8: A Classification of Linear Single-Strand Polymers (1988)

PREAMBLE

The polymer literature lacks, at present, a widely applicable, internally consistent, and easily recognizable system for classifying polymers. This situation prevails in spite of the large number of polymers that are already known or will be synthesized in the future. The classification scheme to be presented here facilitates logical indexing, including through the use of computer techniques, information storage and retrieval. At the present time, the scheme is limited to linear single-strand organic and inorganic polymers. It is consistent with previous IUPAC recommendations [1-5].

GENERAL PRINCIPLES

The classification consists of a hierarchical scheme for naming polymers according to the chemical constitution of the repeating units in the main chain (backbone). It can be applied to homopolymers, alternating copolymers and other macromolecular substances in which the constitutional repeating units can be identified. All existing linear single-strand polymers are embraced by this classification, which has been designed so as to be capable of extension to include any new structures of this type. In view of the open-ended nature of the classification, the tables below can only be illustrative, not comprehensive.

Four hierarchical levels are used; in order of decreasing importance, they are: classes, subclasses, groups and individual polymers.

CLASSES

Polymers are divided into two principal classes on the basis of the constitution of the main chain. *Homochain polymers* are those in which the main chains are constructed from atoms of a single element; *heterochain polymers* are those in which the main chains are constructed from atoms of two or more elements.

Rule 1.1

Homochain polymers are named by placing the name or symbol of the element in the main chain immediately before the expression '-chain polymer'.

Examples (see also 'Subclasses', p. 149, and Fig. 8.1)

- 1. Carbon-chain polymer or C-chain polymer.
- 2. Sulfur-chain polymer or S-chain polymer.

Prepared by a working group consisting of N.A. Platé (USSR) and I.M. Papisov (USSR). Reprinted from *Pure Appl. Chem.* **61**, 243-254 (1989).



Fig. 8.1 Examples of subclasses of homochain polymers.

Rule 2.1

Heterochain polymers are named by placing the names or symbols of all the elements in the main chain, in parentheses, immediately before the expression '-chain polymer'.

Examples (see also 'Subclasses', p. 149, and Fig. 8.2)

- 1. (Oxygen, carbon)-chain polymer or (O, C)-chain polymer.
- 2. (Oxygen, nitrogen, carbon)-chain polymer or (O, N, C)-chain polymer.

Rule 2.2

The order of citation of the elements in heterochain polymers is that conventionally used in inorganic nomenclature [6]. For the common elements, the order of citation is as follows: O, S, N, P, C, Si, B. Note that in those cases where the main chain has bonds in common with cyclic structures, *all* atoms in the rings must be considered for classification purposes. Thus I is a homochain polymer, whereas II is a heterochain Dolymer.



On the other hand, a polymer such as III, in which the main chain has no bonds in common with the cyclic structure, is classified as a homochain polymer.





Fig. 8.2 Examples of subclasses of heterochain polymers.

Rule 3.1

The presence of specific side groups, or specific elements in side groups, is indicated by placing the name of the side group, or of the element in the side group, immediately before the expression '-side-group polymer'.

Rule 3.2

Where more than one element, or more than one side group, is to be specified, the names of the elements or side groups are placed in parentheses.

Examples

- 1. Oxygen-side-group polymer.
- 2. Hydroxy-side-group polymer [for poly(l-hydroxyethylene), etc].
- 3. Ether-side-group polymer [for poly(l-methoxyethylene), etc].
- 4. (O, N, P)-side-group polymer.
- 5. (Ether, amide)-side-group polymer.

SUBCLASSES

Each class of polymers can be divided into various subclasses, according to the nature of the elements in the main chain. Examples are given in Rules 1.1, 2.1, as well as in Figs 8.1 and 8.2.

GROUPS

Each subclass can be further divided into groups having similar chemical structures. Examples of carbon-chain polymers are polyalkylenes, polyarylenes, etc (Fig. 8.3). Examples of (oxygen, carbon)-chain polymers are polyethers, polycarbonates, etc (Fig. 8.4). Examples of other types can be found in Figs 8.5 and 8.6.

It is convenient to retain such widely accepted terminology as polyacetals, polycarbonates, polyamides, polyesters, nucleic acids, etc, for naming the groups of polymers.

INDIVIDUAL POLYMERS

The lowest hierarchical ranking is given to the individual polymers, which are named in accordance with accepted IUPAC nomenclature practice. The reader is referred to References [2] and [3] for recommendations for naming organic and inorganic single-strand polymers, respectively.



Fig. 8.3 Examples of groups of carbon-chain polymers.



Fig. 8.4 Examples of groups of (oxygen, carbon)-chain polymers.



Fig. 8.5 Examples of groups of (sulfur, carbon)-chain polymers.



Fig. 8.6 Examples of groups of (nitrogen, carbon)-chain polymers.

It is to be noted that, for polymers of complex structure, assignment to more than one subclass and/or group is sometimes possible. For example, the polymer

0 -O—CH₂—…

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may be classified as follows:

class:heterochainsubclass:(O, N, C)-chain polymergroups:polycarboxylate and/or pyridine-chain polymerAdditional examples are given in Table 8.1 and the Appendix.

Group	Individa	ual polymer
	Structure	Name
polyalkylenes	CH ₃ -(CCH ₂) n CH ₃	poly(1,1-dimethylethylene) polyisobutylene
polyalkenylenes	$-(C=CHCH_2CH_2)_{\pi}$	poly(1-chloro-1-butenylene) polychloroprene
polyethers	-(O-())n	poly(oxy-1,4-phenylene) poly(phenylene oxide)
polyamides	O O ∥ ∥ - [NHC(CH ₂)₄CNH(CH ₂) ₆] ,	poly(iminoadipoyliminohexamethylene) poly(hexamethylene adipamide)

Table 8.1 Examples of individual polymers

REFERENCES

- 1 IUPAC. Basic definitions of terms relating to polymers 1974. *Pure Appl. Chem.* **40**, 477-491 (1974). Reprinted as Chapter 1, this volume.
- 2 IUPAC. Nomenclature of regular single-strand organic polymers (rules approved 1975). *Pure Appl. Chem.* **48**, 373-385 (1976). Reprinted as Chapter 5, this volume.
- 3 IUPAC. Nomenclature for regular single-strand and quasi-single-strand inorganic and coordination polymers (recommendations 1984). *Pure Appl. Chem.* **57**, 149-168 (1985). Reprinted as Chapter 6, this volume.
- 4 IUPAC. Stereochemical definitions and notations relating to polymers (recommendations 1980). *Pure Appl. Chem.* **53**, 733-752 (1981). Reprinted as Chapter 2, this volume.
- 5 IUPAC. Report on nomenclature in the field of macromolecules, J. Polym. Sci. 8, 257-277 (1952).

6 Rule IP-2.1 in Ref. [3].

Individual po	olymer	Group	Subclass	Class
1(S) "	catena-poly[sulfur]		S-chain	homochain
2. +	poly(1,4-phenylene)	polyarylenes	C-chain	homochain
3. $H_2 H_2 H_1 H_1 H_2$ $C-C C-C C-C H-CH_2 - CH_2 H_2$ $H H_2 H_2 H_2$	poly(spiro[4.5]dec-2,8-yleneethylene)	polycycloalkylenes	C-chain	homochain
4. $(1 + 1)^{-CH_2 - CH_2 + 1}$	poly(2,6-biphenylyleneethylene)	polyarylenes	C-chain	homochain
5. CH_3 $-(C-CH_2)_{n-1}$ $C\equiv N$	poly(1-cyano-1-methylethylene)	polyalkylenes	C-chain	hornochain
6. CI +(Si) , CI CI	<i>catena</i> -poly[dichlorotin]	1	Sn-chain	homochain

APPENDIX

Individual p	polymer	Group	Subclass	Class
7. F CH ₃ + $(Si-Si)_{n}$ + $(Si-Si)_{n}$ F CH ₃	<i>catena</i> -poly[(difluorosilicon)(dimethyl- silicon)]		Si-chain	homochain
8. $+0-CH_2-CH_2-0-C$	- poly(oxyethyleneoxyterephthaloyl)	polyesters of carboxylic acids	(O, C)-chain	heterochain
9. $+$ $+$ $+$ $+$ $+$ $+$ $+$ $+$ $+$ $+$	poly[(2-propyl-1,3-dioxane- 4,6-diyl)methylene]	polydioxanediyls, polyacetals	(O, C)-chain	heterochain
10. 0 $+0-C-CH-CH_2-C)_{\overline{n}}$	poly[oxy(2-chlorosuccinyl)]	polyanhydrides of carboxylic acids	(O, C)-chain	heterochain
11. CH ₃ Br ⁻ + N ⁺ -CH ₂ -CH ₂) ⁿ CH ₃	poly[(dimethyliminio)- ethylene bromide]	polymeric quaternary ammonium salts	(N, C)-chain	heterochain
12. + CH) CH)	poly(4,2-pyridinediylimino- 1,4-cyclohexylenebenzylidene)	polyamines and/or polypyridinediyls	(N, C)-chain	heterochain

Individua H	l polymer	Group	Subclass	Class
–n (poly(4,2-pyridinediyl-4 <i>H</i> - 1,2,4-triazole-3,5-diylmethylene)	polypyridinediyls and/ or polytriazolediyls	(N, C)-chain	heterochain
	poly([2,3'-bipyridine]-4,5'-diyl)	polypyridinediyls	(N, C)-chain	heterochain
	poly[imino(1-oxoethylene)]	polyamides (or polypeptides)	(N, C)-chain	heterochain
	<i>catena</i> -poly[(diphenylsilicon)- <i>µ</i> -oxo] poly(diphenylsiloxane)	polysiloxanes	(O, Si)-chain	heterochain
	<i>catena</i> -poly[(hydridoaluminium)-μ- (phenylimido)]	1	(N, Al)-chain	heterochain
	<i>catena</i> -poly[titaniumtri-μ-chloro]	1	(Cl, Tì)-chain	heterochain
	CH ₂ —CH ₂) n poly(oxycarbonylimino- 1,4-phenyleneimino- carbonyloxyethylene)	polyurethanes	(O, N, C)-chain	heterochain

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