IUPAC- Polymer Division IV

Subcommittee on Polymer Terminology

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INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

INTRODUCTION

In 1952, the Sub-commission on Nomenclature to the **IUPAC Commission on Macromolecules** published its first recommendations. In 1968 IUPAC formally established the Commission on Macromolecular Nomenclature (Commission IV.1), which became the leading nomenclature body in the field of polymers. In 2002 the Commission became the Subcommittee on Macromolecular Terminology, and in 2005 was renamed the **Subcommittee on Polymer** Terminology.

As the former Commission, rules were developed for naming regular single-strand macromolecules, copolymer molecules, irregular macromolecules, ladder and spiro macromolecules, and nonlinear and network polymers. Rules for representing the structures of macromolecules were also developed. Latterly, while still addressing issues of **polymer nomenclature**, the Subcommittee has worked to **standardize** the **terminology** used in polymer science. Amongst other topics, it has developed a glossary of basic terms, and made recommendations concerning the terminology of assemblies of polymer molecules and non-linear macromolecules, polymer solutions, polymer crystals, types of polymerization, kinetics and thermodynamics of polymerization, degradation and aging of polymers, and the mechanical behavior of polymers.

As well as being tasked with establishing terminological rules and definitions, the Subcommittee also advises the Chemical Nomenclature and Structure Representation Division (VIII) on the development of polymer nomenclature.

Since its inception, the Subcommittee has attracted the participation of exceptional scientists from academia, publishing houses, and the polymer industry.

ONGOING PROJECTS

Project number	Acronym	TGL	Project title
2023-007-1-400	MASSIVE	Keddie	Clarifications of Definitions for Polymer Molar Mass Averages
2022-006-2-400	R-BGN	Hiorns	Revision of the Brief Guide to Polymer Nomenclature
2020-024-3-400	SUPRA	Gosecka	Nomenclature and terminology for supramolecular polymers
2019-043-2-400	GOLDEN	dos Santos	Gold Book Updates for Polymers
2019-041-3-400	SEQ	Theato	Nomenclature of Sequence-Controlled Polymers
2019-036-1-800	STARS2	Chen	Structure-based nomenclature for irregular linear, star, comb and brush polymers with different types of constitutional repeating units (CRU)
2019-027-1-400	OVER	Matson	Basic classification and definitions of polymerization reactions
2019-010-2-400	AGGREGATES	Nakano	Terminology of Polymer Aggregates
2018-033-1-400	ADDIPLAST	(Malinconico) Giuntini	Additives intended to promote the degradation of polyolefin-based thermoplastic materials
2016-050-3-400	μSTRUCTURE	Stingelin	Definition of Terms Pertaining to Polymers in the Solid State: Molecular Arrangement from the Nano- to the Micrometer Scale
2017-039-2-800	GRAPHIC	Theato	Graphical Representation of Polymer Structures
2015-050-1-400	ULTIMATE	Adhikari	Definition of Terms Relating to the Ultimate Mechanical Properties of Polymers
2015-049-1-400	CHAR	Topham	Brief Guide to the Characterisation of Polymers
2015-032-2-400	WIKI	Hess	Synchronizing Wikipedia: Polymer Definitions and Terminology
2015-014-1-400	SEMIS	Walter	Guide (and Brief Guide) to Polymer Semiconductors
2014-014-1-400	MODSIM	Meille	Terminology for Modeling and Simulation of Polymers
2013-049-1-400	SEPARATION	Hess	Terminology on the separation of macromolecules
2011-035-1-800	TINCOPS	Jones	Terminology and nomenclature of inorganic and coordination polymers – a extended revision of Nomenclature for regular single-strand and quasi- single-strand inorganic and coordination polymers (1984)

Reconsidering Terms for Mechanisms of Polymer Growth: The "Step-Growth" and "Chain-Growth" Dilemma

Chin Han Chan, Jiun-Tai Chen, Wesley S. Farrell, Christopher M. Fellows, Daniel J. Keddie, Christine K. Luscombe, John B. Matson, Jan Merna, Graeme Moad, Gregory T. Russell, Patrick Théato, Paul D. Topham, Lydia Sosa-Vargas



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



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1) Introduction branch points. This structure is noticeably different from the dendriti The International Union of Pure and Applied Chemistry (IUPAC) macromolecule which is tree-like and carries one or more dendrons.⁶ A publishes definitions of terms to enable communication of information related class is that of macromor er which has an end-group allowing worldwide. Definitions of terms commonly used in polymer chemistry it to act as a monome are paraphrased here with hyperlinks and screen-tips to approved A homopolymer is made from one real or apparent monome

definitions in the Gold and Purple Books, or the original source whereas a copolymer contains two or more. The monomeric units in documents. This document complements the Brief Guide to Polymer statistical and random copolymers, respectively, are distributed Nomenclature,¹ the Brief Guide to Polymerization Terminology² and following statistical laws or placed independently from the nature of the other forthcoming brief guides. 2) Macromolecules and Polymers^{3,4}

adjacent units. A periodic copolymer has more than two monomeric units in a regular sequence, while an alternating copolymer has only two units in strict alternation

An ionic polymer is made of macromolecules containing ionic or

Isomers have the same atomic composition but different line or reochemical formulae. An isomerization is a reaction that yields a

product that is isomeric to the reactant. Configuration is a spatial

be a chiral center, a rigid group, or a cyclic moiety, as exemplified in

Z and E, respectively, denoting the lesser preferred terms, *cis* and *tran*

carbons are described using R and S in accordance with

The terms macromolecule and polymer do not mean the same thing. A polymer is a substance composed of macromolecules of high molar ionizable groups.⁷ An ionomer and a polyelectrolyte are composed of mass (M). An oligomer molecule is of intermediate molar mass such macromolecules, respectively, with a small or a substantial number of that a change in the number of units will noticeably alter its properties. CUs carrying ionic or ionizable groups or both. An ampholytic p The degree of polymerization (X) indicates the number of monomeric units making up a macromolecule. Each sample normally contains a contains both anionic and cationic groups, or corresponding ionizable range of chain lengths. Dispersity (D) quantifies the breadth of this groups. A zwitterionic polymer contains ionic groups of opposite signs, distribution and is defined by $\mathcal{D} = M_{\rm m}/M_{\rm n}^{1.5}$ The number-average molar often on the same pendent group. mass (M_n) and mass-average molar mass $(M_m \text{ or } M_w)$ (unit g mol⁻¹), can

be calculated using the equations, respectively:

 $\overset{\circ}{\underset{\to}{\operatorname{and}}} (w_{\mathrm{M}} / \overline{M}) \quad \text{and} \quad M_{\mathrm{m}} \overset{\circ}{\underset{\to}{\operatorname{and}}} M_{\mathrm{w}} = \overset{\circ}{\underset{\to}{\operatorname{and}}} w_{\mathrm{M}} M$ in which $w_{\rm M}$ is the mass fraction of molar mass M.

A constitutional unit (CU) consists of one or more atoms that makes up an essential part of a macromolecular structure. A monomeric unit is the largest CU that can be identified as coming from a monomer ating units (CRUs) are the CIP priority rules. Diastereoisomers are stereoisomers that are not molecule. Importantly, smallest CUs that can be used to identify the structure of the whole mirror images. chain. A regular macromolecule can be described by a single CRU joined in the same way throughout, whereas an irregular macromolecule



3) Configuration and Stereoisomerism^{8,9,10}

arrangement of atoms or groups about a stereois

Fig. 2. Rigid centers are described using the preferred ste

ethene-1.2-divl]: polv[(Z)-cvclopentane-1,3-divl] & polv[(E)-cyclopentane-1,3-divl]; & poly[(R)-oxy(1-methylethane-1,2-diyl)] & poly[(S)-oxy(1-methylethane-1,2-diyl)]

onal unit, whereas a CRU with at least one stereoisomer is l base unit (CBU). The smallest series of CBUs that describe a configurational repetition of step sm in the mai

We do not recommend new terms here. Instead, members of SPT detail our concerns with these terms and seek suggestions from the community on how to provide **clear**, **simple**, and **consistent** terms to describe the **two major mechanisms** of polymer growth.

Reference. *Polym. Chem.* **2022**, *13*, 2262–2270. doi: 10.1039/d2py00086e



Polymers are classified by their macromolecular skeletal structure, i.e., the sequence of atoms that defines their essential topological are single-strand, and those with connected rings such as ladder and spiro macromolecules are double-strand. A block macromolecule is composed of linear sequences of blocks joined at a junction unit. A star le has at least three chains at the junction unit. The graft le has one or more side chains connected to a main chain, with different structural features from the main chain. However, a comb macromolecule typically has a higher density of side chains which do

IUPAC. Pure Appl. Chem. 84, 2167 (2012).

chain is a configurational repeating unit (CFRU). A CRU having stereoisomeric configurations at all main chain sites is a ste unit (SRU). The tacticity of a polymer defines the orderliness of CFRUs in the main chain (please see Fig. 3). A tactic macromolecul identical CFRUs, while isotactic and syndiotactic macromolecules have representation, as shown in Fig. 1. Those with CUs joined by two atoms CBUs with chiral atoms in the main chain uniquely or alternately arranged with respect to their adjacent CUs, respectively. An atactic macromolecule has CBUs in a random sequence. A diad comprises two stereoisomeric centers next to each other. When they are the same, m is used as a descriptor, and when they are different r is used.¹¹ Thus, syndiotactic chains have only r diads, isotactic chains are all m diads, while atactic chains have both m and r diads in a random sequence.

not need to be different from the main chain. A network polymer is highly interconnected, bonding each CU with many others. A e can be a cyclic macromolecule or just a cyclic part of a structure. Other structures include the branched polymer which has Fig. 3. The position of CBUs in stereoisomeric polymers.

IUPAC. Pure Appl. Chem. 78, 2067 (2006) ⁸ IUPAC. Pure Appl. Chem. 68, 2193 (1996)
⁹ IUPAC. Pure Appl. Chem. 74, 915 (2002).

¹⁰ IUPAC. Pure Appl. Chem. **53**, 733 (1981).
¹¹ IUPAC. Pure Appl. Chem. **92**, 1769 (2020).

 ² IUPAC. Pure Appl. Chem. **94**, 2107 (2012).
³ IUPAC. Pure Appl. Chem. **68**, 2287 (1996). ⁴ IUPAC. Pure Appl. Chem. 81, 1131 (2009).
⁵ IUPAC. Pure Appl. Chem. 81, 351 (2015); Erratum ibid, 81, 779 (2009). 6 IUPAC. Pure Appl. Chem. 91, 523 (2019).

Page 1 of 2

RECENT PUBLICATIONS

DE GRUYTER

Pure Appl. Chem. 2022: 94(9): 1093-1147

Pure Appl. Chem. 2022; 94(5): 559-571

IUPAC Recommendation

Christopher M. Fellows, Richard G. Jones[†], Daniel J. Keddie, Christine K. Luscombe, John B. Matson, Krzysztof Matyjaszewski, Jan Merna, Graeme Moad*, Tamaki Nakano, Stanislaw Penczek, Gregory T. Russell and Paul D. Topham

Terminology for chain polymerization (IUPAC Recommendations 2021)

https://doi.org/10.1515/pac-2020-1211 Received December 19, 2020; accepted June 9, 2022

Abstract: Chain polymerizations are defined as chain reactions where the propagation steps occur by reaction between monomer(s) and active site(s) on the polymer chains with regeneration of the active site(s) at each step. Many forms of chain polymerization can be distinguished according to the mechanism of the propagation step (e.g., cyclopolymerization – when rings are formed, condensative chain polymerization – when propagation is a condensation reaction, group-transfer polymerization, polyinsertion, ring-opening polymerization – when rings are opened), whether they involve a termination step or not (e.g., living polymerization – when termination is absent, reversible-deactivation polymerization), whether a transfer step is involved (e.g., degenerative-transfer polymerization), and the type of chain carrier or active site (e.g., radical, ion, electrophile, nucleophile, coordination complex). The objective of this document is to provide a

[†]Deceased (1939–2021).

Article note: Sponsoring bodies: IUPAC Polymer Division, Sub-Committee on Polymer Terminology

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UPAC Recommendations	
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DE GRUYTER

Michel Vert*, Jiazhong Chen, Andrey Yerin, Karl-Heinz Hellwich, Roger C. Hiorns, Richard Iones[†], Graeme Moad and Gerard P. Moss

Terminology and the naming of conjugates based on polymers or other substrates (IUPAC Recommendations 2021)

https://doi.org/10.1515/pac-2020-0502 Received May 13, 2020; accepted January 9, 2022

Abstract: A number of human activities require that certain complex molecules, referred to as active species (drugs, dyes, peptides, proteins, genes, radioactive labels, etc.), be combined with substrates, often a macromolecule, to form temporary or permanent conjugates. The existing IUPAC organic, polymer, and inorganic nomenclature principles can be applied to name such conjugates but it is not always appropriate. These nomenclatures have two major shortcomings: (1) the resulting names are often excessively long and (2) identification of the components (substrate, active species, and link) can be difficult. The new IUPAC naming system elaborates rules for unambiguous and facile naming of any conjugate. This naming system is not intended to replace the existing nomenclature but to provide a suitable alternative when dictated by necessity. Although the rules are intended to be primarily applicable to the naming of polymer conjugates, they are also applicable to naming conjugates with other substrates, which include micelles, particles, minerals, surfaces, pores, etc. The naming system should be used when recognition of the substrate and active substance is essential and will also be useful when constraints of name length make the otherwise preferred IUPAC nomenclatures untenable. The proposed rules for the new naming system are complemented by a glossary of relevant terms.

Keywords: Active species; biologically active conjugate; carrier; conjugate; conjugation; drug delivery; pharmacologically active conjugate; protein-based conjugate; substrate; support.

CONTENTS

	CONJ-1	Preamble		56
CONJ-2		Structures and limitations		
		CONJ-2.1	Structural base conjugation	56
		CONJ-2.2	Conjugations in a conjugate	56

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IUPAC Recommendations

Jiazhong Chen*, Edward S. Wilks*, Alain Fradet, Karl-Heinz Hellwich, Roger C. Hiorns, Tamaki Nakano, Claudio G. dos Santos and Patrick Theato

Pure Appl. Chem. 2021; 93(9): 963-995

Structure-based nomenclature for irregular linear, star, comb, and brush polymers (IUPAC Recommendations 2020)

https://doi.org/10.1515/pac-2020-0103 Received January 10, 2020; accepted January 25, 2021

Abstract: The existing recommendations for the structure-based nomenclature of regular single-strand organic polymers are extrapolated to complex polymers. The key proposal is that polymeric moieties may be named substituents. The types of polymers covered include linear and branched polymers containing more than one block of a single type of constitutional repeating unit (CRU) and branched polymers containing a main chain from which one or more polymeric side chains emanate.

Keywords: Brush-shaped polymers; comb-shaped polymers; IUPAC Division of Chemical Nomenclature and Structure Representation; IUPAC Polymer Division; linear polymers; Nomenclature Recommendations; starshaped polymers; structure-based polymer names.

SCB-1 Introduction

Between 1984 and 2012, the IUPAC published several documents containing recommendations for the nomenclature of a wide variety of polymer types such as regular linear single-strand [1, 2], irregular singlestrand [2, 3], organic regular double-strand [2, 4], and cyclic organic macromolecules [5], non-linear macromolecules and macromolecular assemblies [2, 6], and quasi-single-strand inorganic and coordination polymers [7]. More recently a document on source-based nomenclature for single-strand homopolymers and copolymers was published in 2016 [8], and a document on nomenclature for dendrimers and hyperbranched polymers was published in early 2019 [9]. However, structure-based nomenclature for certain types of

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Pure Appl. Chem. 2020; 92(11): 1861–1891

IUPAC Recommendations

Richard G. Jones*, Christopher K. Ober, Teruaki Hayakawa, Christine K. Luscombe and Natalie Stingelin

Terminology of polymers in advanced lithography (IUPAC Recommendations 2020)

https://doi.org/10.1515/pac-2018-1215 Received December 18, 2018: accepted July 15, 2020

Abstract: As increasingly smaller molecular materials and material structures are devised or developed for technological applications, the demands on the processes of lithography now routinely include feature sizes that are of the order of 10 nm. In reaching such a fine level of resolution, the methods of lithography have increased markedly in sophistication and brought into play 2terminology that is unfamiliar, on the one hand, to scientists tasked with the development of new lithographic materials or, on the other, to the engineers who design and operate the complex equipment that is required in modern-day processing. Publications produced by scientists need to be understood by engineers and *vice versa*, and these commonly arise from collaborative research that draws heavily on the terminology of two or more of the traditional disciplines. It is developments in polymer science and material science that lead progress in areas that cross traditional boundaries, such as microlithography. This document provides the exact definitions of a selection of unfamiliar terms that researchers and practitioners from different disciplines might encounter.

Keywords: microlithography; nanotechnology; polymers; recommendations; terminology.

CONTENTS

AL-1	Introduct	ion	
AL-2	Terminol	ogy	
	AL-2.1	absorbance, A, A ₁₀ , A _e , B	
	AL-2.2	absorption	
	AL-2.3	adhesion	
	AL-2.4	adhesion promoter	
	AL-2.5	aerial image	
	AL-2.6	annealing (in polymer science)	
		AL-2.6.1 solvent vapor annealing	
		AL-2.6.2 thermal annealing (in lithography)	

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bodies: IUPAC Chemical Nomenclature and Structure Representation Division and IUPAC Polymer Division: see more details on page 994

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PERSPECTIVES - List of envisioned projects

- Degradation of Polymers (Gardette)
- Revision of Purple Book (Theato)
- Polymers of Relevance to Human Health (Stingelin)
- Polymers for 3D printing (Walter)
- Terminology for constitutionally-dynamic polymers (Vohlídal)
- Terminology of renewable and recycled polymers (Vairon)
- Electronic Formulae of Polymers (Yerin)
- Drawing of chemical structures of polymeric networks (Theato)
- Sustainable Polymers (Topham)
- Terminology of copolymerization (Moad)
- Polyaddition/polycondensation ...



