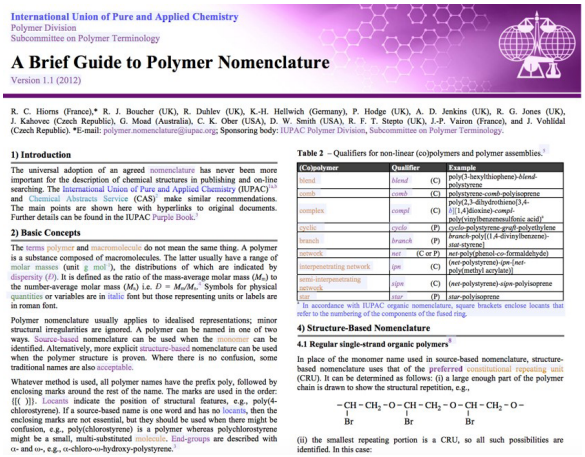
Brief Guide to Polymerization Terminology

A project has been initiated under the Subcommittee of Polymer Terminology (SPT) in the Polymer Division entitled "The Brief Guide to Polymerization Terminology". The project aims to produce a short summary of existing documents related to polymerization terminology in a form that can be readily disseminated and is publicly accessible by students and researchers. The rationale behind the *Brief Guide* is that, while fully elaborated IUPAC recommendations on polymerization terminology exist, confusion still remains in the field. Many researchers and students using a variety of different terms for the same concept, some of which are incorrect or misleading based on the current understanding of polymerizations. We aim to bridge the gulf between IUPAC recommendations and scientific/educational use of terms so that we can all speak the same language when referring to concepts related to polymerization.

While SPT has developed rich terminology that communicates state-of-the-art, precise understanding of polymerizations, there are relatively few publishing academic scientists who use such terms. Examples of such terms include "polydispersity index" instead of "dispersity"; "chain-growth" instead of "chain polymerization"; "step-growth" instead of "polycondensation"; and the frequently incorrectly used term "living polymerization". This is all the more surprising given the extremely high value of such understanding to the worldwide industrial development of advanced polymer-based materials. The SPT has coined terms that both communicate and encapsulate complex concepts in a self-explanatory manner. All their publications are freely accessible, and can be reprinted in whole without constraint. However, few working publishers, scientists, students, industrialists, educators, and authors know where to obtain, how to use, and distribute this work. Our goal is to create an easily accessible and portable document to discourage the use of misleading terms.

This project will address this problem by delivering a short (two-page) document that explains and summarizes the most important terms, and will provide active hyperlinks that will link directly to the original source documents. Liberal use of links to the IUPAC color books will also be made so that any word that might cause confusion to a novice reader will be clarified. In effect, this short guide will provide a robust stairway for users to quickly gain a working knowledge



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.[5]

Table 2 – Qualifiers for non-linear (co)polymers and polymer assemblies.[6]

(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.,

$$-\mathrm{CH}(\mathrm{Br})-\mathrm{CH_2}-\mathrm{O}-\mathrm{CH}(\mathrm{Br})-\mathrm{CH_2}-\mathrm{O}-\mathrm{CH}(\mathrm{Br})-\mathrm{CH_2}-\mathrm{O}-$$

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

"The Brief Guide to Polymerization Terminology" will follow a similar format as "A Brief Guide to Polymer Nomenclature", shown above.

of the concepts and terminology surrounding polymer chemistry today. This project is now all the more important given the incredible explosion in polymerization techniques over the last twenty or so years, thus requiring correct terminology to distinguish the variant methodologies.

This project follows the recently completed and high impact project 'A brief guide to polymer nomenclature' *Pure Appl. Chem.* 84, 2167-2169 (2012). The proposed *Brief Guide for Polymerizations* will follow a similar format.

The terms to be used in the proposed Brief Guide for Polymerizations will be heavily based on recommendations from three projects: "Basic classification and definitions of polymerization reactions (IUPAC Recommendations 1994)", *Pure Appl. Chem.* 66, 2483-2486 (1994); "Glossary of terms related to kinetics, thermodynamics, and mechanisms of polymerization", *Pure Appl. Chem.* 80, 2163-2193 (2008); and the ongoing project 2010-007-1400 entitled "Terminology for Chain Polymerization". The work will begin by identifying the most important terms described in these two documents/three projects. Finally, a project web page will be set up such that updated versions of the document can be downloaded in subsequent years. The resulting *Brief Guide* will be shared with a number of leading publishers that carry polymer journals including Nature, ACS, RSC, and Wiley.

For further information, contact the Task Group Chair Christine Luscombe <luscombe@u.washington.edu> or Graeme Moad <graeme.moad@csiro.au>

www.iupac.org/project/2015-013-1-400