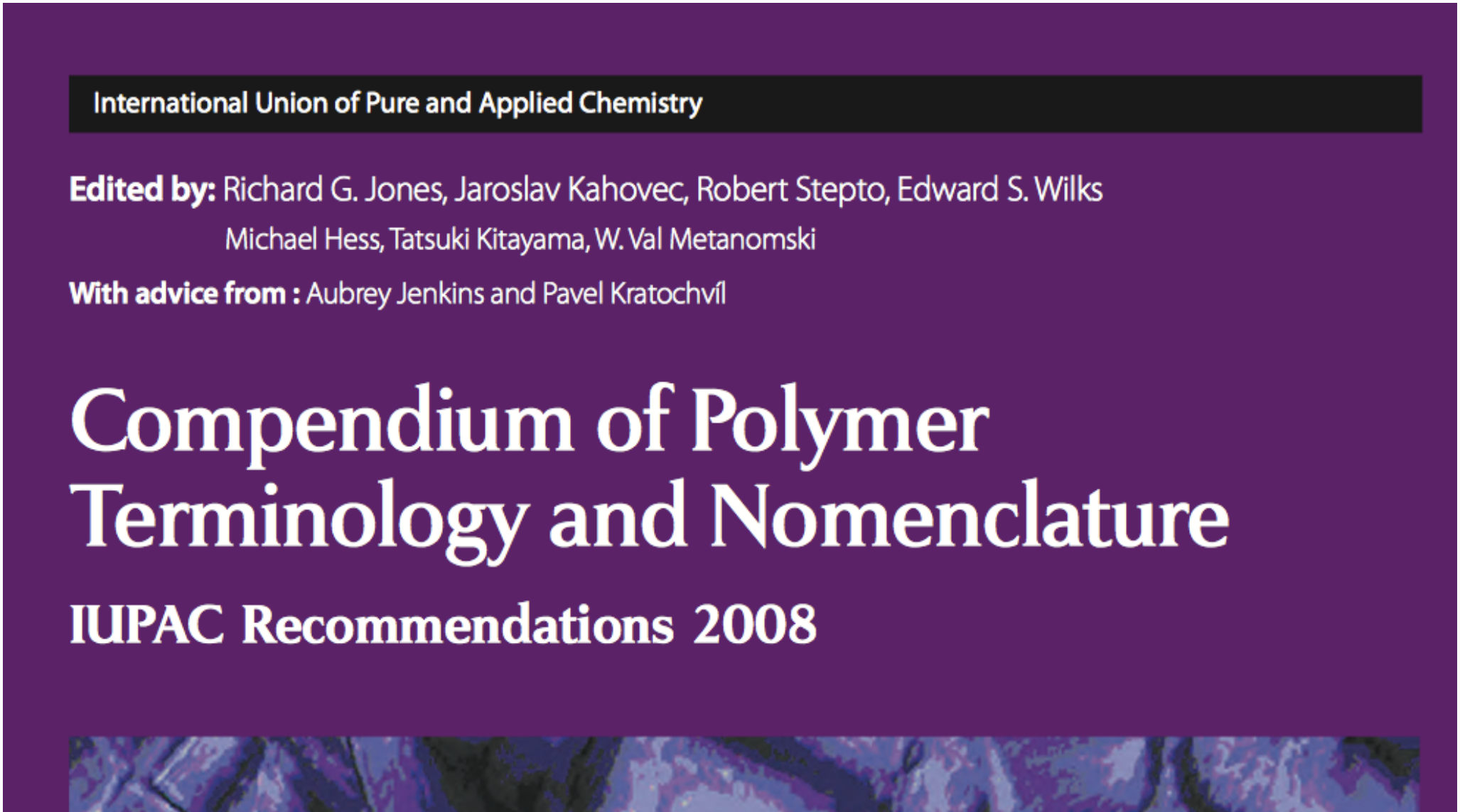
[3] Polystyrene is inexpensive to produce, so the cost of recycling it needs to be very low in order to make recycling commercially viable. This is particularly true for expanded polystyrene (EPS) or polystyrene foam because the 'gas bubbles' cause problems in the recycling process.

[4] Styrene, or ethenylbenzene or phenylethene, may contain the inhibitor 4-(dimethylethyl)-benzene-1,2-diol (4-tert-butyl catechol) which needs to be removed by washing with 1 mol L^{-1} NaOH(aq) then with water in a separating funnel. Dry the phenylethene over anhydrous sodium sulfate, $Na_2SO_4(s)$, for 10 minutes. Wash all equipment in propanone (acetone), CH_3COCH_3.

Further reading

Purple Book

http://www.iupac.org/fileadmin/user_upload/publications/e-resources/ONLINE-IUPAC-PB2-Online-June2014.pdf



Acknowledgements

Wikipedia

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Multilingual

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Brief Guide

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).

Acknowledgements

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IUPAC

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY