Polymer Nomenclature and Structure: A Comparison of Systems Used by CAS, IUPAC, MDL, and DuPont. 4. Stereochemistry, Inorganic, Coordination, Double-Strand, Polysiloxanes, Oligomers, Telomers

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Polymer nomenclature styles and structure representation systems described, recommended, or used by Chemical Abstracts Service (CAS), the International Union of Pure and Applied Chemistry (IUPAC), MDL Information Systems, Inc. (MDL), and DuPont are compared and contrasted. Structure-based versus source-based nomenclature and structural representations are discussed. The topics covered in this paper (part 4 of 4) are stereochemistry in polymers, regular and quasi-single-strand inorganic and coordination polymers, regular double-strand (ladder and spiro) organic polymers, polysiloxanes, and oligomers and telomers.

7. STEREOCHEMISTRY IN POLYMERS

Stereochemical features in polymer structures are treated differently by the four systems.

7.1. CAS Nomenclature and Structure Representation. Stereochemistry of polymers is represented by text descriptor terms when the necessary information is reported; such terms include isotactic, syndiotactic, *threo*-diisotactic, *erythro*-diisotactic, and disyndiotactic.[1a] The term "atactic" (for a random configuration) is not employed by CAS in indexing specific polymers.

In addition to the special terms above, polymer stereochemistry is defined, when appropriate, by the stereo descriptors *E*, *Z*, *R*, *S*, *R**, and *S**.[1b] Six examples (one structure-based and five source-based) are shown below.

Example 7.1.1. Threodiisotactic poly(tetrahydro-2,5-furandiyl)

REGISTRY COPYRIGHT 1995 ACS
RN 93060-00-5 REGISTRY
CN Poly(tetrahydro-2,5-furandiyl), threo-diisotactic (9CI) (CA INDEX NAME)
MF (C4 H6 O)n
CI PMS
PCT Polyether, Polyether only
LC STN Files: CA, CAPLUS
DES *
:

Example 7.1.2. Isotactic polypropylene

COPYRIGHT 1995 ACS
RN 25085-53-4 LREGISTRY
CN 1-Propene, homopolymer, isotactic (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Propene, polymers, isotactic (8CI)
OTHER NAMES:
:
CN Isotactic polypropene
CN Isotactic polypropylene
CN Isotactic propene polymer
CN Isotactic propylene polymer
CN Propene isotactic polymer
CN Propylene isotactic polymer
:
MF (C3 H6)x
CI PMS, COM
PCT Polyolefin
:
DES 8:PM,ISOTACTIC
:

Example 7.1.3. Syndiotactic poly(vinyl chloride)

COPYRIGHT 1995 ACS
RN 25037-47-2 REGISTRY
CN Ethene, chloro-, homopolymer, syndiotactic (9CI) (CA INDEX NAME)
OTHER NAMES:
:
CN Syndiotactic poly(vinyl chloride)
CN Syndiotactic PVC
:
MF (C2 H4)x
CI PMS, COM
PCT Polyolefin
:

Example 7.1.4. Threo-diisotactic (E,E)-2,4-hexadiene

REGISTRY COPYRIGHT 1995 ACS
RN 87278-95-3 REGISTRY
CN 2,4-Hexadiene, (E,E)-, homopolymer, threo-diisotactic (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF (C6 H10)x
CI PMS
PCT Polyolefin
LC STN Files: CA, CAPLUS
DES *
:

Example 7.1.5. Erythro-diisotactic cyclobutene

REGISTRY COPYRIGHT 1995 ACS
RN 90693-96-2 REGISTRY
CN Cyclobutene, homopolymer, erythro-diisotactic (9CI) (CA INDEX NAME)

[⊗] Abstract published in *Advance ACS Abstracts,* February 15, 1997.

S0095-2338(96)00164-3 CCC: $14.00

MF (C4 H6)x
CI PMS
PCT Polyother, Polyother only
LC STN Files: CA, CAPLUS
DES *
:

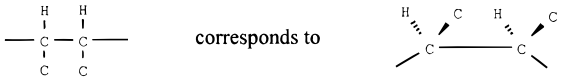
Example 7.1.6. (Z)-2-Butene/erythro-diisotactic ethene copolymer

REGISTRY COPYRIGHT 1995 ACS
RN 89162-96-9 REGISTRY
CN 2-Butene, (Z)-, polymer with ethene, erythro-diisotactic (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethene, polymer with (Z)-2-butene, erythro-diisotactic (9CI)
FS STEREOSEARCH
MF (C4 H8 . C2 H4)x
CI PMS
PCT Polyolefin
LC STN Files: CA, CAPLUS
DES *
:

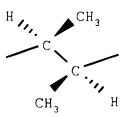
7.2. IUPAC Nomenclature and Structure Representation. The first extensive IUPAC publications on stereochemistry in high polymers were published in the early 1960s, and subsequently in 1966 as a single article.[2] In addition to more conventional polymer names, e.g., polyethylidene and polypropylene, the "-amer" nomenclature (previously introduced in 1952[3]) was used. IUPAC basic definitions relating to stereochemistry, e.g., tacticity, isotactic polymer, etc., were published in 1974.[4]

A major 1981 IUPAC document[5] discusses polymer stereochemistry in depth. Key chapters of the document deal with basic definitions (configurational unit, configurational base and repeating units, stereorepeating unit, different types of tacticity, tactic block polymers, and stereoblock polymers), sequences, conformations, and supplementary definitions. Most of the illustrations use the rotated Fischer projections, but some three-dimensional representations are included.

Example 7.2.1. The rotated Fischer projection



and hence to the zigzag chain



7.3. MDL Graphic Representation. To indicate tacticity an Sgroup data field, such as TACTICITY or STEREO, is created in order to attach tacticity information to a polymer Sgroup.[6]

7.4. SCION Nomenclature and Structure Representation. Stereochemistry in polymers is not currently represented at the structure level. Tactic and atactic polymers are given the same registration number, i.e., tactic polymers are registered as if they were atactic. Controlled terms such as TACTICITY, ISOTACTIC POLYMERS, or SYNDIOTACTIC POLYMERS are added to the appropriate indexing link(s). Indexing is thus relatively simple, but the disadvantage of this approach is that a search for a polymer with specific stereo attributes cannot pinpoint a specific polymer if such a controlled term is in the same indexing link together with registration numbers for several polymers that can have stereo attributes. In this situation, screening of the source document is necessary to resolve the problem.

8. REGULAR AND QUASI-SINGLE-STRAND INORGANIC AND COORDINATION POLYMERS

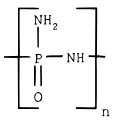
Inorganic and coordination polymers are discussed in this section. A polymer need not be completely inorganic to qualify for this classification; an inorganic backbone is sufficient, even if there are organic moieties attached to a backbone atom.

A regular linear polymer that can be described by a preferred SRU in which only one terminal constituent subunit is connected through a single atom to another identical SRU or to an end group is a quasi-single-strand polymer; i.e., it does not fit the definition of a regular single-strand polymer, but it can be named in the same manner.[7]

8.1. CAS Nomenclature and Structure Representation. Single-strand inorganic polymers are indexed by both structure-based and source-based methods. Other papers on phosphazenes presented at a symposium[8a] show the structures with nitrogen mostly on the left, although some are drawn with phosphorus on the left. Example 8.1.1 shows a typical structure-based record; nitrogen is senior to phosphorus and might be expected to appear on the left. It should be pointed out, however, that the actual image retrieved from a search has no connection with nomenclature; some images appear correctly with the head atom on the left, while others are "mirror-image" when compared with the name.

Example 8.1.1. Structure-based record; poly[imino(aminophosphinylidene)]

REGISTRY COPYRIGHT 1995 ACS
RN 74418-71-6 REGISTRY
CN Poly[imino(aminophosphinylidene)] (9CI) (CA INDEX NAME)
:
MF (H3 N2 O P)n
CI PMS
PCT Polyother, Polyother only
LC STN Files: CA, CAOLD, CAPLUS



:

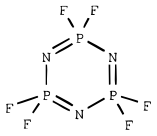
Source-based polymers are typically indexed as shown in example 8.1.2.

Example 8.1.2. Source-based record; homopolymer from "hexafluorotriazatriphosphorine"
REGISTRY COPYRIGHT 1995 ACS
RN 56581-26-1 REGISTRY
CN 1,3,5,2,4,6-Triazatriphosphorine, 2,2,4,4,6,6-hexafluoro-2,2,4,4,6,6-hexahydro-, homopolymer (9CI) (CA INDEX NAME)
:

MF (F6 N3 P3)x
CI PMS
PCT Polyphosphazene, Polyphosphazene formed
:

CM 1

CRN 15599-91-4
CMF F6 N3 P3



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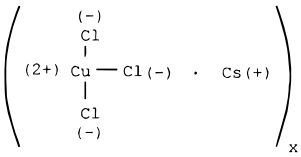
When SRUs are bridged only by metals, systematic polymer nomenclature is not used;[1a] instead, the substance is indexed either at the monomeric salt name or by coordination nomenclature,[1c] with a modification phrase, in either case, such as "homopolymer" or "polymer with...".

Example 8.1.3. Cuprate(1-), trichloro-, cesium, homopolymer

Structure[1c]

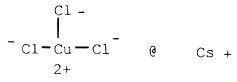


Online record

REGISTRY COPYRIGHT 1995 ACS
RN 36006-29-8 REGISTRY
CN Cuprate(1-), trichloro-, cesium, homopolymer (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Cesium trichlorocuprate(II), polymers (7CI)
MF (Cl3 Cu . Cs)x
CI PMS
LC STN Files: CA, CAOLD, CAPLUS

CM 1

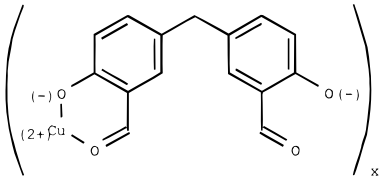
CRN 18437-47-3 (15697-18-4)
CMF Cl3 Cu . Cs
CCI CCS



:

Note on example 8.1.3: The @ symbol in an online text-type terminal display indicates the dot used to separate multicomponent ("dot-disconnect") substances.

Example 8.1.4. Copper, [[3,3′-methylenebis[6-hydroxybenzaldehydato]](2-)-O^1,O^6]-, homopolymer



8.2. IUPAC Nomenclature and Structure Representation. IUPAC[7] presents a system of nomenclature for regular single-strand and quasi-single-strand inorganic and coordination polymers. The system is based on the selection and naming of an SRU defined[4] as the smallest structural unit the repetition of which describes the polymer structure. The name of the polymer is the name of this repeating unit prefixed by the terms "poly", "catena", or other structural indicator, and designations for end groups, if desired.

Rules are described for determining an unambiguous, although not necessarily unique, name for each SRU. Further rules are presented for determining a unique name. The complete list of rules is too lengthy to reproduce here; the most important rules are given below, together with selected examples.

SRUs are oriented so that the head atom (the constitutional subunit of the SRU at which citation of the SRU begins) is the central atom or coordination center of highest seniority, i.e., the most preferred central atom according to the following sequence: F, Cl, Br, I, At, O, S, Se, Po, N, P, As, Sb, Bi, C, Si, Ge, Sn, Pb, B, Al, Ga, In, Tl, Zn, Cd, Hg, Cu, Ag, Au, Ni, Pd, Pt, Co, Rh, Ir, Fe, Ru, Os, Mn, Tc, Re, Cr, Mo, W, V, Nb, Ta, Ti, Zr, Hf, Sc, Y, La through Lu, Ac through Lr, Be, Mg, Ca, Sr, Ba, Ra, Li, Na, K, Rb, Cs, Fr, He, Ne, Ar, Kr, Xe, Rn.

IUPAC has created further rules for situations when further choice is needed for selection of a senior subunit in an SRU.

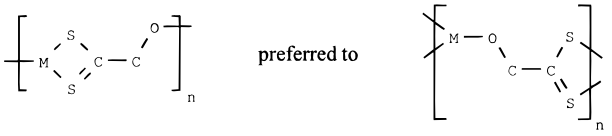
The preferred direction along the polymer chain from the head atom for the sequential citation (from left to right) of the other constituent subunits in the SRU is governed by three major factors considered in order until a definitive decision is reached.

(1) A single-strand SRU is preferred to a quasi-single-strand SRU; i.e., an SRU with both terminal constituent subunits connected to other identical SRUs or to an end group through single atoms is preferred to an SRU with only one terminal constituent subunit to other SRUs or to an end group through a single atom.

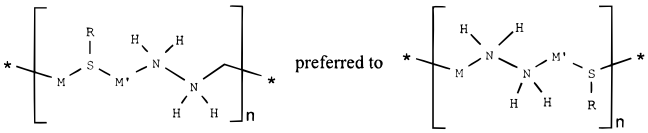
(2) The preferred direction is defined by the shortest path, measured in terms of the number of atoms, in the polymer backbone from the head atom to a subunit of equal seniority (i.e., the next occurrence of the head atom in the chain), or to a subunit next in seniority.

(3) When all paths between the head atom and a subunit of equal seniority, or to a subunit next in seniority, are equal in length, the preferred direction is along the path that includes constituent subunits of greater seniority. The paths between subunits of equal seniority or between the senior subunit and the subunit next in seniority necessarily involve subunits of lesser seniority and often will consist of organic ligands. Hence, the hierarchical order of subunits prescribed for linear organic polymers[9,10] may be needed to determine the preferred direction.

Example 8.2.1. [M is a metal—illustration of rule 1 above]



Example 8.2.2. [M = central atom—the one-atom path through the thiolato ligand is preferred to the two-atom path through the hydrazine ligand—illustration of rule 2 above]



Regular single-strand inorganic and coordination polymers are named by inserting the name of the preferred constitutional repeating unit into the appropriate general polymer name. SRUs with homatomic backbones are named by citing each mononuclear central atom, together with any side groups named as ligands.

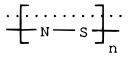
Example 8.2.3. *catena*-Poly[sulfur]

Example 8.2.4. *catena*-Poly[dimethyltin]

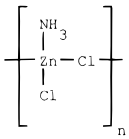
According to the rules for naming linear organic polymers,[9,10] these two polymers could be named poly(sulfanediyl) and poly(dimethylstannylene), respectively.

SRUs with backbones consisting of a mononuclear central atom and one bridging ligand are named by citing the central atom prefixed by its associated nonbridging ligands followed by the name of the bridging ligand prefixed by the Greek letter μ (.mu.).

Example 8.2.5. *catena*-Poly[nitrogen-μ-thio]

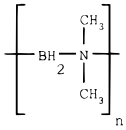


Example 8.2.6. *catena*-Poly[(amminechlorozinc)-μ-chloro]

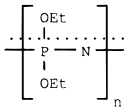


If there is a choice for the central atom, the element occurring *later* in the general element sequence (F, Cl, .. through Rn) shown above is the central atom.

Example 8.2.7. *catena*-Poly[(dihydroboron)-μ-(dimethylamido)]

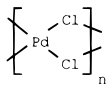


Example 8.2.8. *catena*-Poly[(diethoxophosphorus)-μ-nitrido]

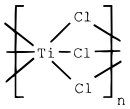


SRUs with backbones consisting of one mononuclear central atom and two or more bridging ligands, alike or different, or a chelating ligand, are named by citing the name of the central atom, prefixed by the names of its associated nonbridging ligand(s), followed by the names of the bridging ligands each prefixed by the Greek letter μ (.mu.). The number of identical bridging ligands, if more than one, is indicated by an appropriate numerical prefix; different bridging ligands are cited in alphabetical order and all enclosed in appropriate enclosing marks.

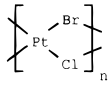
Example 8.2.9. *catena*-Poly[palladium-di-μ-chloro]



Example 8.2.10. *catena*-Poly[titanium-tri-μ-chloro]



Example 8.2.11. *catena*-Poly[platinum(μ-bromo-μ-chloro)]

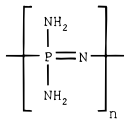


The following are also covered: single-strand and quasi-single-strand coordination polymers with polynuclear coordination centers; regular single-strand and quasi-single-strand inorganic and coordination polymers with ionic SRUs; stereochemical configurations for SRUs; end groups of linear inorganic or coordination polymers.

8.3. MDL Graphic Representation. MDL[6] gives no specific examples, but it may be possible to represent such structures in a MACCS-type database.

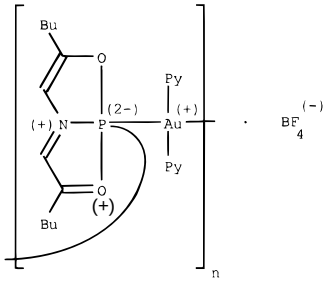
8.4. SCION Nomenclature and Structure Representation. For single-strand inorganic polymers, SCION rules follow CAS rules in broad principle, except that, as in the case of organic polymers, the head atom is the one with the highest atomic number.[11]

Example 8.4.1. Poly((diaminophosphinidyne)nitrilo)



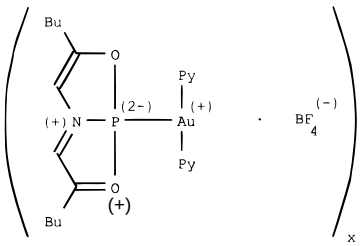
When SRUs are bridged only by metals, systematic polymer nomenclature is not used. The substance is initially named either as the monomeric salt name or by coordination nomenclature, and the name is then prefixed by POLY-.

Example 8.4.2. The SRU polymer of structure



(where Py = pyridine ligand)

is stored as the source-based polymer of structure:



Polymer name: POLY-GOLD(1+), (2,6-DIBUTYL-1,3,2-OXAZAPHOSPHOLE-P8)BIS(PYRIDINE)-, TETRAFLUOROBORATE

Textual descriptor: POLY-HOMO

9. REGULAR DOUBLE-STRAND (LADDER AND SPIRO) POLYMERS

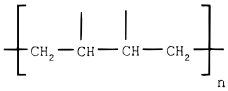
Double-strand ladder and spiro polymers contain no open-chain bonds in the backbone. Polymers containing some open-chain backbone bonds (called partial ladder, imperfect ladder, step-ladder, or block ladder polymers) are not considered to be true ladder or spiro polymers; they are excluded from discussion.

The CAS and IUPAC nomenclature and structure representation systems are very similar. The SCION nomenclature and structure representation system is radically different.

Other prominent articles on double-strand polymers include those by Overberger and Moore,[12] DeWinter,[13] and Bailey;[14] this reference contains a short "proposed nomenclature" section[14a] that is essentially a reprint of part of the ACS publication.[10]

9.1. CAS Nomenclature and Structure Representation. Linear double-strand polymers may sometimes be named as a chain of quadrivalent radicals. Two pairs of locants, separated by a colon, indicate the distribution of bonds.[1a]

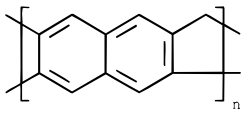
Example 9.1.1. Poly(1,4:2,3-butanetetrayl)



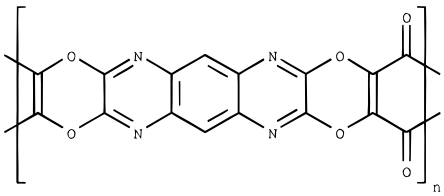
Note on structure 9.1.1: This publication[1a] unfortunately shows this ladder polymer drawn in a horizontal manner, perhaps to save space. The diagram should be rotated clockwise 90° so that it appears identical with the structure of example 9.2.3.

When a ladder polymer must be named as an SRU of one or more quadrivalent radicals linked through one or more bivalent radicals (here, these terms are extended to mean radicals attached to four or two different atoms, not only to radicals with four or two free valence bonds), the direction of citation is from the most favored quadrivalent radical by the shortest path to the next most favored quadrivalent radical, and so on, and then toward the most favored bivalent radical. Rings are broken (a) to minimize the number of free valencies of the total "mer", (b) to maximize the number of most preferred hetero atoms in the ring system, and (c) to maintain intact the most preferred ring system.[1d] End groups, when known, are identified by α and α′ (at the left terminus as the structure is drawn) and by ω and ω′ (at the right terminus) as locants for substituent prefixes in the modification, e.g., α, α′-dihydroxy-ω, ω′-dihydro-.

Example 9.1.2. Poly(2,3:6,7-naphthalenetetrayl-6-methylene)



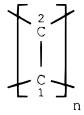
Example 9.1.3. Poly([1,4]dioxino[2,3-*b*]-1,4-dioxino[2′,3′:5,6]pyrazino[2,3-*g*]quinoxaline-2,3:9,10-tetrayl-9,10-dicarbonyl)



9.2. IUPAC Nomenclature and Structure Representation. IUPAC defines a ladder or spiro polymer as a double-strand polymer the molecules of which are formed by an uninterrupted sequence of rings with adjacent rings having one atom in common (spiro polymer) or two or more atoms in common (ladder polymer).[15]

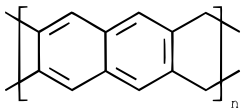
IUPAC presents a comprehensive system for (a) identifying, (b) orienting, and (c) naming the preferred SRU, and subsequently (d) naming the polymer. Full presentation of these rules is beyond the scope of this paper; a key point of the system is that the acyclic SRU that results from breaking a ring is oriented in such a way that the lowest free valence locant is at the lower left. Some examples are given below to illustrate the method:

Example 9.2.1. Poly(ethane-1,2:2,1-tetrayl)

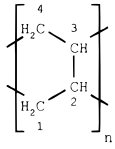


Note on example 9.2.1: Not poly(ethane-1,2:1,2-diylidene)

Example 9.2.2. Poly(naphthalene-2,3:6,7-tetrayl-6,7-dimethylene)



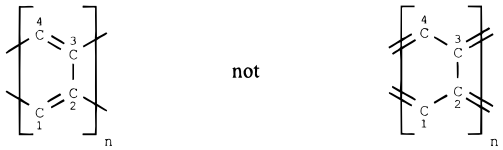
Example 9.2.3. Poly(butane-1,4:2,3-tetrayl)



Note on example 9.2.3: Compare example 9.1.1.

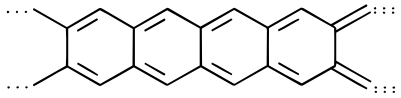
Example 9.2.4. Poly(buta-1,3-diene-1,4:3,2-tetrayl)

Note on example 9.2.4: When an aromatic ring is broken, normally delocalized bonds are fixed as single or double bonds. Free valences in the total SRU are minimized, i.e., single bonds are broken in preference to double bonds.



Although example 9.2.4 represents linear (as opposed to spiral) "poly-benzene", at first glance it appears not to do so; this is because it is customary to think of every ring as containing either six normalized bonds (or three single and three double bonds), and one double bond thus appears to be missing from the structure. This becomes clearer if several contiguous repeats of the "poly-benzene" SRU are drawn—see example 9.2.5.

Example 9.2.5. Linear "poly-benzene"



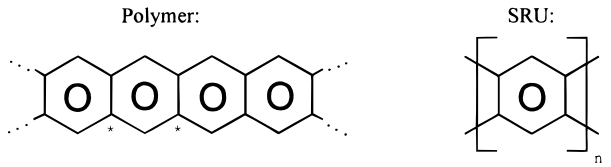
9.3. MDL Graphic Representation. MDL[6] shows no specific examples for storage of ladder or spiro polymer structures.

9.4. SCION Nomenclature and Structure Representation. In SCION, a ladder polymer is defined as a polymer composed of two or more linear polymer backbones connected by cross-links repeated regularly along the multiple-strand backbone; thus, all backbone atoms are in fused or spiro rings.

The novel SCION nomenclature and structural representation system differs markedly from the CAS and IUPAC systems, which require ring fracture, naming of complete ring assemblies, and occasional use of nomenclature to determine final orientation of SRUs.[16] The advantages of the SCION system are as follows: SRU identification and orientation are completely independent of nomenclature; no rings are fractured, so that the integrity of all rings is retained; except in one special situation, each ring is named separately; names of complete ring assemblies are not required.

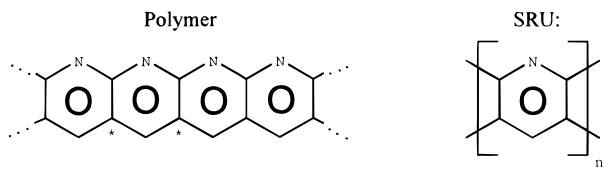
Full presentation of these rules, including an explanation of the one special situation mentioned, is beyond the scope of this paper; some examples are given below to illustrate the method. Asterisks within each structure in this section denote the start and finish of the SRU within the structure, and an O within a ring denotes aromaticity.

Example 9.4.1. POLY-LADDER-(1,2)BENZENE(5,4)

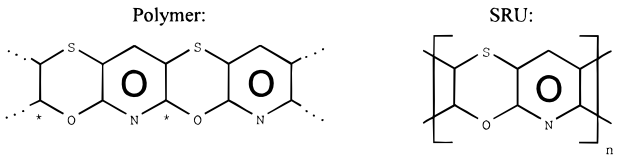


Note on example 9.4.1: Compare example 9.2.4.

Example 9.4.2. POLY-LADDER-(2,3)PYRIDINE(6,5)

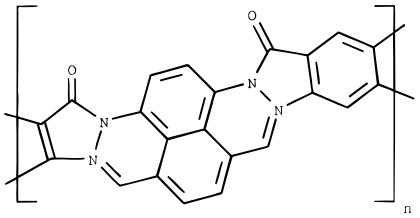


Example 9.4.3. POLY-LADDER-(3,2)1,4-OXATHIIN(5,6)-(3,2)PYRIDINE(5,6)



Note on example 9.4.3: In SCION, S is senior to O and to N. Therefore, the ring containing S is senior to the ring containing N; it is placed on the left with the S atom in the top-leftmost position possible.[16a]

Example 9.4.4. POLY-LADDER-(3,4)(2-OXO-3-PYRROLINE)(1,5)-(1,2)(1,4-DIHYDROPYRIMIDINE)(6,5,4)-(1,-8A,8)NAPHTHALENE(4,4A,5)-(4,5,6)(3,6-DIHYDROPYRIMIDINE)(3,2)-(1,5)(5-OXO-3-PYRROLINE)(4,3)-(1,2)BENZENE(5,4)



10. POLYSILOXANES

Although IUPAC classifies polysiloxanes as inorganic polymers,[7] there is sufficient interest and diversity in them as a group for them to warrant discussion separate from other inorganic polymers.

Polysiloxanes occupy a virtually unique position in the world of polymers. Many polysiloxanes comprise a partly or wholly inorganic backbone built from alternating silicon and oxygen atoms; in contrast, pendent groups or side chains attached to silicon atoms are usually organic. Types discussed in this section include regular single-strand, hyperbranched, ladder, and spiro polysiloxanes.

10.1. CAS Nomenclature and Structure Representation. Polysiloxanes prepared by hydrolytic polymerization of alkoxysilanes or halosilanes typically have been indexed in the CA File at the controlled-term heading "Siloxanes and Silicones" with no polymer registration. Polysiloxanes described only in terms of SRUs also have been indexed at this heading with no polymer registration.[17]

Beginning with volume 121 (1994) of CAS Chemical Abstracts, structural representation and machine registration was begun for polymers previously handled only as text terms in the CA File. Backfile maintenance is not planned.[17]

This policy change affects the following areas [CAS's *exact* phraseology (including use of parentheses, vice brackets, for SRUs) is used below; in most cases, when words such as siloxanes or silsesquioxanes are cited, what is meant is *poly*siloxanes or *poly*silsesquioxanes]: siloxanes or silsesquioxanes prepared by hydrolytic polymerization of alkoxysilanes or halosilanes; siloxanes described only in terms of single-unit SRUs of the type $(-O-SiRR'-)_n$ (R, R′ = monovalent radical); siloxanes described only in terms of multiunit SRUs of the type $(-O-SiR_2-)_x(-O-SiR'_2-)_y$ or $(-R_2SiO-)_x(-R'SiO_{1.5}-)_y$ (R, R′ = monovalent radical); ceramers (hybrid organic−inorganic networks) prepared by

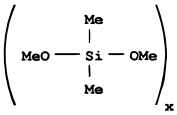
hydrolytic polymerization (sol−gel process) of tetraalkoxysilanes containing organic moieties, which may be trialkoxysilyl-terminated organic polymers; end groups for siloxane SRUs; copolymers containing siloxane components; trade names for siloxanes and silsesquioxanes; silicone rubbers.

Examples 10.1.1 through 10.1.5 demonstrate some registration enhancements.

Example 10.1.1. Siloxanes from hydrolytic polymerization of alkoxysilanes are indexed as monomer-based polymers; an SRU entry is also made for single-unit types of SRU. Additionally, a CA File entry is made.

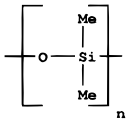
A siloxane from hydrolytic polymerization of $Me_2Si(OMe)_2$ is registered thus

Structure



Polymer name: Silane, dimethoxydimethyl-, homopolymer [25498-04-8]

Structure

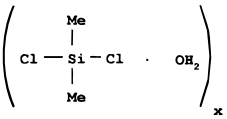


Polymer name: Poly[oxy(dimethylsilylene)] [9016-00-6]
CA File entry: siloxanes and silicones

Example 10.1.2. For siloxane polymers formed by hydrolysis of halosilanes, water is included in the registration; the name includes the term "hydrolytic". An SRU entry is also made for single-unit types of SRU. Additionally, a CA File entry is made.

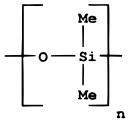
A siloxane from hydrolytic polymerization of Me_2SiCl_2 is registered thus:

Structure



Polymer name: Silane, dichlorodimethyl-, homopolymer, hydrolytic [158158-00-0]

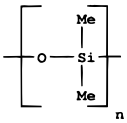
Structure



Polymer name: Poly[oxy(dimethylsilylene)] [9016-00-6]
CA File entry: siloxanes and silicones

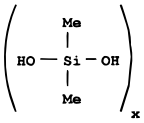
Example 10.1.3. Single-unit siloxane SRUs receive an SRU entry, a monomer-based polymer entry (with the assumption of a hydroxysilane as monomer), and a CA File entry.

Structure



Polymer name: Poly[oxy(dimethylsilylene)] [9016-00-6]

Structure

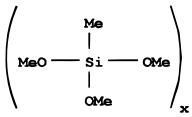


Polymer name: Silanediol, dimethyl-, homopolymer [31900-57-9]
CA File entry: siloxanes and silicones

Example 10.1.4. Silsesquioxanes with repeating RSiO1.5 units are registered as monomer-based polymers from assumed hydroxysilane monomers. Ladder-type entries are made for silsesquioxanes represented by a single type of RSiO1.5 repeat unit, e.g., R = Me.

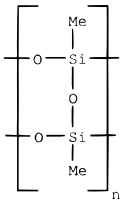
The methyl silsesquioxane from hydrolytic polymerization of MeSi(OMe)3 is registered thus

Structure 10.1.4a



Polymer name: Silane, trimethoxymethyl-, homopolymer [25498-03-7]

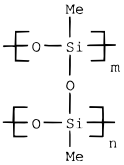
Structure 10.1.4b



Polymer name: Poly[(1,3-dimethyl-1,3:1,3-disiloxanediylidene)-1,3-bis(oxy)] [153315-80-1]
CA File: silsesquioxanes

Note on example 10.1.4: The assumption that the SRU equivalent 10.1.4b of the source-based structure 10.1.4a is a ladder polymer is probably only partly correct; the hyperbranched structure 10.1.4c is also likely to form by hydrolytic polymerization of $MeSi(OMe)_3$, and the structure of the polymer is therefore probably a blend of 10.1.4b and 10.1.4c. However, since the CAS Registry System cannot currently register structures such as 10.1.4c, structure 10.1.4b is the only way of representing this as a structure-based polymer.

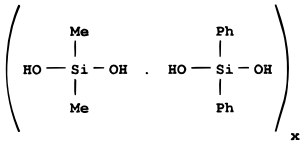
Structure 10.1.4c



Example 10.1.5. Siloxanes described only in terms of the type $(-O-SiR_2-)_x(-O-SiR'_2-)_y$ or $(-R_2SiO-)_x(-R'SiO_{1.5}-)_y$ (R, R′ = monovalent radical) cannot be registered as SRUs (see point 10.1.1); instead, they are registered as monomer-based polymers with the assumption of hydroxysilanes as monomers. A CA File entry is also made.

The polymer $(-O-SiMe_2-)_x(-O-SiPh_2-)_y$ is registered thus

Structure

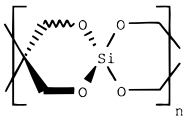


Polymer name: Silanediol, dimethyl-, polymer with diphenylsilanediol
CA File entry: siloxanes and silicones

Point 10.1.1: Since the CAS Registry System can register any SRU with an even number of crossing bonds, the CAS statement that polymers of the type $(-R_2SiO-)_x(-R'SiO_{1.5}-)_y$ "cannot be registered as SRUs" probably reflects a decision of policy not to try to construct linear and ladder SRUs to cover all the possibilities. The CAS statement that polymers of the type $(-O-SiR_2-)_x(-O-SiR'_2)_y$ "cannot be registered as SRUs" is not strictly true, because the CAS Registry System is capable of registering copolymers such as $([-O-SiMe_2-]_n.[-O-SiPh_2-]_n)_x$. The statement "cannot be registered as SRUs" should be rephrased "are not registered as SRUs", because it is currently CAS registration policy to register unterminated copolymers of SRUs as source-based polymers and not as structure-based copolymers $([SRU\_A]_n.[SRU\_B]_n)_x$—see section 5.1.1.

The final example in this section is a silicon-containing spiro polymer.

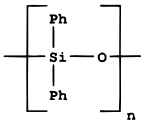
Example 10.1.6. Poly[1,3-dioxa-2-silacyclohexane-5,2-diylidene-2,2-bis(oxymethylene)]



Note on example 10.1.6: Not poly[1,3-dioxa-2-silacyclohexane-2,5-diylidene-5,5-bis(methyleneoxy)]; the direction is determined by the shortest path from the heteroatom in the ring to the acyclic heteroatom.

10.2. IUPAC Nomenclature and Structure Representation. For linear polysiloxanes, IUPAC[7] states that if there is a choice for the central atom, the element occurring *later* in the general element sequence table (see point 10.2.1) is the central atom. The linear polysiloxane (diphenylsilylene)-oxy is represented by the structure shown as example 10.2.1. The IUPAC name also differs appreciably from that of CAS.

Example 10.2.1. Poly[(diphenylsilylene)oxy]



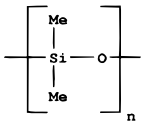
Polymer name: *catena*-poly[(diphenylsilicon)-μ-oxo]
Synonym: poly(diphenylsiloxane)[18]

According to the rules for linear organic polymers, this polymer would be oriented and named poly[oxy(diphenylsilylene)].[7]

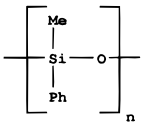
Point 10.2.1: The general element sequence table lists all elements. Order of precedence begins in the top, right-hand corner of the periodic table and proceeds (in vertical columns) toward the bottom, left-hand corner. Atom seniority is F, Cl, Br, I, At, O, S, Se, Te, Po, N, P, As, Sb, Bi, C, Si, ... Li, Na, K, Rb, Cs, Fr, He, Ne, Ar, Kr, Xe, Rn.

Lichtenwalner and Sprung[19] present some IUPAC nomenclature for polysiloxanes. They cite the following:

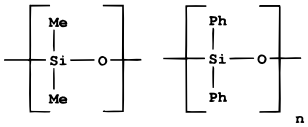
Example 10.2.2. Poly(dimethylsiloxane)



Example 10.2.3. Poly(methylphenylsiloxane)



Example 10.2.4. Poly(dimethylsiloxane-*co*-diphenylsiloxane)

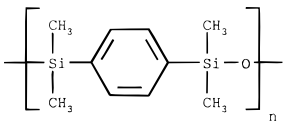


Example 10.2.5

$(C_6H_5SiO_{1.5})_n$ - poly(phenylsiloxane)

Note on example 10.2.5: No structure is given; the commonly used name for this polymer that does not follow the IUPAC system is poly(silsesquioxane).

Example 10.2.6. Poly(1-dimethylsil-4-dimethyloxysilphenylene)

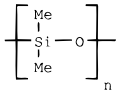


Other papers on polysiloxanes in a 1988 symposium publication[8b] show the structures with silicon mostly on the left, although some are drawn with oxygen on the left.

10.3. MDL Graphic Representation. MDL[6] shows no specific examples for storage of polysiloxanes.

10.4. SCION Nomenclature and Structure Representation. Because silicon has a higher atomic number than oxygen, in polysiloxanes comprising backbones composed only of alternating Si and O atoms the head atom is always Si. This is illustrated by example 10.4.1.

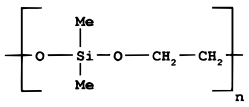
Example 10.4.1. "Poly-dimethylsiloxane"



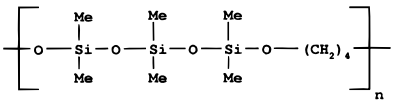
Polymer name: POLY-(DIMETHYLSILYLENE)OXY

In the case of polysiloxanes containing carbon atoms in the backbone, the SRU head atom is Si unless other heteroatoms are positioned between a silicon atom and a carbon atom; in these cases, the atom of highest atomic number that is also joined to a carbon atom is selected as head atom. The reason for this is to preserve the complete functional group as a single moiety (see section 4.7.4 for the definition of a complete functional group). As always, the SRU is oriented so that the head atom is leftmost with the next senior atom to its right. Examples 10.4.2 through 10.4.5 illustrate the method.

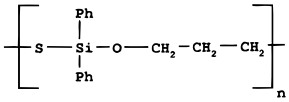
Example 10.4.2. POLY-OXY(DIMETHYLSILYLENE)-OXYETHYLENE



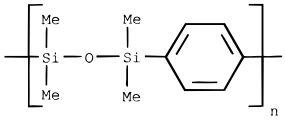
Example 10.4.3. POLY-OXY(HEXAMETHYL-1,5-TRISILOXANEDIYL)OXYTETRAMETHYLENE



Example 10.4.4. POLY-THIO(DIPHENYLSILYLENE)-OXYTRIMETHYLENE



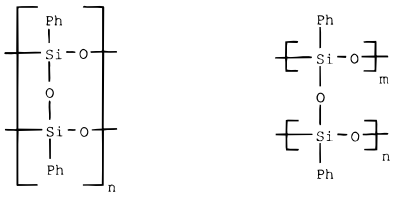
Example 10.4.5. POLY-(TETRAMETHYL-1,3-DISILOXANEDIYL)-P-PHENYLENE



Note on example 10.4.5: This is the same polymer as example 10.2.6, but oriented and named according to SCION rules.

Polysilsesquioxanes classically represented by structures such as $[CH_5SiO_{1.5}]_n$ [called poly(phenylsiloxane) by IUPAC—see example 10.2.5] are represented in SCION by double-strand, nonladder SRUs. These are hyperbranched structures; ideally, they would be represented by a structure such as that shown in example 10.4.6b, in which the two −Si−O− chains are in different geometrical planes. Owing to CAS Registry System limitations, they are represented by structures such as that shown in example 10.4.6a.[11,16] It is emphasized that the structure of example 10.4.6a does *not* represent a ladder polymer in SCION.

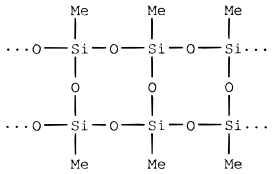
Example 10.4.6. Polysilsesquioxane $[C_{12}\ H_{10}\ O_3\ Si_2]_n$



(a) (b)

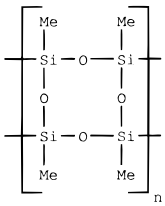
The ladder polymer represented by the structure shown in example 10.4.7 is represented by CAS as the structure shown in example 10.1.4b.

Example 10.4.7. Typical siloxane ladder polymer

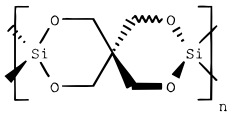


In SCION, this polymer is represented by the structure shown as example 10.4.8.

Example 10.4.8. POLY-LADDER-(2,4)(2,4,6,8-TETRAMETHYLCYCLOTETRASILOXANE)(8,6)



Example 10.4.9. POLY-LADDER-(2,2)1,3-DIOXA-2-SILACYCLOHEXANE(5,5)-(5,5)1,3-DIOXA-2-SILACYCLOHEXANE(2,2)



Note on example 10.4.9: This example is identical with example 10.1.6.

SCION nomenclature of ladder and spiro polymers is described in more detail elsewhere.[16]

An example of a comb polymer with a siloxane backbone was given in section 6.4.4.

11. OLIGOMERS AND TELOMERS

Qualitatively, oligomers are "short polymers", and telomers are "short polymers with specific end groups".

IUPAC defines an oligomer as a substance composed of molecules containing a few of one or more species of atoms or group of atoms (constitutional units) repetitively linked to each other for which the physical properties vary with the addition or removal of one or a few constitutional units from its molecules.[4]

The terms telogen and telomerization were defined many years ago to describe an innovative method for the free-radical polymerization of ethylene.[20] The essence of telom-

erization, as described by a 1942 patent,[20a] involves reaction of a telogen XY (also called a chain-transfer agent) with an ethylenic molecule to give a telomer of structure:

$$X-(A)_n-Y$$

In the product telomer, fragments of the chain-transfer agent are attached to the termini of the molecule.[20]

Example 11.1. CCl_4 is added as chain-transfer agent in the polymerization of ethylene

$$CCl_4 + nCH_2{=}CH_2 \rightarrow Cl_3C-[-CH_2-CH_2-]_n-Cl$$

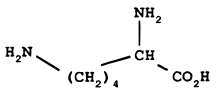
11.1. CAS Nomenclature and Structure Representation. Oligomers of definite structures are indexed as specific compounds by the regular principles of index nomenclature. When the precise structure is not known but the number of units is specific, "dimer", "trimer", etc., is expressed in the modification at the name of the monomer. The term "oligomeric" may be cited after "homopolymer" or "polymer with ..." if this aspect is stressed in the original document.[1a] Oligomeric, if applicable, is expressed in the text modification part of the index name and is not part of the CAS Registry record, except for some records marked with an asterisk.[21] Examples 11.1.1 and 11.1.2 demonstrate these last two rules.

Example 11.1.1. Trimer of unknown structure

REGISTRY COPYRIGHT 1995 ACS
RN 137243-06-2 REGISTRY
CN L-Lysine, trimer (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF (C6 H14 N2 O2)3
CI PMS
SR CA
LC STN Files: CA, CAPLUS

CM 1

CRN 56-87-1
CMF C6 H14 N2 O2
CDES 5:L



:

Example 11.1.2. Oligomeric homopolymer of 1,3-butadiene

REGISTRY COPYRIGHT 1995 ACS
RN 68441-52-1 REGISTRY *
* Use of this CAS Registry Number alone as a search term in other STN files may result in incomplete search results. For additional information, enter HELP RN* at an online arrow prompt (⟹).
CN 1,3-Butadiene, homopolymer, oligomeric (CA INDEX NAME)
MF Unspecified
CI PMS, MAN, GRS
PCT Manual registration
:

Note on example 11.1.2: Records with registry numbers marked with an asterisk such as those shown in these two examples do *not* represent CAS indexing and naming policies. These numbers and names are created by CAS for regulatory agencies to meet their need in identifying articles of commerce.[21] Such registry numbers usually have few or no postings in bibliographic files such as the CA File.

Inorganic oligomers, even as short as dimers, are indexed as polymers—see example 11.1.3.

Example 11.1.3. Water dimer

REGISTRY COPYRIGHT 1995 ACS
RN 25655-83-8 REGISTRY
CN Water, dimer (8CI, 9CI) (CA INDEX NAME)
:
MF (H2 O)2
AF H4 O2
CI PMS, COM
:

CM 1

CRN 7732-18-5
CMF H2 O
H_2O
:

Telomers with a definite structure are named systematically.[1a]

Example 11.1.4. Oligomeric poly(ethylene) telomer with CCl_4

Structure: $Cl-[-CH_2-]_6-CCl_3$

Name: heptane, 1,1,1,7-tetrachloro-

Note on example 11.1.4: The term "oligomeric" is part of the CAS Registry record only in records marked with an asterisk.

Example 11.1.5. Methylene chloride/vinylidene fluoride telomer

Structure: $Cl-[-CF_2-CH_2-]_n-CHCl_2$

Polymer name: poly(1,1-difluoro-1,2-ethanediyl), α-chloro-ω-(dichloromethyl)-

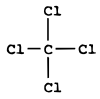
Telomers of unknown structure are indexed as copolymers with the term "telomer with..." cited in the modification.[1a]

Example 11.1.6. 1-Hexene, telomer with tetrachloromethane

REGISTRY COPYRIGHT 1995 ACS
RN 50320-18-8 REGISTRY
CN 1-Hexene, telomer with tetrachloromethane (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Methane, tetrachloro-, telomer with 1-hexene (9CI)
OTHER NAMES:
CN Carbon tetrachloride-1-hexene telomer
MF (C6 H12)x . C Cl4
PCT Polyolefin
LC STN Files: CA, CAPLUS

CM 1

CRN 56-23-5
CMF C Cl4

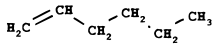


CM 2

CRN 25067-06-5
CMF (C6 H12)x
CCI PMS

CM 3

CRN 592-41-6
CMF C6 H12



:

11.2. IUPAC Nomenclature and Structure Representation. The IUPAC definition of an oligomer was given above. As of November 1996 IUPAC has published no definitions for "telomer" or "telomerization". A draft IUPAC document[22] defines "telomer" and "telomerization" essentially as follows:

•Telomer: an oligomer obtained by a telomerization process.

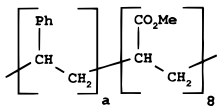
•Telomerization: an oligomerization by chain polymerization carried out in presence of a large amount of chain transfer agent, so that the end groups are essentially fragments of the chain transfer agent.

No recommendations have been published on how structure-based and source-based oligomers and telomers are to be named and represented graphically.

IUPAC references to oligomers and telomers are rare. Example 4.7.2.1.2 (in section 4.7.2.1) is an example of a telomer.[23a]

One published example of an oligomer[24a] is shown as example 11.2.1; note that IUPAC uses sub-a, vice sub-n, to indicate oligomers.

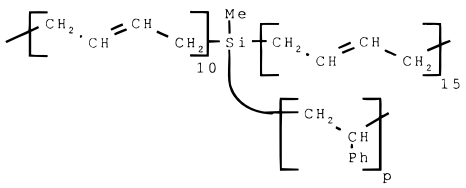
Example 11.2.1. Oligostyrene-*block*-octakis(methyl acrylate)



See also section 6.3.2.2.

Another oligomer, shown as example 11.2.2, utilizes the specific numerical prefixes "deca" and "pentadeca" in a star polymer containing two butadiene chains of specific length.[24b]

Example 11.2.2. Deca(buta-1,3-diene)-*block*-(methylsilanetriyl-*graft*-polystyrene)-*block*-pentadeca(buta-1,3-diene)



Two source-based names that use the prefix "oligo", vice "poly",[23b] are shown as examples 11.2.3 and 11.2.4.

Example 11.2.3. Oligo[(adipic acid)-*alt*-(1,4-butanediol)]

Example 11.2.4. Oligo[(2,4-tolylene diisocyanate)-*co*-(trimethylolpropane)]

11.3. MDL Graphic Representation. MDL[6] has not indicated how oligomers and telomers are to be indexed.

11.4. SCION Nomenclature and Structure Representation. Oligomers and telomers are named and structured in the SCION chemical file as if they were high polymers. In the SCION bibliographic file (corresponding to File CA), an appropriate controlled term such as OLIGOMERS or TELOMERS is indexed in the same indexing link as the CNUM of the oligomer or telomer. Additionally, a controlled term such as OLIGOMERIZATION or TELOMERIZATION is used when a preparation is reported in the source document. Specific textual descriptors at the polymer level such as OLIGOMER or TELOMER are not used. If the end groups are known, they are added as components of the oligomer or telomer. The polymer of example 11.1.6 is shown again as example 11.4.1 to demonstrate the method and illustrate the difference between the CAS method and the SCION method.

Example 11.4.1. "1-Hexene, telomer with tetrachloromethane"

Structure: (CH_2=CH-$(CH_2)_3$-CH_3 . .Cl . .CCl_3)$_x$

Telomer name: POLY-1-HEXENE, END GROUP CHLORO, END GROUP TRICHLOROMETHYL

SUMMARY AND CONCLUSIONS

Polymer nomenclature styles and structure representation systems described, recommended, or used by Chemical Abstracts Service, the International Union of Pure and Applied Chemistry, MDL Information Systems, Inc., and DuPont have been compared and contrasted. Structure-based versus source-based nomenclature and structural representations have been presented. Types covered include regular single-strand organic polymers, irregular single-strand organic polymers, including alternating and other periodic, block, comb, cross-linked, dendritic, graft, hyperconnected (i.e., hyperbranched, hypercross-linked), post-treated, and star. Stereochemistry in polymers, regular and quasi-single-strand inorganic and coordination polymers, regular double-strand (ladder and spiro) organic polymers, polysiloxanes, and oligomers and telomers were also covered. Nomenclature styles and structural representations of end groups were included.

Principal conclusions are as follows:

CAS and IUPAC are very close in their overall approach to nomenclature and structural representations of polymers. There are key differences in the areas of name inversion versus natural language and polysiloxane structures and nomenclature.

MDL has an interesting and versatile system; the "flexmatch" search capabilities are unique in that they offer simultaneous structure-based and source-based structure searching and a solution to the "phase-shift" problem of SRU polymer structure representation.

SCION concepts are mostly in accordance with CAS concepts, but there are key differences: SRU head atom rules; ladder and spiro polymer nomenclature and structure representation; polysiloxane structures and nomenclature.

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