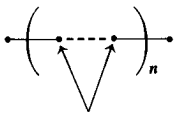
6: Nomenclature for Regular Single-Strand and Quasi-Single-Strand Inorganic and Coordination Polymers (1984)

PREAMBLE

The system for naming polymers in terms of structure previously published [1, 2] dealt with linear organic polymers, primarily those defined [2] as regular single-strand polymers, and followed as closely as possible established principles of organic nomenclature [3]. Accordingly, constituent subunits of the smallest repeating structural unit, named as bivalent radicals, are combined additively to form the name of the constitutional repeating unit. Extension of this method to linear inorganic and/or coordination polymers is seriously limited by the general lack of a system for naming bivalent radicals, because of the basic difference in philosophy between inorganic nomenclature and organic nomenclature. Furthermore, the constituent units of the constitutional repeating unit in most inorganic and coordination polymers are not bivalent radicals in the usual sense.

The present system is designed to name, uniquely and unambiguously, regular inorganic and/or coordination linear polymers, the constituent subunits of which can be formulated according to usual chemical principles of covalent and/or coordinate covalent bonding and the structures of which can be described by a constitutional repeating unit with at least one terminal constituent subunit that is connected through only one atom to other identical constitutional repeating units, or to an end group. 'Ladder' structures are thus excluded.

A *regular linear polymer* that can be described by a preferred constitutional repeating unit in which *both* terminal constituent subunits are connected through single atoms to the other identical constitutional repeating units or to an end group is called a *regular single-strand polymer* (see also Reference [2]).



single atoms

A *regular linear polymer* that can be described by a preferred constitutional repeating unit in which *only one* terminal constituent subunit is connected through a single atom to the other identical constitutional repeating units or to an end group is a *quasi-single-strand polymer,* i.e. it does not fit the definition of regular single-strand polymers [2c], but can be named in the same manner.

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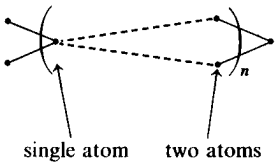
Based on the document *'A Structure-Based Nomenclature for Polymers. II. One-Dimensional Inorganic and Semi-Organic Polymers'* prepared by the Nomenclature Committee of the American Chemical Society's Division of Polymer Chemistry (1977).



Established principles of inorganic and coordination nomenclature [4] are used as far as is consistent with the definitions [5] and basic principles [1,2] of polymer nomenclature already published. As in the nomenclature of organic polymers, these rules apply to structures, not substances, that may be idealized representations of complex systems. Polymeric substances usually include a number of different structures, and a complete description of a polymer molecule would have to include such items as degree of steric regularity, chain imperfections, random branching, etc, resulting in extremely complex nomenclature. In any event, it is useful to consider a polymer in terms of a single structure that may itself be idealized. To the extent that an inorganic or coordination polymer can be represented as a linear combination of regularly repeating constitutional (structural) units, it can be named by the following rules. End groups may be included, if desired.

A few polymers with inorganic backbones in which the bonding is primarily covalent have trivial or semisystematic names of long standing, e.g. poly(dimethylsiloxane) for $-[-Si(CH_3)_2-O-]_n-$* and poly(dichlorophosphazene) for $-[-PCl_2=N-]_n-$† ; some of these polymers can also be named by the principles for naming organic polymers, i.e. by using bivalent radicals [1, 2], e.g. poly[oxy-(dimethylsilylene)] for $-[-Si(CH_3)_2-O-]_n-$, and poly[nitrilo(dichlorophosphoranylidyne)] for $-[-PCl_2=N-]_n-$. There is no objection to the use of trivial or semisysternatic names as long as they are clear and unambiguous, nor is there objection to the use of names based on the principles for naming organic polymers, if names for the bivalent radicals in the structure are clearly established. However, for some structures, the use of the rules given below provides unambiguous names with much less artificiality.

FUNDAMENTAL PRINCIPLES

The system of nomenclature for regular single-strand and quasi-single-strand inorganic and coordination polymers presented here is governed by the same fundamental principles of polymer nomenclature developed for single-strand organic polymers [2]. It is based on the selection and naming of a constitutional repeating unit (CRU), defined [5a] 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.

The name of the CRU is formed by citing, in order of appearance along the chain of the CRU, the names of its constituent subunits, which are the *longest structural fragments* of the CRU that can be

*Trivial names of 'siloxane' polymers are based on a $-SiH_2-O-$ repeating unit named siloxane which, together with substituents, is enclosed in parentheses or brackets and preceded by the prefix 'poly'. Names of low-molecular-weight siloxane polymers can be named by using the prefix 'oligo' or a numerical prefix in place of 'poly' as described in the organic polymers rules [1, 2].

On the other hand, names of specific, low-molecular-weight, acyclic siloxanes with the general formula $H_3Si-[-O-SiH_2-]_n-O-SiH_3$ are formed according to Rule D-6.22 [3a]. This results in similar, yet not identical names; for example, when n = 2 in the general formula above, the name would be tetrasiloxane. In these names, substituents are cited as prefixes to such parent names, for example, decamethyttetrasiloxane.

† This name is a hybrid of additive and substitutive nomenclature that does not satisfy fully the rules of either system.

named by the established principles of inorganic and/or coordination nomenclature.* Accordingly, bridging ligands are not broken into subunits smaller than those named by principles of coordination nomenclature for ligands [4].

Although this procedure will result in an unambiguous name, it will not necessarily give a unique name. To obtain a unique name, a single, preferred CRU must be selected. This may be accomplished by the following procedure:

1. *identify* the CRU and its constituent subunits;
2. *orient* the CRU, i.e. determine the subunit that will begin the citation of the CRU and the direction to proceed along the backbone of the polymer chain in writing the rest of the CRU from left to right;
3. *name* the CRU in two basic steps: (i) *name the subunits* by established inorganic and/or coordination nomenclature principles; (ii) *assemble the names* of the subunits according to the preferred direction of citation to form the name of the CRU.

Note

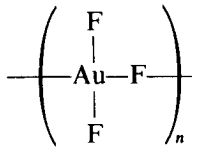
It is important to identify and orient the CRU as far as possible before assembling the name of the CRU. However, occasionally the choice of a unique orientation will depend on names for individual subunits.

Identification of the constitutional repeating unit (CRU)

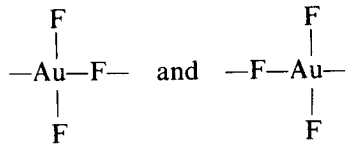
In many cases, the polymer structure is simple enough that the CRU and its constituent subunits can readily be identified.

Example

In the polymer



the two possible CRUs are:



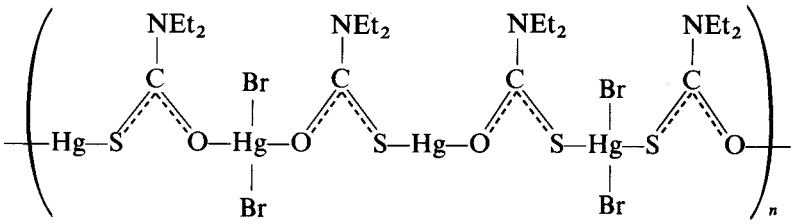
However, in more complex cases and occasionally in some simple cases it may be necessary to draw out a fairly long segment of the polymer chain in order to identify the possible constitutional repeating units.

Examples

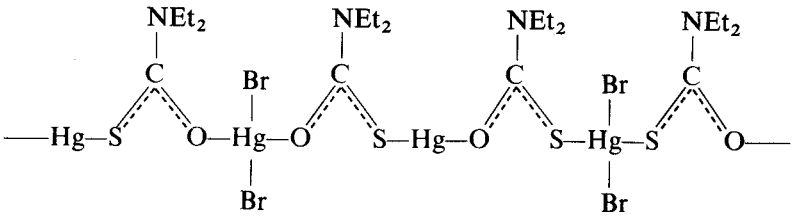
1. In the polymer $-(-Ag-CN-Ag-CN-)_n-$, the possible CRUs are: —Ag—CN—; —Ag—NC—; —CN—Ag—; and —NC—Ag—. (As already stated the bridging ligand —CN— is not broken up into smaller subunits.)

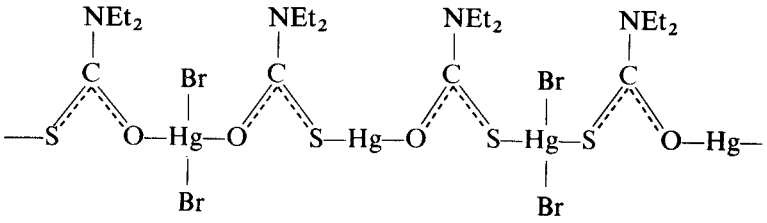
*In the rules for naming organic, polymers [1, 2], the constituent subunits of the CRU are the largest structural fragments that can be named as bivalent or multivalent radicals according to the established principles of organic nomenclature [3]. Single central atoms, mononuelear coordination centres, and bridging ligands are constituent subunits of CRUs in regular single-strand and quasi-single-strand inorganic and coordination polymers. Polymiclear coordination centres are used as subunits only under certain conditions (see discussion in 'Naming the constitutional repeating unit', p. 114).

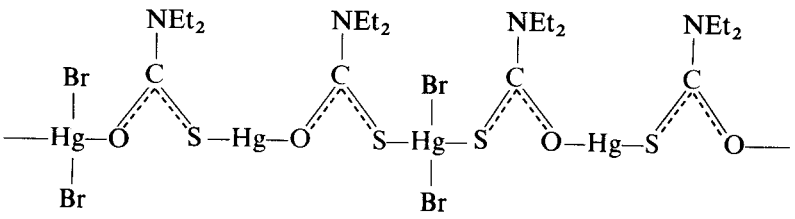
2. In the polymer

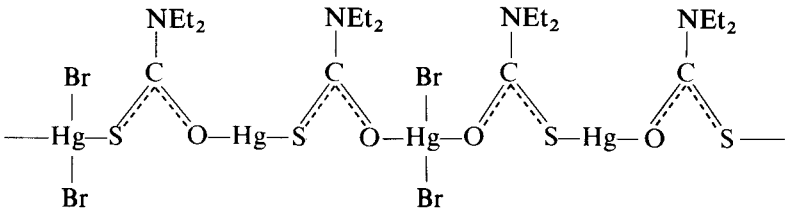


the possible constitutional repeating units are:









Orientation of the constitutional repeating unit

The constituent subunit of the CRU at which the citation of the CRU begins is the central atom (or coordination centre) of highest seniority, i.e. the most preferred central atom according to the set of hierarchical rules given in Rule IP-2.0, below. This centre is normally written as the *left* terminal subunit of the CRU.

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

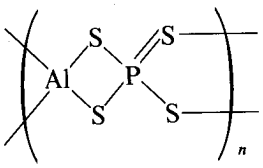
1. A single-strand CRU is preferred to a quasi-single-strand CRU, i.e. a CRU with *both* terminal constituent subunits connected to other identical constitutional repeating units or to an end group through single atoms is preferred to a CRU with only *one* terminal constituent subunit connected to other constitutional repeating units 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 senior subunit to a subunit of equal seniority, or to a subunit next in seniority.
3. When all paths between the senior subunit and a subunit of equal seniority, or a subunit ranking next in seniority, are of equal length, the preferred direction is along the path that includes constituent subunits of higher 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 [1, 2] may be needed to determine the preferred direction.

Further refinements to these general principles are given under Rule IP-2 and are illustrated in subsequent sections dealing with-the naming of specific polymers.

Naming the constitutional repeating unit

The name of a CRU of a single-strand and quasi-single-strand inorganic or coordination polymers is based on a backbone consisting of central atoms and bridging ligands where present. All inorganic or coordination polymers have one or more central atoms, but may or may not have bridging ligands. Homoatomic inorganic polymers are considered to consist of central atoms only. Coordination centres, mononuclear or polynuclear, and their associated ligands, except for ligands between central atoms in the backbone, if any, are named by the usual principles of coordination nomenclature. Bridging ligands are named as ligands prefixed by the Greek letter *m*

Selection of the largest structural fragments in the backbone that can be assigned multivalent radical names as subunits of a CRU is a fundamental principle in naming linear organic polymers. For naming inorganic and coordination polymers, this principle is applied to the selection of bridging ligands in the CRU. When there is a choice, the largest group that can be named by the accepted methods for naming polydentate ligands is chosen. For example, in the polymer shown below the CRU could be considered as two central atoms connected by



sulfur ligands. However, the principle of 'largest bridging ligand' requires the bridging ligand to be phosphorotetrathioato(3–). Strict application of this principle to inorganic or coordination polymers would lead to the selection of polynuclear coordination centres as the 'largest' structural fragment in the backbone. Since, at the present time, there are no officially accepted rules for uniquely naming and/or numbering certain types of polynuclear coordination centres, it is not yet convenient in some cases to use polynuclear coordination centres as subunits of a CRU in inorganic and coordination polymers. Hence, the principle of largest subunit is not always applied to coordination centres of a CRU and, in this set of rules, polynuclear coordination centres are used as subunits of CRUs only when it is *not* convenient to express such structural units in terms of their mononuclear coordination centres (see Rule IP-5). However, for illustrative purposes, names using polynuclear subunits are given as alternatives for some of the examples in the rules that follow.

Once the names of the constituent subunits of the CRU are determined, the CRU name is formed

by citing the name of the senior subunit followed by the names of the other constituent subunits as they occur in the preferred direction along the polymer chain.

RULE IP-1 THE GENERAL POLYMER NAME

IP-1.1
A name of a polymer, for which the CRU is known, but with a dimensional structure* that may not be known, or that need not be specified, consists of the prefix 'poly' followed by the name of the constitutional repeating unit (see Rules IP-3-IP-7) enclosed in square brackets, e.g. poly[CRU].†

IP-1.2
If it is desired to specify the number of constitutional repeating units, the appropriate numerical prefix [3b] may be used in place of the prefix 'poly', e.g. deca[CRU].

IP-1.3
A linear (one dimensional) polymer is indicated by the italicized prefix '*catena*' added to the name of the polymer formed according to Rules IP-1.1 and IP-1.2‡, e.g. *catena*-poly[CRU].

IP-1.4
End groups of a polymer molecule may be specified, if desired, by appropriate prefixes identified by the Greek letters α and ω, which are added to the name of the polymer formed as given by Rules IP-1.1 or IP-1.2 and IP-1.3, e.g. α-(end group)-ω-(end group)-*catena*-poly[CRU]. For details see Rule IP-8.

RULE IP-2 SENIORITY RULES FOR SELECTION OF A PREFERRED CONSTITUTIONAL REPEATING UNIT

Many regular single-strand and quasi-single-strand inorganic or coordination polymers can be represented as multiples of a repeating unit most conveniently represented as a series of smaller subunits. The following rules are concerned with various seniority considerations necessary for the derivation of a preferred CRU. Refinements of these basic rules and their application to specific polymers are illustrated in the sections that follow.

IP-2.1 Choice of the senior constituent subunit

IP-2.1.1
The constituent subunit of highest seniority, i.e. the first subunit to be cited, in the preferred CRU of

*Linear (chain), crosslinked, branched, etc.

†Although the rules for naming linear organic polymers [1,2] do not provide for describing dimensional structure, such specification would allow the prefix 'poly' to be a very general descriptor having no structural implications other than the presence of a number of constitutional repeating units.

‡The prefix *'catena'* is consistent with the existing rules for naming coordination compounds with 'extended' structures [4a, 4b]. In mineralogy and geochemistry, silicate chains have been denoted by the prefix *'ino'*; and the prefixes *'phyllo'* and *'tecto'* are used for sheet (two-dimensional) and three-dimensional structures, respectively [4c]. The term *catena* should not be confused with terms such as catenane, or catena compounds, used to describe interlocking organic ring compounds.

an inorganic or coordination polymer must contain one or more central atoms; bridging groups between central atoms in the backbone of the polymer cannot be senior subunits.*

IP-2.1.2

When there are two (or more) central atoms in a CRU of a linear inorganic or coordination polymer, the senior subunit is the one containing the central atom occurring latest in the general element sequence table (Fig. 6.1) [4d] shown below, as the line through the table is followed starting at the upper right corner.†

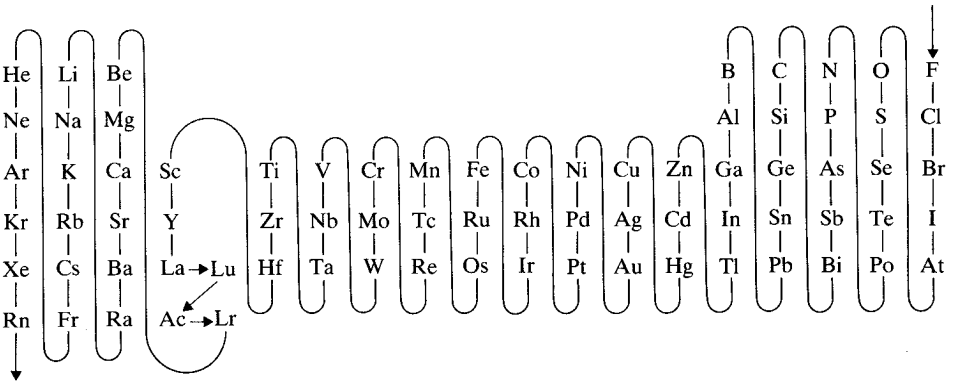


Fig. 6.1 Element sequence table.

IP-2.1.3

When a further choice is needed for the selection of a senior subunit in a CRU of a linear inorganic or coordination polymer, preference is given, in order, to:

1. a polynuclear coordination centre, in order of decreasing number of central atoms, provided the use of polynuclear centres as a subunit of a CRU is necessary (see discussion in 'Naming the constitutional repeating unit', p. 114);
2. the central atom or coordination centre with the greatest number of attached coordinating atoms, excluding coordinating atoms of bridging ligands in the backbone of the polymer chain;
3. the central atom or coordination centre the name of which, including ligands and their multiplying prefixes, if any, other than the bridging ligands in the backbone of the polymer chain, occurs earliest in the alphabet.

IP-2.2 Choice of the preferred direction along the polymer chain for the sequential citation of the constituent subunits of the CRU

After the senior subunits of the CRU have been determined by satisfying all of the seniority considerations of Rule IP-2.1, the following general principles are applied in order, where applicable.

IP-2.2.1

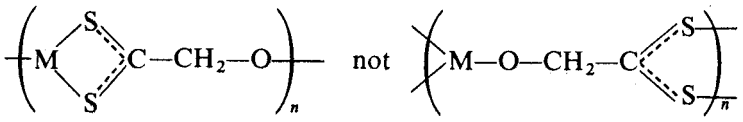
When it is possible to have either a single-strand or a quasi-single-strand CRU, the preferred

*This is consistent with the principles of coordination nomenclature in which the emphasis is always on the coordination centre. There is always at least one coordination centre in each inorganic or coordination polymer.

† Note that this seniority order is not the same as the seniority order for hetero atoms given in the organic polymer rules [2].

direction is that given a single-strand CRU*,

Example (M =central atom)

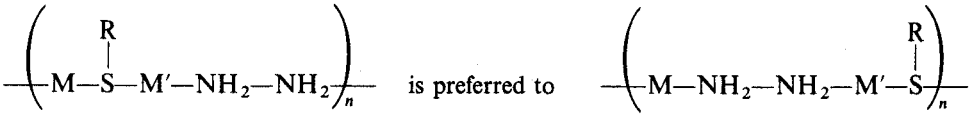


IP-2.2.2 Shortest path

The preferred direction along a polymer chain for the sequential citation of the constituent subunits of the CRU is the direction that leads first through the shortest path from the subunit of highest seniority to a subunit of equal seniority or to a subunit of next highest seniority. The length of the path between these subunits is the number of atoms in the most direct continuous chain of atoms from one unit to the other.

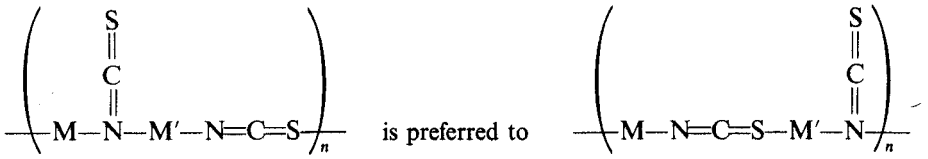
Examples (M=central atom)

1.



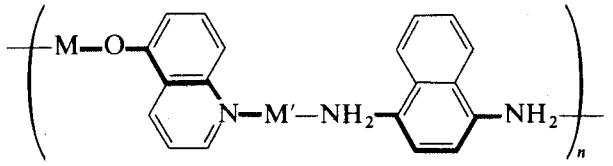
The one-atom path through the thiolato ligand is preferred to the two-atom path through the hydrazine ligand.

2.

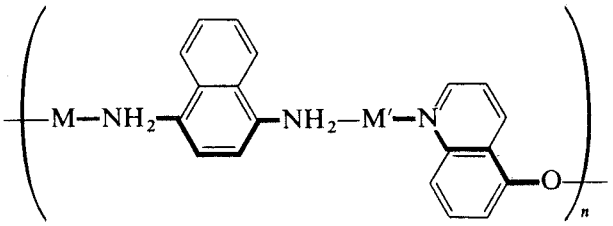


The one-atom path through the nitrogen atom of the isothiocyanato ligand is preferred to the threeatom path through all of the atoms of the isothiocyanato ligand.

3.



is preferred to



*This principle is quite analogous to that of minimizing free valences of constitutional repeating units in naming linear organic polymers when it is necessary to choose between a bivalent and a higher valent CRU after all factors concerned with the determination of subunit of highest seniority have been observed [2c].

The five-atom path through the 5-quinolinolato ligand is preferred to the six-atom path through the 1,4-naphthalenediamine ligand.

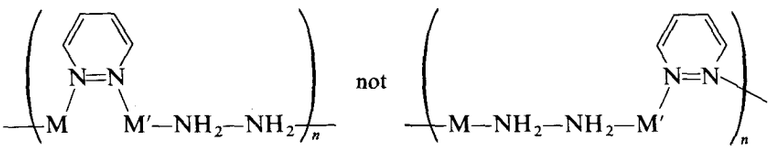
IP-2.2.3

When there are paths of equal (shortest) length between two subunits of equal highest seniority or between a subunit of highest seniority and a subunit ranking next in seniority, the preferred direction is determined by the kinds of structures and atoms included in the path and does not depend on actual names for subunits used in the final CRU name, unless there is no other choice remaining.

IP-2.2.3.1. For the selection of a preferred path, the same principles are used as in the organic polymer rules [2c], in which the fundamental order of seniority is (i) heterocycles; then (ii) acyclic hetero atoms; then (iii) carbocycles; and then (iv) acyclic carbon atoms or chains (see Rule 2.1.2, Reference [2c]). Seniority priority within these classes as given by the organic rules are also followed: for heterocycles*, see Rule 2.2.3 [2c]; for acyclic hetero atoms†, see Rule 2.3.1 [2c]; for carbocycles, see Rule 2.4.1 [2c]; for acyclic chains, see Rule 2.4.2 [2c].

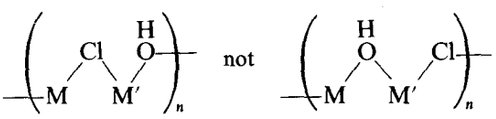
Examples (M = central atom)

1.



The heterocycle is preferred to the acyclic hetero chain.

2.



The Cl ligand is preferred to the O ligating atom.

IP-2.2.3.2. Substituents on atoms or groups in the path are used to determine priority between otherwise identical paths according to the principles in Rule 2.4.2 of the organic polymer rules [2c].

IP-2.2.3.3. If a further choice is necessary between otherwise identical paths, the preferred path leads by the shortest path, in the sense of Rule IP-2.2.2, from the senior subunit to the most preferred structural feature in the path.

Examples (M= central atom)

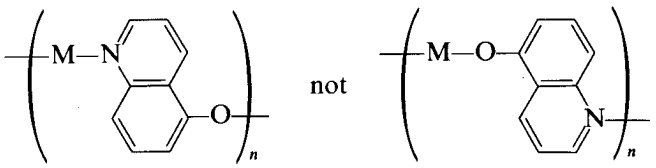
1.

–M–N C–$_n$ not –M–C N–$_n$

The hetero atom N is preferred to the carbon atom, and hence is preferred for citation closest to the senior subunit, M, in the preferred CRU.

*It is important to note that the seniority order for hetero atoms in ligands prescribed here is not the same as the seniority order for coordination centres, for which see Rule IP-2.1.2 in these rules.

2.



not

The heterocycle is preferred to the hetero atom O, and hence is preferred for citation closest to the senior subunit, M, in the preferred CRU.

IP-2.2.3.4. If a further choice is needed, the preferred path contains the ligand whose name occurs earliest in the alphabet.

RULE IP-3 REGULAR SINGLE-STRAND INORGANIC AND COORDINATION POLYMERS

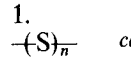
Regular single-strand inorganic and coordination polymers are named by inserting the name of the preferred constitutional repeating unit into the appropriate general polymer name as given by Rule IP-1.

IP-3.1

Constitutional repeating units with homoatomic backbones are named by citing each mononuclear central atom, together with its side groups, if any, named as ligands.

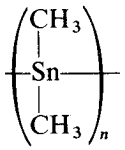
*Examples**

1.



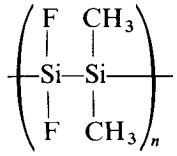
catena-poly[sulfur] [4e]

2.



catena-poly[dimethyltin]

3.



catena-poly[(difluorosilicon)(dimethylsilicon)]
(the subunit with the alphabetically earliest side group is the senior subunit)

IP-3.2

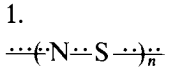
Constitutional repeating units with backbones consisting of a mononuclear central atom and one bridging ligand are named by citing the central atom prefixed by its associated non-bridging ligands followed by the name of the bridging ligand prefixed by the Greek letter *m*†

*According to the rules for naming linear organic polymers [1, 2], these inorganic homoatomic polymers could
be named: (1) poly(sulfanediyl); (2) poly(dimethylstannylene) or poly(dimethylstannanediyl); (3) poly(1,1difluoro-2,2-dimethyldisilane-1,2-diyl).

†Note that the bridging ligand is not included with the other ligands attached to the central atom. However, bridging ligands of polynuclear coordination centres that are not backbone units of the polymer are cited in their usual position in the name of the polynuclear coordination centre (see Rule IP-5).

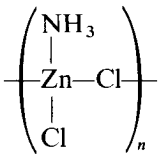
Examples

1.



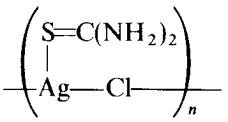
catena-poly[nitrogen-μ-thio]
(see Rule IP-3.2.1)

2.



catena-poly[(amminechlorozinc)-μ-chloro]

3.



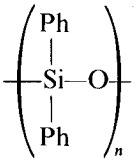
catena-poly[[(thiourea-*S*)silver]-μ-chloro]

IP-3.2.1

If there is a choice for the central atom, the element occurring later in the general element sequence table (see Rule IP-2.1.2) is the central atom.

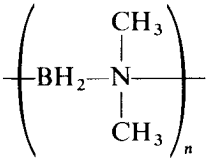
Examples

1.



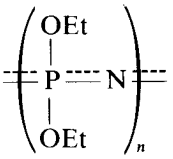
catena-poly[(diphenylsilicon)-μ-oxo]*

2.



catena-poly[(dihydroboron)-μ-(dimethylamido)]

3.



catena-poly[(diethoxophosphorus)-μ-nitrido]†

IP-3.2.2

Italicized element symbols indicating the coordinating atoms of bridging ligands in the backbone are cited in the order of the direction of citation of the CRU and are separated by a colon. Hence, element symbols cited before the colon refer to the central atom occurring just before the bridging

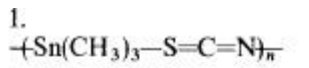
*According to the rules for linear organic polymers [1,2], this polymer would be oriented and named poly[oxy(diphenylsilylene)].

†According to the rules for linear organic polymers [1,2], this inorganic polymer would be oriented and named poly[nitrilo(diethoxyphosphoranylidyne)].

ligand in the CRU and element symbols cited after the colon refer to the central atom occurring immediately after the bridging ligand in the CRU or in the polymer chain.

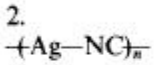
Examples

1.



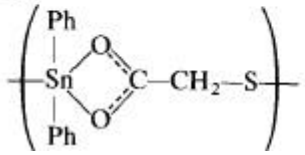
catena-poly[(trimethyltin)-μ-(thiocyanato-*S*:*N*)]

2.



catena-poly[silver-μ-(cyano-*N*:*C*)]
(not *catena*-poly[silver-μ-(cyano-*C*:*N*)]; see Rule IP-2.2.3.3)

3.



catena-poly[(diphenyltin)-μ-[mercaptoacetato(2−)-*O*,*O*′:*S*]
(direction of citation chosen by Rule IP-2.2)

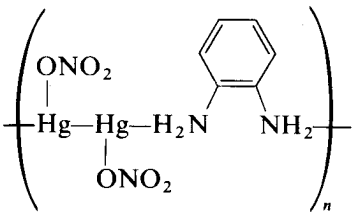
When a choice of direction for citation of the constituent subunits in the CRU remains after application of the principles in Rule IP-2.2, the direction is chosen so that the italicized element symbols denoting coordinating atoms of the bridging ligand are cited in lowest alphabetic order (see Example 6 under Rule IP-3.3).

IP-3.3

Constitutional repeating units consisting of more than one central atom and no more than one bridging ligand between each central atom of the polymer, are named by extending the principles of Rule IP-3.2. The senior central atom is selected according to Rule IP-2.1 and the direction of citation is determined by Rule IP-2.2.

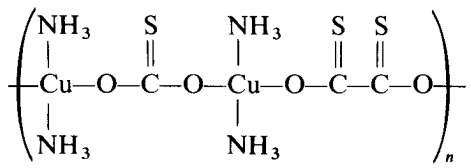
Examples

1.



catena-poly[(nitratomercury)(nitratomercury)-μ-(*o*-phenylenediamine-*N*:*N*′)]
(not *catena*-poly[(nitratomercury)-μ-(*o*-phenylenediamine-*N*:*N*′)-(nitratomercury)];
Rule IP-2.2.2)*

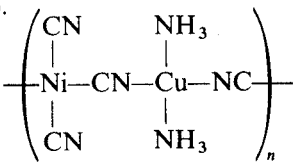
2.



catena-poly[(diamminecopper)-μ-[thiocarbonato(2−)-*O*:*O*′]-(diamminecopper)-μ-[dithiooxalato(2−)-*O*:*O*′]]
(direction selected according to Rule IP-2.2.2)

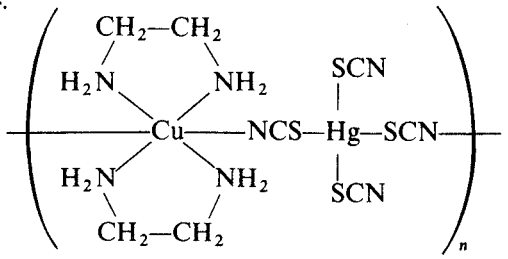
*The omission of an indication for metal-metal bonding in this example is consistent with existing coordination rules for di- and polynuclear complexes [4f].

3.



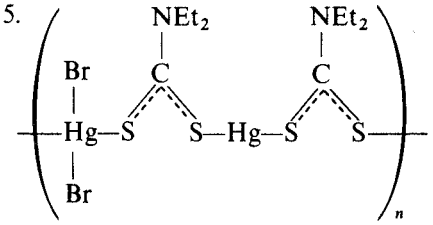
catena-poly[[bis(cyano-*C*)nickel]-μ-(cyano-*C*:*N*)-(diamminecopper)-μ-(cyano-*N*:*C*)]
(senior subunit chosen according to Rule IP-2.1.2)

4.



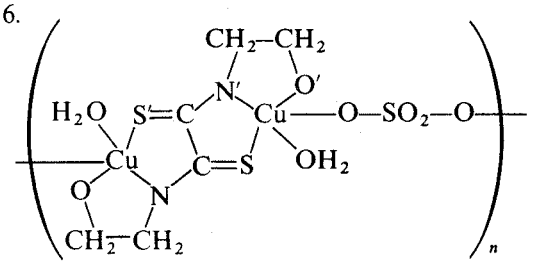
catena-poly[[bis(ethylenediamine-*N*,*N*′)copper]-μ-(thiocyanato-*N*:*S*)-[bis(thiocyanato-*S*)mercury]-μ-(thiocyanato-*S*:*N*)]

5.



catena-poly[(dibromomercury)-μ-(diethyldithiocarbamato-*S*:*S*′)-mercury-μ-(diethyldithiocarbamato-*S*:*S*′)]
(senior subunit chosen according to Rule IP-2.1.3)

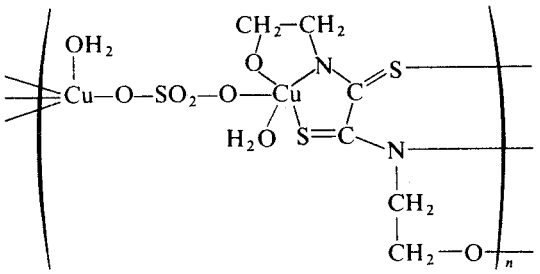
6.



catena-poly[(aquacopper)-μ-[*N*,*N*′-bis(2-hydroxyethyl)dithiooxamido(2−)-*N*,*O*,*S*′:*N*′,*O*′,*S*]-[aquacopper)-μ-[sulfato-(2−)-*O*:*O*′]]*

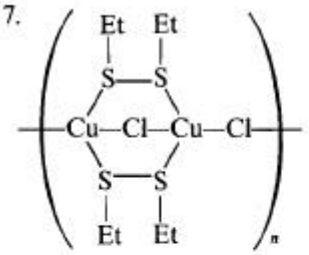
---

*Orientations of the CRU that begin with either copper central atom and proceed first through the sulfato ligand are ruled out by Rule IP-2.2.1. These orientations produce the less preferred quasi-single-strand polymeric structure as shown below.



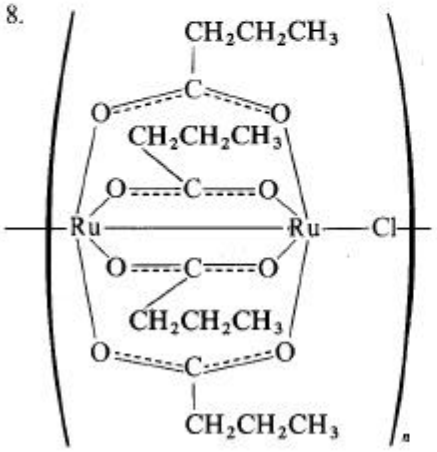
Multiple bridging ligands between the same pair of central atoms are cited in alphabetic order each preceded by the Greek letter μ, and all are enclosed in square brackets to reduce the possibility of misinterpretation.

7.



catena-poly[copper-[μ-chloro-bis-μ-(diethyl disulfide-*S*:*S'*)]-copper-μ-chloro]
(direction of citation chosen by Rule IP-2.2.1)*

8.



catena-poly[[ruthenium-tetrakis-μ-(butyrato-*O*:*O'*)-ruthenium(*Ru*-*Ru*)]-μ-chloro]
(direction of citation chosen by Rule IP-2.2.1)†

RULE IP-4 REGULAR QUASI-SINGLE-STRAND COORDINATION POLYMERS

Regular quasi-single-strand coordination polymers are named by inserting the name of the preferred constitutional repeating unit into the appropriate general polymer name as given by Rule IP-1.

Footnote *continued*

The choice between the remaining two orientations is made according to the second paragraph of Rule IP-3.2.2. In the preferred orientation, the letter locant order for the bridging ligand, *N,O,S':N',0',S,* is lower than *N',0',S:N,O,S'.*

*It might be convenient in such cases to treat the two copper central atoms as a binuclear complex as follows: *catena*-poly[[*m*-chloro-bis-*m*-(diethyl disulfide-S:S')-dicopper]-*m*-chloro].

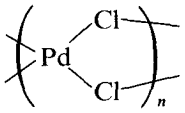
†It does not seem quite consistent with the philosophy of polymer nomenclature to cite a metal-metal bond in this fashion; hence, it would probably be more acceptable here to treat the two ruthenium central atoms as a binuclear complex, perhaps as follows: *catena*-poly[[tetrakis-*m*-(butyrato-O:O')-diruthenium(*Ru*-*Ru*)]-*m*-chloro].

IP-4.1

Constitutional repeating units 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 non-bridging ligand(s), followed by the names of the bridging ligands each prefixed by the Greek letter ***m*** The number of identical bridging ligands, if more than one, is indicated by an appropriate numerical prefix; different bridging ligands are cited in alphabetic order and all are enclosed in appropriate enclosing marks.

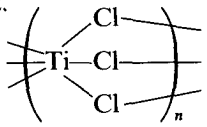
Examples

1.



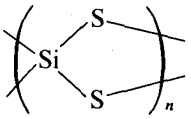
catena-poly[palladium-di-μ-chloro]
(*catena*-di-μ-chloro-palladium in the 1970 IUPAC Inorganic Rules [4g])

2.



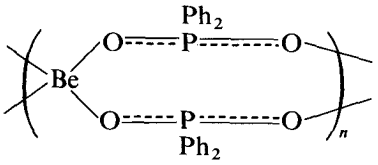
catena-poly[titanium-tri-μ-chloro]

3.



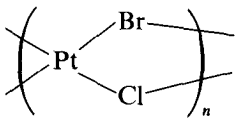
catena-poly[silicon-di-μ-thio]

4.



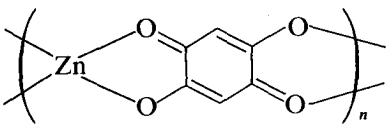
catena-poly[beryllium-bis-μ-[diphenylphosphinato(1−)-*O*:*O*′]]

5.



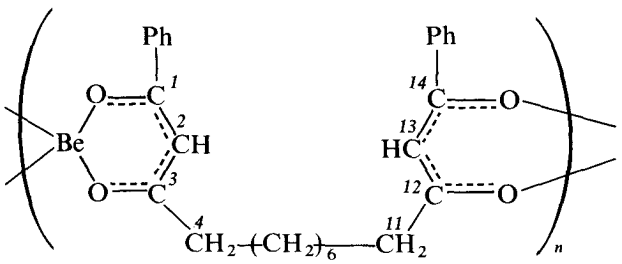
catena-poly[platinum(μ-bromo-μ-chloro)]

6.



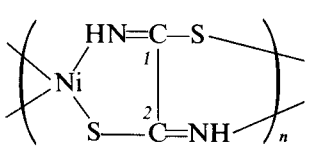
catena-poly[zinc-μ-[2,5-dihydroxy-*p*-benzoquinonato(2−)-O^1,O^2:O^4,O^5]]

7.



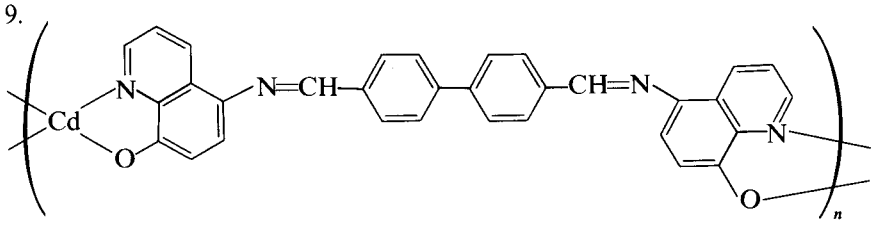
catena-poly[beryllium-μ-[1,14-diphenyl-1,3,12,14-tetradecanetetronato(2−)-O^1,O^3:O^{12},O^{14}]]

8.



catena-poly[nickel-μ-[dithiooximidato(2−)-N^1,S^2:N^2,S^1]]

9.



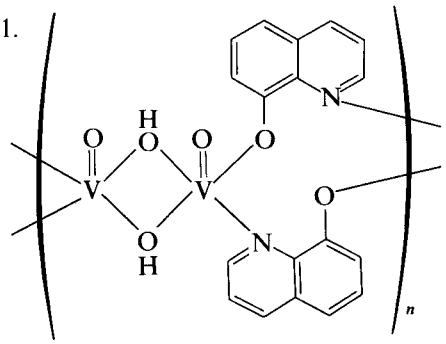
catena-poly[cadmium-μ-[[5,5′-[4,4′-biphenylylenebis(methylidynenitrilo)]di-8-quinolinolato](2−)-N^1,O:$N^{1'}$,O']]

IP-4.2

Constitutional repeating units containing more than one central atom are named by extending the principles of IP-4.1. The senior central atom is selected according to Rule IP-2.1, and the direction of citation is determined by Rule IP-2.2.

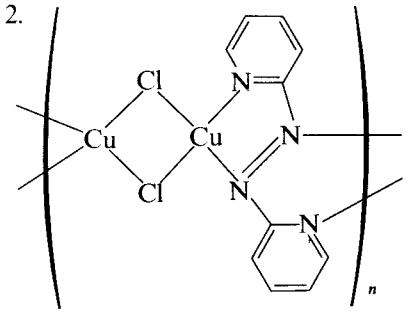
Examples

1.



catena-poly[(oxovanadium)-di-μ-hydroxo-(oxovanadium)-[μ-(8-quinolinolato-N:O)-μ-(8-quinolinolato-O:N)]]
(the direction of citation is determined by Rule IP-2.2.2)

2.



catena-poly[copper-di-μ-chloro-copper-μ-[2,2′-(azo-N:N')dipyridine-N':N]]
(the direction of citation is determined by Rule IP-2.2.2)

RULE IP-5 SINGLE-STRAND AND QUASI- SINGLE- STRAND COORDINATION POLYMERS WITH POLYNUCLEAR COORDINATION CENTRES

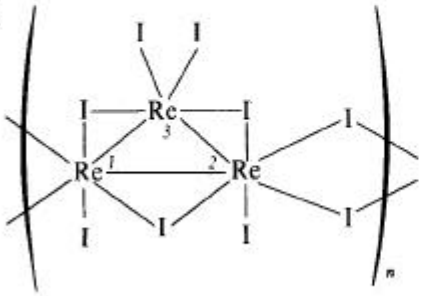
Single-strand and quasi-single-strand coordination polymers with one polynuclear coordination centre are named in much the same manner as coordination polymers having only mononuclear centres. The polynuclear centre is the senior subunit and begins the citation of the subunits in the name of the CRU. Both positions on the polynuclear complex where the bridging ligand is attached are indicated by numerical locants, inserted between the name of the polynuclear centre and the names of the bridging ligand and separated by a colon; locants before the colon refer to the preceding polynuclear centre in the CRU and locants following the colon refer to the next polynuclear centre in the polymer chain.

Examples

1. $-(-[\textit{octahedro}\text{-}W_6(\mu\text{-}Br_8)(2,3,4,5\text{-}Br_4)]-(6:1)-(Br_4)-)_n-$

catena-poly[(octa-μ-bromo-2,3,4,5-tetrabromo-*octahedro*-hexatungsten)-6:1-μ-[tetrabromido(2−)]]

2.



catena-poly[[1,2:1,3:2,3-tri-μ-iodo-1,2,3,3-tetraiodo-*triangulo*-trirhenium(3*Re-Re*)]-2,2:1,1-di-μ-iodo]*

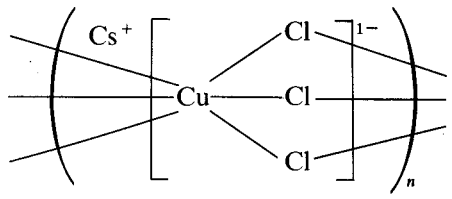
RULE IP-6 REGULAR SINGLE-STRAND AND QUASI-SINGLE-STRAND INORGANIC AND COORDINATION POLYMERS WITH IONIC CONSTITUTIONAL REPEATING UNITS

Regular single-strand and quasi-single-strand inorganic and coordination polymers with ionic CRUs are named in the same general manner as described in Rules IP-3, IP-4 and IP-5. The charge of the CRU may be indicated by an Ewens-Bassett number cited after the name of the ionic portion of the CRU. Stock numbers may be used to denote the oxidation state of the central atom; if so, they are attached to the name of the central atom in the usual manner.

*Numbering rules for polynuclear complexes have not yet been fully defined and are under study by the IUPAC Commission on Nomenclature of Inorganic Chemistry. The numbering shown here is arbitrary and only for convenience in defining the structure of this polymer for this document.

*Examples**

1.

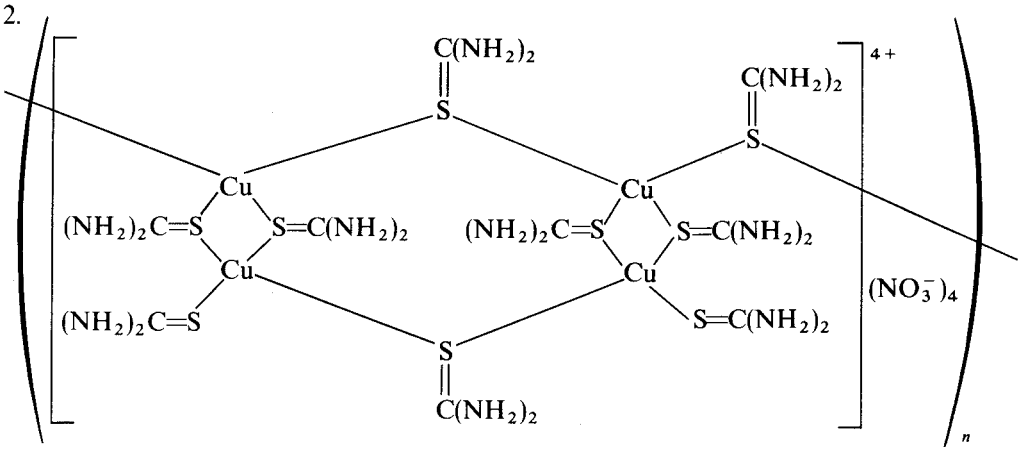


catena-poly[caesium [cuprate-tri-μ-chloro](1−)]

or

catena-poly[caesium [cuprate(II)-tri-μ-chloro]]

2.



catena-poly[[[bis-*m*(thiourea-S,S)-2-(thiourea-S)dicopper]-1,2:1,2-[bis-*m*(tbiourea-S:S)][bis-*m*(thiourea-S,S)-2-(thioureaS)dicopper]-1:1-*m*(thiourea-S:S)](4+) tetranitrate]

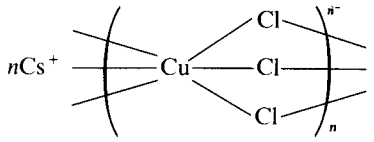
or

catena-poly[[[bis-*m*(thiourea-S,S)-2-(thiourea-S)dicopper(I)]-1,2:1,2-[bis-*m*(thiourea-S:S)] [bis-*m*(thiourea-S:S)-2(thiourea-S)dicopper(I)-1:1-*m*(thiourea-S:S)] tetranitrate]

RULE IP-7 STEREOCHEMICAL CONFIGURATION OF A CONSTITUTIONAL REPEATING UNIT

Stereochemical configuration of a constitutional repeating unit consisting of a mononuclear central atom and one bridging ligand may be designated by suitable prefixes cited before the appropriate complete polymer name.†

* From an inorganic viewpoint, it might be better to consider these polymers to be salts of polymeric ions as illustrated below:



caesium *catena*-poly[[cuprate-tri-μ-chloro](1−)]

or

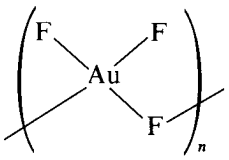
caesium *catena*-poly[cuprate(II)-tri-μ-chloro]

† An alternative format in which the stereochemical prefix is inserted between the prefix `poly' and the name of the CRU, as shown below for both examples under this rule, would be more consistent with inorganic nomenclature practice, as shown by the names below.

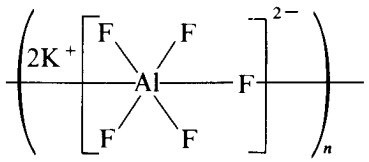
1. *catena*-poly [*cis*-[(difluorogold)-*m*-fluoro]]
2. *catena*-poly [*trans*-[dipotassium [[(tetrafluoroaluminate)-*m*-fluoro](2–)]]] or
   catena-poly [*trans*-[dipotassium [[tetrafluoroaluminate(III)]-*m*-fluoro]]]

However, the recommendation in this Rule (IP-7) is in accord with the stereochemical notation recommended for organic polymers [6].

Examples

1. 

cis-catena-poly[(difluorogold)-μ-fluoro]

2. 

trans-catena-poly[dipotassium [[(tetrafluoroaluminate)-μ-fluoro](2−)]]
or
trans-catena-poly[dipotassium [[tetrafluoroaluminate(III)]-μ-fluoro]]
(inorganic nomenclature practice would not require use of the Stock number for aluminium)

RULE IP-8 END GROUPS OF LINEAR INORGANIC OR COORDINATION POLYMERS

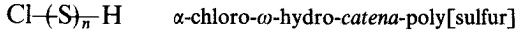
End groups of linear inorganic or coordination polymers are specified by prefixes cited in front of the name of the polymer (see Rule IP-1.4).

IP-8.1

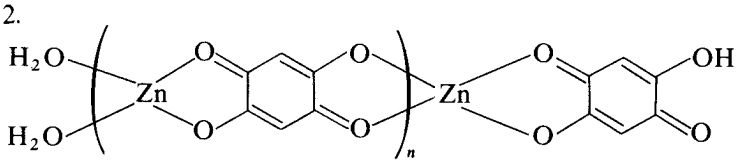
The groups attached to the first constituent subunit of the preferred CRU, i.e. the senior coordination centre written as the left terminal subunit in the CRU, are named as ligands and designated by the Greek letter ***α***.

End groups attached to the other terminal subunit of the preferred CRU are named as ligands if attached to a central atom, or, if attached to a bridging ligand, are named as a central atom by the usual principles of coordination nomenclature and are designated by the Greek letter ***ω***.

Examples

1. 

α-chloro-ω-hydro-*catena*-poly[sulfur]

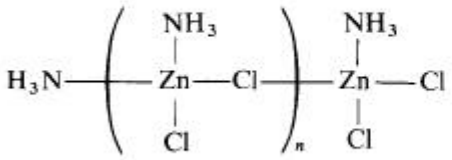
2. 

α,α-diaqua-ω-[[2,5-dihydroxy-*p*-benzoquinonato(1−)-O^1,O^2]zinc]-*catena*-poly[zinc-μ-[2,5-dihydroxy-*p*-benzoquinonato-(2−)-O^1,O^2:O^4,O^5]]

IP-8.2

When a choice is necessary to determine ligands to be cited as an end group or to be included in the constitutional repeating unit, the ligand chosen as the ***α*** end group is the one whose name occurs earliest in the alphabet.

Example



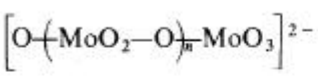
α-ammine-ω-(amminedichlorozinc)-*catena*-poly[(amminechlorozinc)-μ-chloro]

IP-8.3

End groups that may be considered ionic are named by the principles of coordination nomenclature in the usual manner. The amount of charge is indicated by an Ewens-Bassett number cited at the end of the complete polymer name.

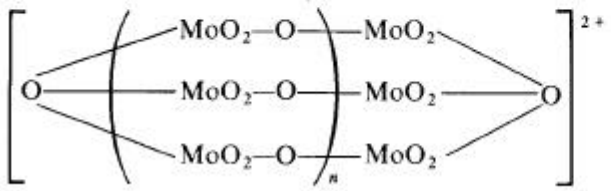
Examples

1.



[α-oxo-ω-(trioxomolybdate)-*catena*-poly[(dioxomolybdenum)-μ-oxo]](2 −)

2.



[α-μ_3-oxo-ω-[μ_3-oxo-tris(dioxomolybdenum)]tris[*catena*-poly[(dioxomolybdenum)-μ-oxo]]](2+)*

REFERENCES

1 American Chemical Society. A structure-based nomenclature for linear polymers. *Macromolecules* **1**, 193-198 (1968).

2 IUPAC. Nomenclature of regular single-strand organic polymers: (a) *IUPAC Inf. Bull. Append.* No. **29** (1972); (b) *Macromolecules* **6**, 149-158 (1973) - a separate publication of the tentative rules (Reference [2a]); (c) *Pure Appl. Chem.* **48**, 373-385 (1976) - the approved rules (1975). Reprinted as Chapter 5, this volume.

3 IUPAC. *Nomenclature of organic chemistry,* Sections A, B, C, D, E, F and H, Pergamon Press, Oxford (1979): (a) Rule 6.22, pp. 411-412; (b) Rule 1.1, p. 5.

4 IUPAC. *Nomenclature of inorganic chemistry,* 2nd Edn., Butterworths, London (1971): (a) Rule 7.62, pp. 71-72; (b) Table Ill, p. 103; (c) Rule 4.14, footnote, p. 27; (d) Table IV, p. 104; (e) Rule 1.4, example 6, p. 12; (f) Rules 7.71 and 7.72, pp. 72-73; (g) Rule 7.62, p. 71.

5 IUPAC. Basic definitions of terms relating to polymers 1974. *Pure Appl. Chem.* **40**, 477-491 (1974): (a) Definition 3.3, p. 482. Reprinted as Chapter 1, this volume.

6 IUPAC. Stereochemical definitions and notations relating to polymers (recommendations 1980). *Pure Appl. Chem.* **53**, 733-752 (198 1). Reprinted as Chapter 2, this volume.

*This is a regular single-strand polymer consisting of three chains linked by a terminal oxo end group.