Project 2001-082-1-800
extension 2004-046-1-800

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION (VIII)
and
POLYMER DIVISION (IV)
COMMISSION ON MACROMOLECULAR NOMENCLATURE*,
SUBCOMMITTEE ON MACROMOLECULAR TERMINOLOGY**

STRUCTURE-BASED NOMENCLATURE FOR CYCLIC MACROMOLECULES

(IUPAC Recommendations 200X)

This document was prepared by a working group consisting of
M. Barón (Argentina), R. B. Fox (USA), A. Fradet (France), K.-H. Hellwich (Germany),
P. Hodge (UK), K. Horie (Japan), J. Kahovec (Czech Republic), P. Kubisa (Poland),
E. Maréchal (France), W. V. Metanomski (USA), W. Mormann (Germany),
R. F. T. Stepto (UK), J. L. Schultz (USA), and E. S. Wilks (USA)

Prepared for publication by
W. Mormann
Universität Siegen, FB 8, Laboratorium für Makromolekulare Chemie, Adolf-Reichwein-Str. 2, 57076 Siegen, Germany
mormann@chemie.uni-siegen.de
and
K.-H. Hellwich
Postfach 100731, 63007 Offenbach, Germany
hellwich.iupac@web.de

IUPAC Provisional Recommendations
For Peer Review Only

***Membership of the Commission on Macromolecular Nomenclature (extant until 2002) during the preparation of this report (1997-200X) was as follows:**

Titular members: M. Barón (Argentina, Titular Member from 1996, *Secretary* from 1998); K. Hatada (Japan, to 1997, Associate Member to 1999); M. Hess (Germany, Associate Member from 1996, Titular Member from 1998, *Chairman* from 2000); K. Horie (Japan, Associate Member from 1996, Titular Member from 1998); R. G. Jones (UK, Pool Titular Member to 1997, Titular Member from 1998); J. Kahovec (Czech Republic, to 1999); P. Kubisa (Poland, Associate Member from 1996, Titular Member from 2000); E. Maréchal (France, Titular Member to 1999, Associate Member 2000-2001); I. Meisel (Germany, Associate Member from 1998, Titular Member from 2000); W. V. Metanomski (USA, to 1999); C. Noël (France, to 1997); V. P. Shibaev (Russia, Associate Member to 1999); R. F. T. Stepto (UK, *Chairman* to 1999); E. S. Wilks (USA, Associate Member from 1998, Titular Member from 2000); W. J. Work (USA, *Secretary* to 1997)

Associate Members contributing to this report: J. He (China, from 2000); J.-Il. Jin (Korea, from 1994); T. Kitayama (Japan, from 2000); S. Penczek (Poland, from 1994); J. Vohlídal (Czech Republik, from 2000).

****Membership of the Subcommittee on Macromolecular Terminology (extant from 2002) during the preparation of this report (1997-200X) was as follows:**

M. Hess (Germany, *Chairman* to 2005, *Secretary* from 2006); M. Barón (Argentina, *Secretary* until 2003); R. G. Jones (UK, *Secretary* 2003 to 2005, *Chairman*, from 2006); G. Allegra (Italy); A. Fradet (France); J. He (China); K.-H. Hellwich (Germany); P. Hodge (UK); K. Horie (Japan); A. D. Jenkins (UK); J.-I. Jin (Korea); J. Kahovec (Czech Republic); T. Kitayama (Japan); P. Kratochvíl (Czech Republic); P. Kubisa (Poland); I. Meisel

(Germany); W. V. Metanomski (USA); V. Meille (Italy); G. Moad (Australia); W. Mormann (Germany); S. Penczek (Poland); L. P. Rebelo (Portugal); M. Rinaudo (France); C. dos Santos (Brazil); I. Schopov (Bulgaria); M. Schubert (USA); V. P. Shibaev (Russia); S. Słomkowski (Poland); R. F. T. Stepto (UK); D. Tabak (Brazil); J. Vohlídal (Czech Republic); E. S. Wilks (USA); W. J. Work (USA).

DRAFT WM 8: FOR PUBLIC REVIEW

References including cross-references are marked in yellow in order to find them readily for renumbering during the final editorial work on the document.

For Peer Review Only
IUPAC Provisional Recommendations

Structure-Based Nomenclature for Cyclic Macromolecules
(IUPAC Recommendations 2006)

ABSTRACT: A structure-based nomenclature system for monocyclic and polycyclic macromolecules is presented. Single-strand mono- and polycyclic macromolecules as well as spiro macrocyclic compounds are covered. However, rotaxanes and catenanes, which contain interlocked rings, and rings or ring systems formed by non-covalent bonds are excluded. The nomenclature of cyclic macromolecules is based on the existing nomenclature of regular and irregular polymers, which in turn is based on the nomenclature of organic chemistry also published by IUPAC. The procedure for naming a cyclic macromolecule consists of transforming it to an open chain molecule in such a way that naming of units proceeds in descending order of seniority. For polycyclic macromolecules *main ring*, *bridge*s and *branch unit*s are identified and locants for *branch unit*s as well as *bridge*s are assigned before naming according to the rules of this document. Wherever possible, examples for illustration of the naming procedure have been chosen from the literature.

For Peer Review Only
IUPAC Provisional Recommendations

CONTENTS

For Peer Review Only
IUPAC Provisional Recommendations

CM-7 REFERENCES

For Peer Review Only
IUPAC Provisional Recommendations

CM-0 INTRODUCTION

This nomenclature of cyclic macromolecules is designed to provide unambiguous names through an extension of structure-based nomenclature for regular [1] and irregular [2] macromolecules. The document includes single-strand mono- and polycyclic macromolecules as well as spiro macrocyclic compounds. However, rotaxanes and catenanes, which contain interlocked rings, and rings or ring systems formed by non-covalent bonds are excluded. They will be dealt with in separate documents because of their specific structural features. A first approach to naming macrocyclic compounds used IUPAC-approved names for bivalent units and concepts of structure-based polymer names [3]. The present document follows this basic principle and adjusts it to the specific requirements of macromolecular structures; at the same time it is extended to more complex structures. The concept is based on transforming a cyclic macromolecule into an open chain regular or irregular macromolecule by a conceptual scission of a ring bond and naming it according to the rules established for these types of macromolecules. The principles of nomenclature for regular and irregular polymers will not be repeated here. They will be used but explained only where necessary for a better understanding of examples.

Nomenclature of polycyclic macromolecules uses the same principles as that of monocyclic macromolecules. Polycyclic macromolecules are named by identifying the *main ring*, *branch point*s, and *bridge*s, and citing them in the appropriate order.

To name cyclic macromolecules, knowledge of nomenclature of organic chemistry [4, 5, 6], at least to the extent it is explained and illustrated by examples in [1], is indispensable.

The intention of this document is to propose a nomenclature applicable to practically all cyclic macromolecules that can be imagined, e.g., by transformation of organic-chemical ring systems to macrocyclic ring systems. One should, however, also take into account the synthetic feasibility of macrocyclic molecules. Most of them will be monocyclic, bicyclic or spiro. Polycyclic macromolecules beyond bicyclics are unsupported by convincing proof of structure and at present should be treated as hypothetical.

Structure-based nomenclature unambiguously names a compound with respect to its constitution. Configurational aspects can be included in the name by means of stereodescriptors added to the structure-based name as affixes. Topology, in particular of polycyclic macromolecules, is not an explicit topic in structure-based nomenclature, although it is inherently contained in a structure-based name (see rule 21, last example, in [1]). The topology of polycyclic macromolecules has been discussed elsewhere in the literature [7, 8].

To assist the reader, throughout the document cross references to terms defined in the following glossary are denoted in italic typeface.

CM-1 GLOSSARY

CM-1.1 block

Portion of a macromolecule, comprising many constitutional units, that has at least one feature which is not present in the adjacent portions ([9] and definition 1.62 in [10]).

CM-1.2 branch point

Point on a chain at which a branch or a *bridge* is attached. (See also [9] and definition 1.54 in [10].)

CM-1.3 branch unit

Constitutional unit in a macromolecule to which a branch or *bridge* is attached. (See also [9] and definition 1.55 in [10].)

CM-1.4 bridge

Block, constitutional unit, or bond, joining two *branch units* of a more senior *macrocycle*, i.e., the macrocycle containing units of higher seniority (See also VB-1 in [11], [9], and R-2.4.2.1, note 29 [5].)

CM-1.5 constitutional unit (CU)

Atom or group of atoms (with pendent atoms or groups, if any) comprising a part of the essential structure of a macromolecule, an oligomer molecule, a *block* or a chain ([9] and definition 1.14 in [10]).

CM-1.6 constitutional repeating unit (CRU)

For Peer Review Only
IUPAC Provisional Recommendations

Smallest *constitutional unit*, the repetition of which constitutes a regular macromolecule, a regular oligomer molecule, a regular *block* or a regular chain ([9] and definition 1.15 in [10]).

CM-1.7 cyclic macromolecule

Macromolecule in which the termini of the backbone are connected to form a ring.

Note: Linear macromolecules comprising constitutional units that include small cyclic structures [e.g., the phenylene groups in poly(ethylene terephthalate)] are not cyclic macromolecules. However, a cyclic molecule comprising such constitutional (repeating) units is a cyclic macromolecule (see also example 1).

CM-1.8 irregular monocyclic macromolecule

Cyclic macromolecule that with a single conceptual scission of a chain bond is converted to an open-chain structure with an irregular distribution of constitutional units, i.e., a structure that cannot be described by a single constitutional repeating unit (See also [9] and definition 1.5 in [10].)

CM-1.9 macrocycle

Cyclic macromolecule or macromolecular cyclic portion of a macromolecule ([9] and definition 1.57 in [10]).

Note 1: A macrocycle is always monocyclic.

Note 2: Rings that can be named by rules of organic chemistry nomenclature are not considered as macrocycles.

Note 3: Macrocycle is also used for molecules of low molar mass that would not be considered to be macromolecules as specified in the definition given above. [12]

CM-1.10 main ring

Macrocycle in a bridged polycyclic macromolecule or polycyclic macromolecular portion that contains the subunits of highest seniority.

Note: In macrocyclic molecules with macrocyclic substituents, the ring that contains the *subunits* of highest seniority is called the parent macrocycle or macrocyclic system.

CM-1.11 path length

Number of polymer main-chain (backbone) atoms between two subunits.

Note: Where a ring or ring system constitutes all or part of a path between two subunits, the shortest continuous chain of atoms in the ring or ring system is selected (see also Glossary in [1]).

CM-1.12 polycyclic macromolecule

Molecule that includes more than one *macrocycle*, all of which have at least one atom in common with another *macrocycle*.

Note 1: Molecules that have two rings without any common atom are not considered polycyclic, e.g., biphenyl. In general terminology, however, they are often regarded as polycyclic.

Note 2: “Multicyclic” or “pluricyclic” have been proposed as alternative terms for polycyclic. In accordance with nomenclature of organic chemistry the term polycyclic is used here, since it does not lead to confusion with respect to poly in polymer. Therefore the use of “multicyclic” or “pluricyclic” is discouraged as an alternative for “polycyclic”.

CM-1.13 preferred constitutional repeating unit

Constitutional repeating unit that begins with the subunit of highest seniority (adopted from [1], p. 1925).

CM-1.14 regular monocyclic macromolecule

For Peer Review Only
IUPAC Provisional Recommendations

Cyclic macromolecule that can be described by a single *constitutional repeating unit*. (See also [9] and definition 1.4 in [10]).

CM-1.15 seniority

Priority in a set of atoms or groups of atoms according to a prescribed order (see also Glossary in [1] and [9]).

CM-1.16 spiro compound

Compound having one atom as the only common member of two rings (see also [9, 13]).

CM-1.17 spiro macromolecule

Macromolecule having one atom as the only common member of two *macrocycle*s.

Note: Spiro macromolecule is also used for double-strand *macromolecule*s in which case the definition is: Double-strand *macromolecule* consisting of an uninterrupted sequence of rings, with adjacent rings having only one atom in common. Alternatively, a spiro macromolecule is a double-strand macromolecule with adjacent *constitutional unit*s joined to each other through three atoms, two on one side and one on the other side of each *constitutional unit* ([9] and definiton 1.43 in [10].

CM-1.18 spiro union

Linkage between two rings consisting of a single atom common to both rings. A 'free spiro union' is a linkage which constitutes the only union direct or indirect between the two rings. The common atom is designated as the 'spiro atom' (R-2.4.3 in [5]; see also [4b], [9] and rule SP-0 in [13]).

CM-1.19 substituent

An atom or a group of atoms that replaces one or more hydrogen atoms attached to a backbone atom. (See also definition R-0.2.2.1 in [5].)

CM-1.20 subunit

Largest segment named as a single unit under nomenclature of organic chemistry rules [4, 5, 6].

Note: A subunit may be a ring or ring system, a heteroatom or a heteroatom chain, or a carbon chain. (See also Glossary in [1].)

CM-2 GENERAL PRINCIPLES

CM-2.1 Seniority

Nomenclature of *cyclic macromolecules* like that of open chain macromolecules [1, 2] is based on the seniority of *constitutional units* and *constitutional repeating units* that are part of the macromolecule. Wherever possible the *constiutional unit, constitutional repeating unit* and *subunits* are named according to the IUPAC nomenclature of organic chemistry [4, 5, 6].

Seniority depends on the atoms, rings, bonds and substituents in a cyclic macromolecule. The order of seniority of subunits is adopted from organic and polymer nomenclature; it is defined in detail elsewhere [1, 2, 4, 5, 6]. The basic order of seniority of subunits is:

heterocyclic units > heteroatoms (according to their position in the periodic table O > S > N > P > Si > B, etc. [4a, 5a, 14]) > carbocyclic units > acyclic carbon units.

Rings for the purpose of determining seniority are those that can be named by conventional nomenclature [4, 5, 6, 15] and that do not contain polymeric units.

Seniority among subunits will be evident from examples that follow. For a concise overview of the principles of seniority of *subunits* see [1].

There is a difference between structure-based nomenclature of irregular polymers as described in [2] and in the present document. In [2], p. 880, it is explicitly stated that seniority of *block*s, which are *constitutional*

For Peer Review Only
IUPAC Provisional Recommendations

repeating units in terms of nomenclature, has not been defined. In the present document, the seniority of a *block* is that of the *constitutional repeating unit*. If the most senior unit in a *cyclic macromolecule* is a *constitutional repeating unit* that has a direction from the *subunit* of highest seniority to that of second highest seniority within the *constitutional repeating unit,* e.g., –[O–CH_2–CH_2]–, this direction automatically defines the direction of citation unless there are two identical *block*s in the *cyclic macromolecule*.

CM-2.2 Conceptual scission

For nomenclature purposes, *polycyclic macromolecules* are broken down to monocyclic structures (cf. CM-4.1 and CM-5.2). By analogy with open chain macromolecules, the structure of a monocyclic macromolecule is described by citing consecutively the names of the subunits as one proceeds around the cycle. In contrast to open chain macromolecules, where naming has to begin at one terminus, in *macrocycles* the sequence of *subunits* could theoretically begin at any point and it is possible to proceed in either direction from that point. Here, rules are provided, which on the basis of seniority, allow unambiguous selection of the correct starting point and identification of the direction to take in the sequence around the cycle. To aid this, conceptual scission is introduced. A conceptual scission of a *cyclic macromolecule* transforms it to an open chain macromolecule that has the most senior *subunit* or *constitutional repeating unit* at the terminus from which naming begins.

CM-2.3 Naming of a cyclic macromolecule or macrocycle

When naming a *cyclic macromolecule* or a *macrocycle* the steps to be followed in order are:

CM-2.3.1 Draw the structure of the *cyclic macromolecule*. Identify the *constitutional repeating units* and minimize the number of *subunits* outside of them (see CM-3.3.1) wherever there is a choice.

Note: Minimization of the number of *subunits* outside the *constitutional repeating unit* in the cyclic macromolecule prevails over citation of a *constitutional repeating* unit beginning with the subunit of highest seniority within that *constitutional repeating* unit (see also examples 8 and 11).

CM-2.3.2 Identify the *main ring* and the *bridges* or macrocyclic substituent (if present) by applying the rules of seniority and conceptual scission.

CM-2.3.3 Name the *cyclic macromolecule* or *macrocycle* according to the rules given in the following sections

CM-3 MONOCYCLIC MACROMOLECULES

CM-3.1 Naming of a monocyclic macromolecule

For naming a monocyclic macromolecule the steps to be followed in order are:

CM-3.1.1 Draw the structure of the monocyclic macromolecule. Identify the *constitutional repeating units* and minimize the number of *subunits* outside them wherever there is a choice.

CM-3.1.2 Irrespective of its location within or outside a *constitutional repeating unit* identify the most senior *subunit* in the *macrocycle* according to rules of organic-chemical [4, 5, 6] and structure-based polymer nomenclature [1, 2].

CM-3.1.3 If the most senior unit is part of a preferred *constitutional repeating* unit the direction within this *constitutional repeating* unit determines the direction of citation.

CM-3.1.4 If the most senior unit is not part of a preferred *constitutional repeating* unit the shortest path to the *subunit* of identical or next lower *seniority* determines the direction of citation. For equivalent *path lengths*, the atoms or units within a *block* (CRU) are senior to the same atoms or units outside the *block*.

CM-3.1.5 Make a *conceptual scission* of the *macrocycle* such that the resulting open chain macromolecule begins with the *constitutional repeating* unit containing the subunit of highest seniority, or with the subunit of highest seniority if that is not part of a *constitutional repeating* unit, and proceed in the direction determined in CM-3.1.3 or in CM-3.1.4.

CM-3.1.6 Name the resulting open chain macromolecule according to the rules established for regular and irregular, single strand macromolecules [1, 2] citing the names of individual subunits reading from left to right, beginning with the most senior *constitutional unit* or *constitutional repeating unit* and proceeding in the direction of the *subunit* next in seniority.

For Peer Review Only
IUPAC Provisional Recommendations

CM-3.1.7 Name the monocyclic macromolecule by adding the prefix “cyclo-” to the structure-based name created in CM-3.1.6 and enclosed within parentheses, square or curly brackets as appropriate.

CM-3.2 Regular monocyclic macromolecules

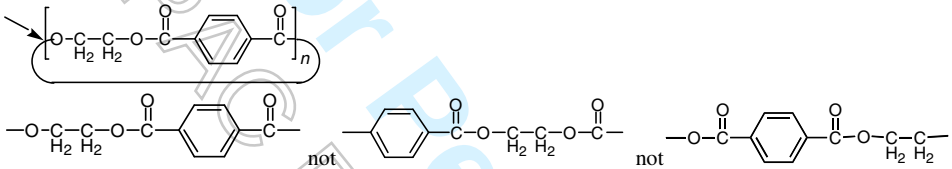
Regular, single-strand, monocyclic macromolecules have a structure such that with a single *conceptual scission* of the *macrocycle* they are converted to an open-chain, regular macromolecule consisting of one *constitutional repeating unit* [1].

The general format for the name of a regular monocyclic macromolecule is **cyclo[poly(constitutional repeating unit)]**.

Note 1: The same format can be used for oligomer nomenclature: cyclo[tetra(constitutional repeating unit)], e.g., cyclo[tetra(oxyethyleneoxyterephthaloyl)]

Note 2: In all of the following examples the open chain structures are those that result from conceptual scission if not stated otherwise.

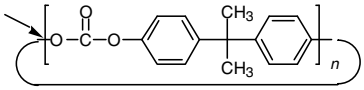
Example 1



Name: cyclo[poly(oxyethyleneoxyterephthaloyl)]

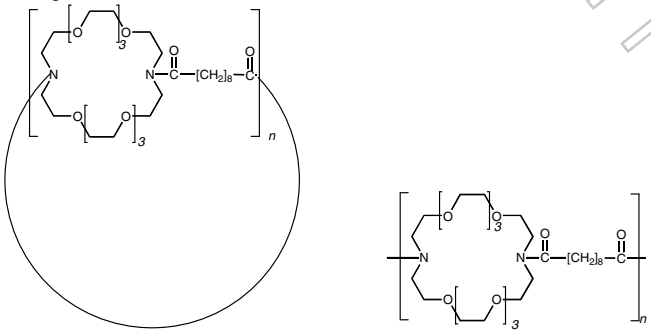
Note: A semi-systematic or trivial name for this polymer is cyclo[poly(ethylene terephthalate)].

Example 2 (taken from [16])



Name: cyclo{poly[oxycarbonyloxy-1,4-phenylene(dimethylmethylene)-1,4-phenylene]}
Alternative correct name: cyclo[poly(oxycarbonyloxy-1,4-phenylenepropane-2,2-diyl-1,4-phenylene)]

Example 3

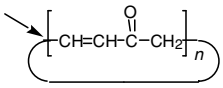


Name: cyclo{poly[(1,4,7,10,16,19,22,25-octaoxa-13,28-diazatriacontan-13,28-diyl)(1,10-dioxodecane-1,10-diyl)]}

For Peer Review Only
IUPAC Provisional Recommendations

Note: The ring containing the nitrogen atoms is not a macrocycle in the sense of this document, as it can be named by nomenclature of organic chemistry. The cyclic polymer (left) is a monocyclic macromolecule while the structure at the right represents a linear macromolecule (see CM-1.9, note 2).

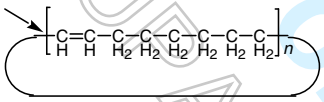
Example 4



Name: cyclo[poly(3-oxobut-1-ene-1,4-diyl)]

Note: The lower locant for the double bond is preferredto the lower locant for the oxo substituent according to seniority rules (p 1929 in [1]).

Example 5 (taken from [17])



Name: cyclo[poly(oct-1-ene-1,8-diyl)]

Note: The name polyoctenamer for the open chain polymer of this example is obsolete and should not be used.

CM-3.3 Irregular monocyclic macromolecules

Single strand, *irregular monocyclic macromolecules* have a structure such that with one conceptual scission of the *macrocycle* they are converted to an irregular, open chain macromolecule.

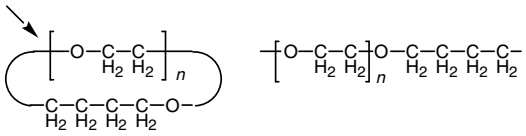
Irregular monocyclic macromolecules are named by prefixing "cyclo-" to the name, in parentheses, square or curly brackets, of the open-chain structure in accordance with the principles of structure-based nomenclature of irregular polymers [2] and the conventions described in CM-2.1 and the principles of section CM-3.1.

A name of a *block* and names of *constitutional units* outside the *block* in the sequence are separated by hyphens in the name of the *macrocycle*.

An irregular polymer or a *block* with unknown distribution of units is written to place its units, separated from each other by a solidus without space before and after it [2], in alphabetical order.

Note: In [2] a dash is used to separate a name of a *block* from names of *constitutional units* outside the *block*. In the present document a hyphen is recommended since hyphens result in more concise names and fulfill the same function. A dash as a special symbol should be reserved for specific cases where a hyphen is inappropriate such as that described in CM-4.7.

Example 6 (taken from [18])



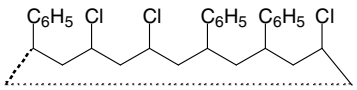
Name: cyclo[poly(oxyethylene)-oxybutane-1,4-diyl]

Note: The oxygen atom within the *constitutional repeating* unit is senior to the oxygen atom outside the *constitutional repeating* unit because the shortest path from one oxygen atom to the next is via the ethylene group within the *block*.

For Peer Review Only
IUPAC Provisional Recommendations

Example 7

A cyclic statistical copolymer of styrene and vinyl chloride joined head-to-tail (a cyclic polymer of example 1.1 from [2])

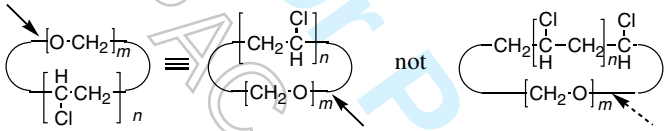


Name: cyclo[poly(1-chloroethylene/1-phenylethylene)]

CM-3.3.1 Minimization of the number of individual subunits

Monocyclic macromolecules are written in such a way that the number of individual *subunits* outside the *constitutional repeating units* is minimized. This requires in some cases that the senior *subunit* in a *constitutional repeating* unit will be located other than at the starting point of the *constitutional repeating unit* [2].

Example 8

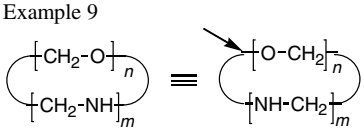


Name: cyclo[poly(oxymethylene)-poly(2-chloroethylene)]
not cyclo[poly(oxymethylene)-methylene-poly(1-chloroethylene)-chloromethylene]

Note 1: Since –[O–CH_2]– is the preferred *constitutional repeating unit* representing a regular *block* in this example it automatically determines the direction of citation.

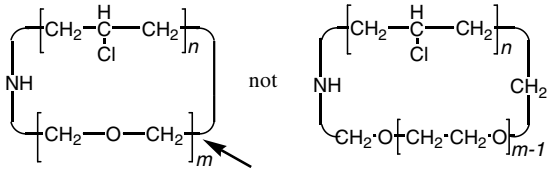
Note 2: Because cyclic macromolecules are ring structures it does not matter which unit is written in the upper left corner of the graphical representation. For naming purposes it may be convenient to write the unit of highest seniority in the upper left corner and proceed clockwise in the order of decreasing seniority.

Example 9



Name: cyclo[poly(oxymethylene)-poly(methyleneimino)]

Example 10



Name: cyclo[poly(methyleneoxymethylene)-imino-poly(2-chloropropane-1,3-diyl)]

Note: This example illustrates that minimization of the number of *constitutional units* takes preference over the order of subunits within a *constitutional repeating* unit, i.e., it can (and often will) prevent the conceptual scission being made at the most senior subunit (for the direction of citation see also CM-3.3.2).

For Peer Review Only
IUPAC Provisional Recommendations

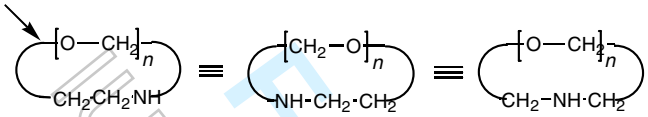
CM-3.3.2 Direction of citation

If the most senior unit is a preferred *constitutional repeating unit* the direction within this unit determines the direction of citation (see example 8). If the most senior unit is not a preferred *constitutional repeating* unit the direction for citation of the units is determined by the shortest *path length* (see CM-1.16) between the most senior unit in a monocyclic macromolecule and the next senior units.

For the case of equal *path lengths* between the unit of highest seniority and that with the next highest seniority, the path selected is the one with a unit of third highest seniority nearest to the unit of highest seniority.

For equivalent *path lengths*, the atoms or units inside a *constitutional repeating unit* are senior to the same atoms or units outside. (see also CM-2.1).

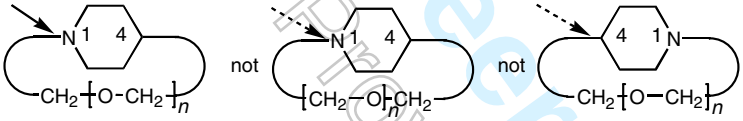
Example 11



Name: cyclo[poly(oxymethylene)-iminoethylene]
not: cyclo[poly(oxymethylene)-methyleneiminomethylene]

Note: Regrouping of the *constitutional repeating* unit of the rightmost structure reduces the number of *subunits* outside the *constitutional repeating* unit from three to two.

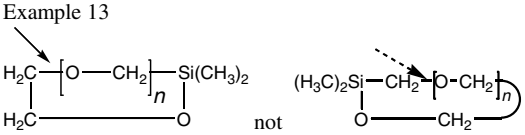
Example 12



Name: cyclo[piperidine-1,4-diyl-poly(methyleneoxy)-methylene]
not cyclo[piperidine-1,4-diyl-methylene-poly(oxymethylene)]
not cyclo[piperidine-4,1-diyl-poly(methyleneoxy)-methylene]

Note: The piperidine ring is the most senior constitutional unit. Because of its fixed numbering and in order to retain the lowest set of locants, the piperidine ring determines the direction of citation.

Example 13

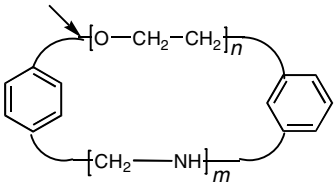


Name: cyclo[poly(oxymethylene)-(dimethylsilanediyl)oxyethylene]
not: cyclo[poly(oxymethylene)-methyleneoxy(dimethylsilanediyl)methylene]

Note: Although oxygen has the highest seniority, followed by silicon, the direction of citation is determined by the smallest number of *subunits* outside of the *constitutional repeating* unit.

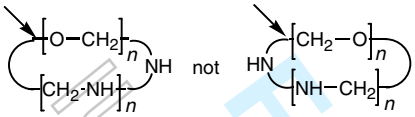
Example 14

For Peer Review Only
IUPAC Provisional Recommendations



Name: cyclo[poly(oxyethylene)-1,3-phenylene-poly(iminomethylene)-1,4-phenylene]

Example 15



Name: cyclo[poly(oxymethylene)-imino-poly(iminomethylene)]
not: cyclo[poly(methyleneoxy)-poly(methyleneimino)-imino]

Note: The direction of the preferred *constitutional repeating* unit determines the direction of citation.

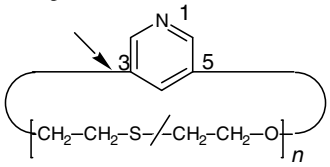
CM-3.3.3 Substituents and locants

Constitutional units containing substituted chain atoms are named as described in detail in [1, 4, 5, 6] and according to the preceding rules.

The name of the each substituent together with its locant are prefixed to the name of the appropriate subunit of the *macrocycle*.

Polyatomic chain or ring units named by nomenclature of organic chemistry such as ethylene, 1,4-phenylene, or pyridine-2,6-diyl retain their own numbering for substitution (see rule 12, p. 1930 [1]). See also examples 12 and 19.

Example 16

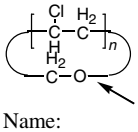


Name: cyclo{pyridine-3,5-diyl-poly[(oxyethylene)/(sulfanediylethylene]}

Note 1: Citation of the name begins with the locant of the atom attached to the point of *conceptual scission*. In this case the lower locant is cited first.

Note 2: Although citation of irregular *block constitutional units* seems to be according to *seniority*, citation follows alphabetical order according to [2].

Example 17

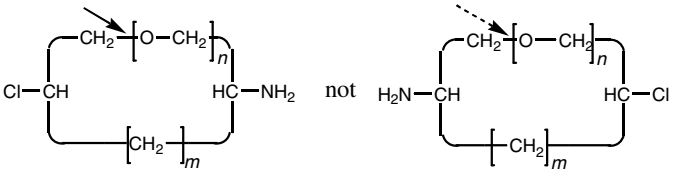


Name: cyclo[oxy-poly(2-chloroethylene)-methylene]
not cyclo[oxymethylene-poly(1-chloroethylene)]

For Peer Review Only
IUPAC Provisional Recommendations

Note: Since the path from oxygen to the chloromethylene group is equal in either direction, the path from oxygen via the methylene group within the *constitutional repeating* unit is preferred. See CM-3.1.4.

Example 18



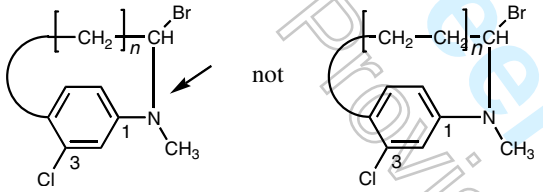
Name: cyclo[poly(oxymethylene)-aminomethylene-poly(methylene)-(1-chloroethylene)]
not: cyclo[poly(oxymethylene)-chloromethylene-poly(methylene)-(1-aminoethylene)]

Note 1: Rule 10, criterion (e) in [1] requires that aminomethylene is senior to chloromethylene.

Note 2: Rule 18, in [1] requires that substituted *subunits* are parenthesized or bracketed; [2] cites these subunits without parentheses or brackets.

Note 3: The unsubstituted version of this example would be named cyclo[poly(oxymethylene)-poly(methylene)].

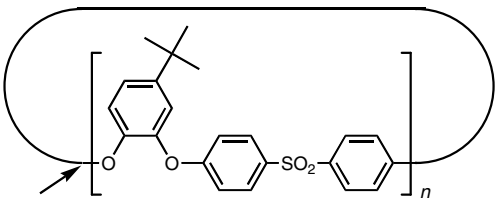
Example 19



Name: cyclo[(methylimino)(3-chloro-1,4-phenylene)-poly(methylene)-(bromomethylene)]

Note: The name cyclo[(methylimino)(3-chloro-1,4-phenylene)-poly(ethylene)-(bromomethylene)] must not be used since in structure-based nomenclature the preferred *constitutional repeating unit* is methylene. (See also footnote, p. 1956 in [1].)

Example 20 (taken from [19])



Name: cyclo{poly[oxy(4-*tert*-butyl-1,2-phenylene)oxy-1,4-phenylenesulfonyl-1,4-phenylene]}

CM-3.3.4 Macrocyclic substituents

A monocyclic macromolecule containing a macrocyclic substituent requires the determination of the senior *macrocycle*.

The *macrocycle* containing the *constitutional (repeating) units* of highest seniority is the senior ring and other *macrocycles* are the substituents (see also CM-4 and CM-5 for *polycyclic macromolecules*). On this basis there are two different way of naming such polymers.

Parent ring nomenclature

IUPAC Provisional Recommendations For Peer Review Only

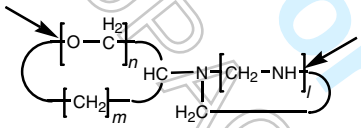
The parent (senior) *macrocycle* is named as described above where the substituents are included in the names of the respective *branch units*. The substituents are named starting from the side of the *branch unit* having units of highest *seniority* (in alphabetical order in irregular macromolecules with unknown sequence of *constitutional units*); name 1 in the following examples.

Ring assembly nomenclature:

Each ring is named separately. *Branch point*s are identified for each ring separately as described in CM-4.3, where the *branch point* of the senior terminal ring has a plain (i.e., unprimed) number, and that of the next ring a primed number. Finally the bond between two rings is specified by the appropriate symbol, i.e., – for a single or = for a double bond between the respective *branch point* locants, all included in square brackets and placed in front of the name, e.g., [B1–B1'] or [B1=B1'], c.f., the valence bond *bridge* description in section CM-4.7; name 2 in the following examples.

The general format for the name according to the alternative nomenclature is
[B1–B1']-cyclo[[B1]ring name 1]-cyclo[[B1']ring name 2]

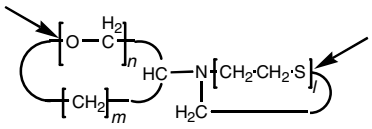
Example 21



Name 1: cyclo[poly(oxymethylene)-{cyclo[poly(iminomethylene)-nitrilomethylene]}methylene-poly(methylene)]

Name 2: [B1–B1']-cyclo[poly(oxymethylene)-[B1]methylene-poly(methylene)]-cyclo[poly(iminomethylene)-[B1']iminomethylene]

Example 22



Name 1: cyclo[poly(oxymethylene)-{cyclo[poly(sulfanediylethylene)-nitrilomethylene]}methylene-poly(methylene)]

Name 2: [B1–B1']-cyclo[poly(oxymethylene)-[B1]methylene-poly(methylene)]-cyclo[poly(sulfanediylethylene)-[B1']iminomethylene]

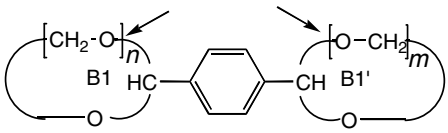
Example 23

Name 1: cyclo[poly(oxymethylene)-oxy{cyclo[poly(oxymethylene)-oxymethanetriyl]methylene}]

Name 2: [B1–B1']-bis{cyclo[poly(oxymethylene)-oxy[B1]methylene]}

Example 24

For Peer Review Only
IUPAC Provisional Recommendations



Name 1: cyclo{poly(oxymethylene)-oxy[({cyclo[poly(oxymethylene)-oxymethanetriyl]}-1,4-phenylene)methylene]}

Name 2: [B1],[B1']-(1,4-phenylene)-bis{cyclo[poly(oxymethylene)-oxy[B1]methylene]}

CM-4 BRIDGED POLYCYCLIC MACROMOLECULES

CM-4.1 Overview

Polycyclic macromolecules (see CM-1.12) are considered to comprise a *main ring* and at least one *bridge* between two atoms of this ring. This section provides rules for the identification of the *main ring*, of *bridges*, *branch points* and *branch units*, and their locants, and how to name each component or segment. *Spiro macromolecules* with a free *spiro union* [5, 6, 13] are not included but will be dealt with in CM-5.

The general format of the name for bridged polycyclic macromolecules is
Bridge(s)-cyclo(main ring)

Note: Treating a *polycyclic macromolecule* in the above manner reduces it to a monocycle, which is why cyclo and not bicyclo or a higher order cyclo-notation appears in the name.

CM-4.2 Selection of the main ring and bridges

The *main ring* is the ring that contains the constitutional units of highest seniority [1, 2, 5, 6]. The remaining parts of the structure are *bridges* connected to the *main ring* with *branch units*.

The *main ring* is named according to the rules described in section 3.

Note: Only *bridges* connecting two *branch points* are allowed. Any connection to an additional *branch point* is considered as a separate *bridge*.

CM-4.3 Locants for branch units

Each *branch unit* in the *main ring*, to which a *bridge* is attached, is identified by the letter "B" to indicate a *branch point*, and by an integer "*n*". *Branch units* are numbered with "*n*" in the order in which they appear in the naming sequence of the *main ring*. This B*n*-expression is preceded, if necessary, by a locant "*l*" that specifies the position within the *constitutional unit* the *branch point* is part of, and a colon.

The representation of these symbols, i.e., the sequence of *branch point* locant *l*, a colon, and the B*n* expression all enclosed within square brackets: [*l*:B*n*] is the locant for the *branch unit*.

In a name, each [*l*:B*n*] expression precedes the name of the *constitutional unit* to which the *branch point* belongs. The square brackets of the representation of this locant do not affect the nesting order of enclosing marks.

Note: Because of the frequent occurrence of letters and numbers that precede ring systems, use of square brackets and a colon are essential to maintain clarity; compare …[3:B1]1*H*-pyrrole-2,5-diyl… with …3-B1-1*H*-pyrrole-2,5-diyl… (cf. example 26).

CM-4.4 Locants for bridges

In the name of a *bridge*, both B*n* expressions for the corresponding *branch units* created during the naming of the macrocyclic *main ring* are cited as locants in ascending order in square brackets **before** the name of the *bridge*. The complete name of a *bridge* thus comprises two B*n* expressions followed by name(s) of the subunit(s) within the *bridge*. When a locant is required to indicate the attachment position within a *bridge*, the locant and a colon precede the corresponding B*n* expression (see example 27).

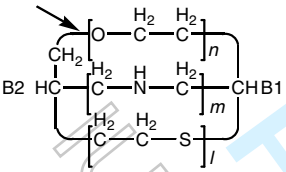
For Peer Review Only
IUPAC Provisional Recommendations

CM-4.5 Naming a bridge

In *bridge* names, *constitutional (repeating) units* are cited in the order in which they appear, beginning at the lower numbered *branch point* and proceeding to the higher numbered *branch point*.

Note: For example, although seniority rules dictate that (iminoethylene) be cited in preference to (ethyleneimino), in bridge names, [B1],[B2]-(ethyleneimino) takes precedence over [B2],[B1]-(iminoethylene). See example 29.

Example 25

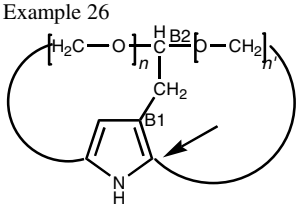


main ring contains the O- and S-containing *constitutional repeating* units
bridge N-containing *block*
branch point 1 [B1]methylene
branch point 2 carbon-1 in an ethylene unit …[1:B2]ethylene…

name for main ring: cyclo[poly(oxyethylene)-[B1]methylene-poly(sulfanediylethylene)-[1:B2]ethylene]
name for the bridge: [poly(methyleneiminomethylene)]
locants for the bridge: [B1],[B2]

Name for the polymer: [B1],[B2]-[poly(methyleneiminomethylene)]-cyclo[poly(oxyethylene)-[B1]methylene-poly(sulfanediylethylene)-[1:B2]ethylene]

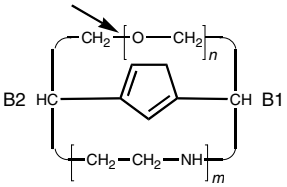
Example 26



Name: [B1],[B2]-(methylene)-cyclo[[3:B1]1*H*-pyrrole-2,5-diyl-poly(methyleneoxy)-[B2]methylene-poly(oxymethylene)]

Note: The first *branch point* is at position 3 within a 1*H*-pyrrole-2,5-diyl unit of the *main ring*.

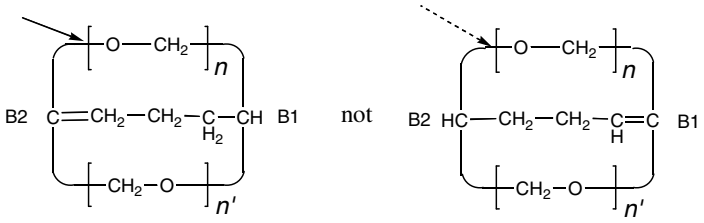
Example 27



Name: [1:B1],[3:B2]-(cyclopenta-1,3-diene-1,3-diyl)-cyclo[poly(oxymethylene)-[B1]methylene-poly(iminoethylene)-[1:B2]ethylene]

Example 28

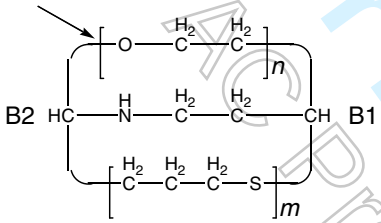
For Peer Review Only
IUPAC Provisional Recommendations



Name: [B1],[B2]-(propan-1-yl-3-ylidene)-cyclo[poly(oxymethylene-[B1]methylene-poly(oxymethylene)-[B2]methylene]

Note: Since in nomenclature of organic chemistry -yl is senior to -ylidene, a lower locant for -yl is preferred if the same locant set would result when both suffixes are considered together. As a result, the first *branch point* should be the one with the single bond, which in turn determines that naming begins with the oxygen atom marked with an arrow.

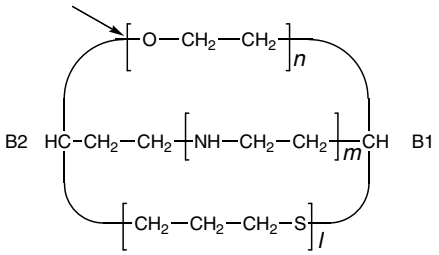
Example 29



Name: [B1],[B2]-(ethyleneimino)-cyclo[poly(oxyethylene)-[B1]methylene-poly(sulfanediylpropane-1,3-diyl)-[B2]methylene]

Note: *Bridge* names used in nomenclature of organic chemistry such as epiminoethano are not used for polymers.

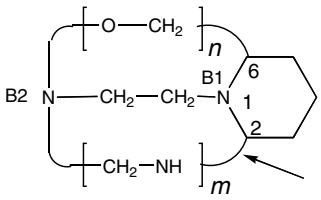
Example 30



Name: [B1],[B2]-[poly(ethyleneimino)-ethylene]-cyclo[poly(oxyethylene)-[B1]methylene-poly(sulfanediylpropane-1,3-diyl)-[B2]methylene]

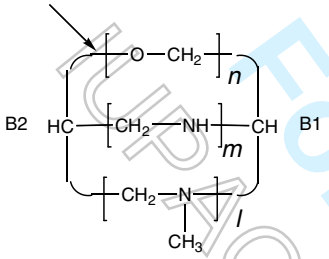
Example 31

IUPAC Provisional Recommendations
For Peer Review Only



Name: [B1],[B2]-(ethylene)-cyclo[[1:B1]piperidine-2,6-diyl-poly(methyleneoxy)-[B2]imino-poly(methyleneimino)]

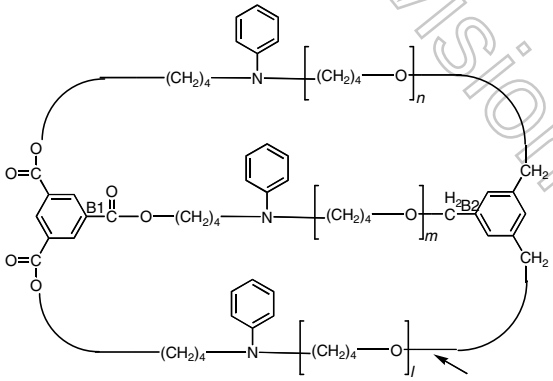
Example 32



Name: [B1],[B2]-[poly(iminomethylene)]-cyclo[poly(oxymethylene)-[B1]methylene-poly[(methylimino)methylene]-[B2]methylene]

Note: A substituted *subunit* in a backbone is senior to the same *subunit* when unsubstituted; thus, –N(Me) – is senior to –NH–, and – $[CH_2–N(Me)]_n$– is senior to – $[CH_2–NH]_n$–.

Example 33 (taken from [20])



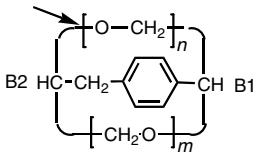
Name: [B1],[B2]-[carbonyl-oxy-butane-1,4-diyl-(phenylimino)-poly(butane-1,4-diyloxy)-methylene]-cyclo[poly(oxybutane-1,4-diyl)-(phenylimino)-butane-1,4-diyl-oxy-[5:B1]isophthaloyl-oxy-butane-1,4-diyl-(phenylimino)-poly(butane-1,4-diyloxy)-methylene-[5:B2]1,3-phenylene-methylene]

CM-4.6 Influence of a bridge on the conceptual scission of the main ring

For *polycyclic macromolecules* having a type of symmetry such that the name of the *main ring* is identical regardless of the direction taken around the ring, path lengths from each senior unit to the senior *constitutional unit* in the *bridge* **must** be considered; the shortest path determines from which *main ring* senior unit the naming starts. See also example 28.

For Peer Review Only
IUPAC Provisional Recommendations

Example 34



Name: [B1],[B2]-(1,4-phenylenemethylene)-cyclo[poly(oxymethylene)-[B1]methylene-poly(oxymethylene)-[B2]methylene]

Note 1: The ethylene two-carbon sequence (with one atom in the *bridge* and the other shared by main chain and *bridge*) must be broken in order to separate the *main ring* atoms from the *bridge* atoms.

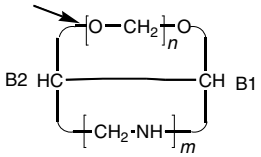
Note 2: The name of the *main ring*, whether it begins from the oxygen atom with the arrow or the oxygen atom of the other block, is cyclo[poly(oxymethylene)-[B1]methylene-poly(oxymethylene)-[B2]methylene]. The *main ring* structure therefore cannot be used to determine from which oxygen atom to begin. Starting from the oxygen atom with the arrow results in the *bridge* name including locants [B1],[B2]-(1,4-phenylenemethylene); starting from the oxygen atom of the other block results in the *bridge* name including locants [B1],[B2]-(methylene-1,4-phenylene). Since a carbocyclic constitutional unit is senior to an acyclic *constitutional unit* [1, 2, 5, 6] the preferred *bridge* name including locants is [B1],[B2]-(1,4-phenylenemethylene). This, in turn, determines that naming of the *main ring* begins at the oxygen atom with the arrow.

CM-4.7 Valence bond bridge

A *bridge* consisting only of a single, double, or (theoretically) triple bond is denoted in square brackets by [B*n*] expressions as locants, between which the appropriate symbol is placed, i.e., [B1–B2], [B1=B2], or [B1≡B2], cited in front of the name of the *main ring* in which the *branch points* are identified as usual (see CM-4.3).

Note: A triple bond as a *bridge* is highly unlikely in a real polycyclic macromolecule.

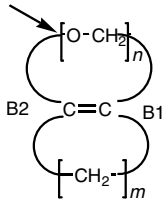
Example 35



Name: [B1–B2]-cyclo[poly(oxymethylene)-oxy-[B1]methylene-poly(iminomethylene)-[B2]methylene]

Note: This example illustrates application of seniority rules [1, 2, 4]; the O–C–O–C–N sequence (clockwise from O with arrow) is preferred to the O–C–O–C–C–N sequence (counter-clockwise from the O not marked with an arrow). Naming therefore proceeds clockwise from the O marked with an arrow.

Example 36



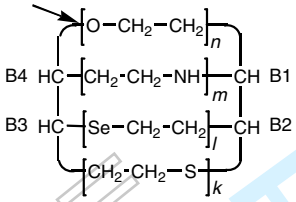
For Peer Review Only
IUPAC Provisional Recommendations

Name: [B1=B2]-cyclo[poly(oxymethylene)-[B1]methylene-poly(methylene)-[B2]methylene]

CM-4.8 Multiple bridges

Multiple *bridges* are named in the order in which the *branch point*s, each identified by the respective [B*n*] expression were assigned during the naming of the *main ring*.

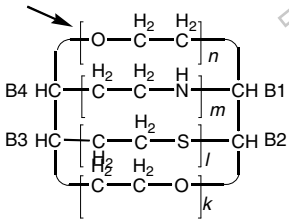
Example 37



Name: [B1],[B4]-[poly(iminoethylene)]-[B2],[B3]-[poly(ethyleneselanediyl)]-cyclo[poly(oxyethylene)-[1:B1][2:B2]ethylene-poly(sulfanediylethylene)-[1:B3][2:B4]ethylene]

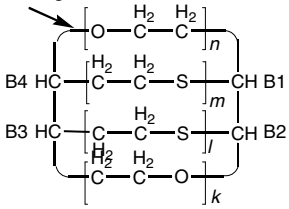
If more than one constitutional unit in the *main ring* can be chosen as the senior unit and the names of the *main ring* thus generated are identical with each other, path lengths from each *main ring* senior unit to the senior *constitutional unit* in each *bridge* must be considered.

Example 38



Name: [B1],[B4]-[poly(iminoethylene)]-[B2],[B3]-[poly(sulfanediylethylene)]-cyclo[poly(oxyethylene)-[1:B1][2:B2]ethylene-poly(oxyethylene)-[1:B3][2:B4]ethylene]

Example 39

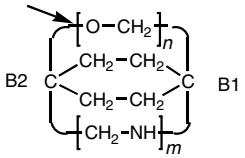


Name: [B1],[B4]-[poly(sulfanediylethylene)]-[B2],[B3]-[poly(sulfanediylethylene)]-cyclo[poly(oxyethylene)-[1:B1][2:B2]ethylene-poly(oxyethylene)-[1:B3][2:B4]ethylene]

or [B1],[B4]:[B2],[B3]-bis[poly(sulfanediylethylene)]-cyclo[poly(oxyethylene)-[1:B1][2:B2]ethylene-poly(oxyethylene)-[1:B3][2:B4]ethylene]

Example 40

For Peer Review Only
IUPAC Provisional Recommendations



Name: [B1],[B2]-(ethylene)-[B1],[B2]-(ethylene)-cyclo[poly(oxymethylene)-[B1]methylene-poly(iminomethylene)-[B2]methylene]

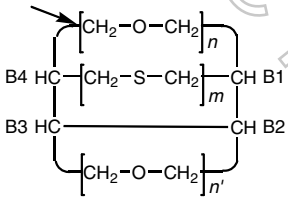
or [B1],[B2]:[B1],[B2]-bis(ethylene)-cyclo[poly(oxymethylene)-[B1]methylene-poly(iminomethylene)-[B2]methylene]

Note: The ring system of this example contains two spiro atoms, which are the *branch points*. Since none of these is a free *spiro union*, the substance must be named as bridged polycyclic macromolecule.

CM-4.9 Seniority of a constitutional unit over valence bond bridge

In *polycyclic macromolecules* containing at least one *bridge* comprising one or more *constitutional units* and at least one *bridge* comprising a valence bond, when more than one *constitutional unit* in the *main ring* can be chosen as the senior unit and the names of the *main ring* thus generated are identical to each other, *bridges* containing *constitutional units* are senior to valence-bond *bridges*.

Example 41



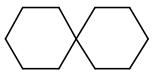
Name: [B1],[B4]-[poly(methylenesulfanediylmethylene)-[B2–B3]-cyclo[poly(methyleneoxymethylene)-[1:B1][2:B2]ethylene-poly(methyleneoxymethylene)-[1:B3][2:B4]ethylene]

Note: In cyclic macromolecules with more than one valence-bond *bridge*, the order of decreasing *seniority* is triple bond > double bond > single bond.

CM-5 SPIRO MACROMOLECULES

CM-5.1 Introduction

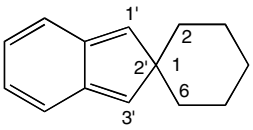
Spiro molecules have a single atom common to two ring systems. In some non-polymeric *spiro compounds* such as spiro[5.5]undecane and others in which all component rings could be named by an established “cyclo...” name, the shared atom is not cited (rule SP-1.1 [13] and R-2.4.3.1 [5]).



spiro[5.5]undecane

In other cases, in which at least one of the rings (or ring systems) has a name not beginning with “cyclo…”, e.g., spiro[cyclohexane-1,2'-indene], the “shared” atom of each *spiro union* is cited twice (rule SP-4.1 [13] and R-2.4.3.3 [5].

For Peer Review Only
IUPAC Provisional Recommendations



spiro[cyclohexane-1,2′-indene]

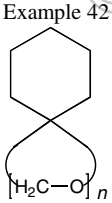
For naming *spiro macromolecules* the second of these methods is recommended as the more general method.

The method described in section 4 for bridged polycyclic macromolecules could also be adapted for spiro macromolecules. This leads to shorter and often easier names for monospiro macromolecules but much more complicated names result for more complex structures when using this method. Both methods are described below. The method using the prefix "spiro" is generally the preferred method.

Only macrocyclic substances containing a free *spiro union*, i.e., those in which the two rings or ring systems sharing the spiro atom are not interconnected by additional *bridge*s, such as in example 40, are named as described in the following sections.

Substances with *spiro unions* to non-macromolecular rings such as cyclohexane, e.g., cyclo[poly(oxymethylene)-cyclohexane-1,1-diyl], example 42, are not regarded as *spiro macromolecules*. These are cyclic macromolecules and named according to the recommendations in CM-3.

Example 42



Name: cyclo[poly(oxymethylene)-cyclohexane-1,1-diyl]

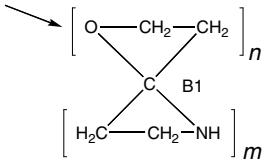
CM-5.2 Bicyclic monospiro macromolecules

Spiro-name: Both rings of a spiro macromolecule containing only two *macrocycles* are named independently according to the recommendations in section 3. The spiro atom is regarded as a *branch point* in each ring and a prime is added to the *branch point* expression referring to the less senior ring. The prefix "spiro" is placed in front of the names of the components, which are cited in order of seniority, enclosed in square brackets regardless of the nesting order. The locants for the spiro atom expressed by the respective *branch point* expression of each of the individual *macrocycles* are placed between the names of the components.

The general format for the name is:
spiro[cyclo(ring name 1)-[B*n*],[B*n*']-cyclo(ring name 2)]
in which [B*n*] and [B*n*'] are the locants for the spiro atom.

Alternative polycyclic macromolecule name: Alternatively the most senior macrocycle may be named according to the recommendations in section 3. The other ring is then regarded as a *bridge* and named according to the recommendations for naming *bridge*s in section 4 and cited in front of the name of the *main ring*. The same locant is cited twice before the name of the *bridge* in order to indicate that both of its ends are attached to the same *branch point* of the *main ring*.

Example 43

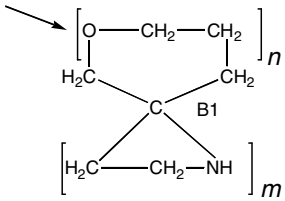


Name: spiro[cyclo[poly(oxyethylene)-[B1]methylene]-[B1],[B1']-cyclo[poly(iminoethylene)-[B1']methylene]]

For Peer Review Only
IUPAC Provisional Recommendations

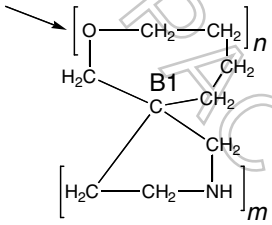
Alternative name: [B1],[B1]-[poly(iminoethylene)]-cyclo[poly(oxyethylene)-[B1]methylene]

Example 44



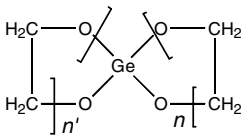
Name: spiro[cyclo[poly(oxyethylene)-[2:B1]propane-1,3-diyl]-[B1],[B1']-cyclo[poly(iminoethylene)-[B1']methylene]]
Alternative name: [B1],[B1]-[poly(iminoethylene)]-cyclo[poly(oxyethylene)-[2:B1]propane-1,3-diyl]

Example 45



Name: spiro[cyclo[poly(oxyethylene)-[3:B1]butane-1,4-diyl]-[B1],[B1']-cyclo[poly(iminoethylene)-[1:B1']ethylene]]
Alternative name: [B1],[B1]-[poly(methyleneiminomethylene)-methylene]-cyclo[poly(oxyethylene)-[3:B1]butane-1,4-diyl]

Example 46 (taken from [21])

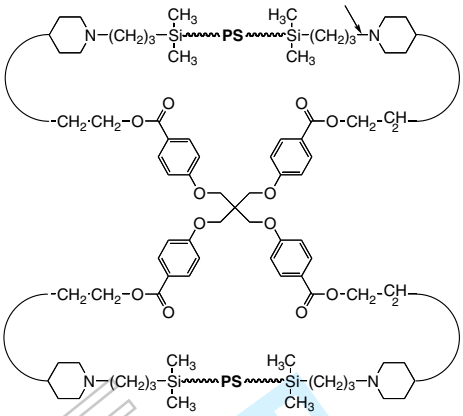


Name: spiro[cyclo[oxy[B1]germanediyl-poly(oxyethylene)]-[B1],[B1']-cyclo[oxy[B1']germanediyl-poly(oxyethylene)]]
or: [B1],[B1']-spirobi[cyclo[oxy[B1]germanediyl-poly(oxyethylene)]]
Alternative name: [B1],[B1]-[poly(oxyethylene)-oxy]-cyclo[poly(oxyethylene)-oxy-[B1]germanediyl]

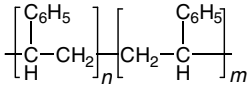
Note: The spirobi[...] method described in SP-2.1 [13] for spiro compounds with two identical spiro-fused rings may also be used, even though the two rings in a spiro macromolecule are most likely of different size.

Example 47 (taken from [22])

For Peer Review Only
IUPAC Provisional Recommendations



PS =



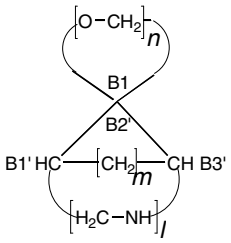
Name: spiro[cyclo[piperidine-1,4-diylethyleneoxycarbonyl-1,4-phenyleneoxy[2:B1]propane-1,3-diyloxy-1,4-phenylenecarbonyloxyethylenepiperidine-4,1-diylpropane-1,3-diyl(dimethylsilanediyl)-poly(1-phenylethylene)-poly(2-phenylethylene)-(dimethylsilanediyl)propane-1,3-diyl]-[B1],[B1']-cyclo[piperidine-1,4-diylethyleneoxycarbonyl-1,4-phenyleneoxy[2:B1']propane-1,3-diyloxy-1,4-phenylenecarbonyloxyethylenepiperidine-4,1-diylpropane-1,3-diyl(dimethylsilanediyl)-poly(1-phenylethylene)-poly(2-phenylethylene)-(dimethylsilanediyl)propane-1,3-diyl]

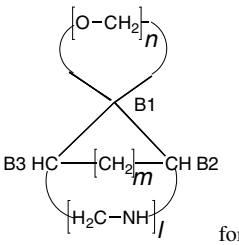
Alternative name: [B1],[B1]-[methyleneoxy-1,4-phenylenecarbonyloxyethylenepiperidine-4,1-diylpropane-1,3-diyl(dimethylsilanediyl)-poly(1-phenylethylene)-poly(2-phenylethylene)-(dimethylsilanediyl)propane-1,3-diylpiperidine-1,4-diylethyleneoxycarbonyl-1,4-phenyleneoxymethylene]-cyclo[piperidine-1,4-diylethyleneoxycarbonyl-1,4-phenyleneoxy[2:B1]propane-1,3-diyloxy-1,4-phenylenecarbonyloxyethylenepiperidine-4,1-diylpropane-1,3-diyl(dimethylsilanediyl)-poly(1-phenylethylene)-poly(2-phenylethylene)-(dimethylsilanediyl)propane-1,3-diyl]

CM-5.3 Spiro macromolecules with additional bridges

If there are additional *bridge*s present in a spiro macromolecule with a free spiro union, the most senior spiro macromolecule that can be named according to section CM-5.2 is selected and named accordingly. *Branch point* expressions are added as appropriate and finally the names of the *bridge*s are placed in front of the name as described in section CM-4.1.

Example 48



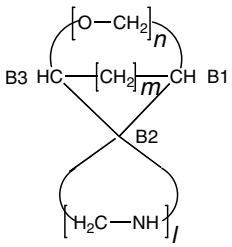


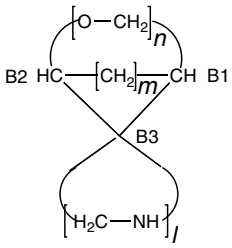
for alternative name

Name: [B1'],[B3']-[poly(methylene)]-spiro[cyclo[poly(oxymethylene)-[B1]methylene]-[B1],[B2']-cyclo[poly(iminomethylene)-[1:B1',2:B2',3:B3']propane-1,3-diyl]]
Alternative name: [B1],[B1]-{[B2],[B3]-[poly(methylene)]-[B2]methylene-poly(iminomethylene)-[B3]methylene}-cyclo[poly(oxymethylene)-[B1]methylene]

Example 49

For Peer Review Only
IUPAC Provisional Recommendations





for alternative name

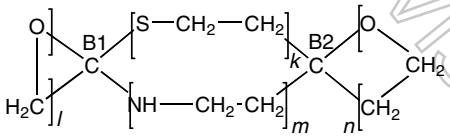
Name: [B1],[B3]-[poly(methylene)]-spiro[cyclo[poly(oxymethylene)-[1:B1,2:B2,3:B3]propane-1,3-diyl]-[B2],[B1']-cyclo[poly(iminomethylene)-[B1']methylene]]
Alternative name: [B1],[B2]-{[B3],[B3]-[poly(iminomethylene)]-[B3]methylene}-cyclo[poly(oxymethylene)-[B1]methylene-poly(methylene)-[B2]methylene]

CM-5.4 Polyspiro macromolecules

For polyspiro macromolecules the principles of CM-5.2 and CM-5.3 are extended in a similar fashion to those published in [13] for non-macromolecular spiro compounds. Briefly, if more than one spiro atom is present in a polymacrocyclic substance a numerical prefix, e.g., di, tri, etc., in front of the prefix "spiro" indicates the number of spiro atoms shared by two macromolecular rings. The component macromolecular rings are cited in order of occurrence beginning with the most senior terminal component. The locants for the spiro atoms expressed by the respective *branch point* expression of each of the individual *macrocycles* are placed between the names of the respective components, with a prime added to the *branch point* expression referring to the second and two primes to those referring to the third component ring, etc.

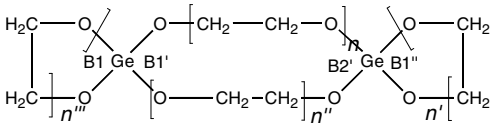
Polyspiro macromolecules with only macrocycles and *bridge*s are rather theoretical. Apart from the difficulty of synthesising such molecules, unambiguous proof of the polyspiro structure would be difficult or even impossible to obtain.

Example 50



Name: dispiro[cyclo[poly(oxymethylene)-[B1]methylene]-[B1],[B2']-cyclo[poly(sulfanediylethylene)-[B1']methylene-poly(ethyleneimino)-[B2']methylene]-[B1'],[B1'']-cyclo[poly(oxyethylene)-[B1'']methylene]]
Alternative name: [B1],[B1]-{[B2],[B2]-[poly(oxyethylene)]-poly(sulfanediylethylene)-[B2]methylene-poly(ethyleneimino)}-cyclo[poly(oxymethylene)-[B1'']methylene]

Example 51 (taken from [23])



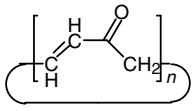
Name: dispiro[cyclo[poly(oxyethylene)-oxy-[B1]germanediyl]-[B1],[B1']-cyclo[poly(oxyethylene)-oxy-[B1']germanediyl-poly(oxyethylene)-oxy-[B2']germanediyl]-[B2'],[B1'']-cyclo[poly(oxyethylene)-oxy-[B1'']germanediyl]]
Alternative name: [B1],[B1]-[poly(oxyethylene)-oxy]-[B2],[B2]-[poly(oxyethylene)-oxy]-cyclo[poly(oxyethylene)-oxy[B1]germanediyl-poly(oxyethylene)-oxy[B2]germanediyl]
or: [B1],[B1]:[B2],[B2]-bis[poly(oxyethylene)-oxy]-cyclo[poly(oxyethylene)-oxy[B1]germanediyl-poly(oxyethylene)-oxy[B2]germanediyl]

For Peer Review Only
IUPAC Provisional Recommendations

CM-6 STEREOISOMERISM

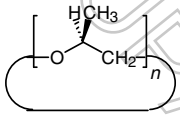
Configuration of stereogenic units in cyclic macromolecules is denoted by conventional stereodescriptors. A more detailed description of possible forms of stereoisomerism will be covered in a future document.

Example 52
E/*Z* isomerism



Name: cyclo{poly[(*E*)-3-oxobut-1-ene-1,4-diyl]}

Example 53
Chiral *constitutional repeating unit*



Name: cyclo(poly{oxy[(1*S*)-1-methylethylene]})

CM-7 REFERENCES

1. IUPAC, "Nomenclature of Regular Single-Strand Organic Polymers", *Pure Appl. Chem.* **74**, 1921 – 1956 (2002); http://www.chem.qmul.ac.uk/iupac/rssop/.

2. IUPAC, "Structure-Based Nomenclature for Irregular Single-Strand Organic Polymers (Recommendations, 1994)", *Pure Appl. Chem.* **66**, 873 – 889 (1994).

3. R. B. Fox "Nomenclature of Macrocyclic Compounds by Sequential Citation", *J. Chem. Inf. Comput. Sci.* **24**, 266 – 271 (1984).

4. IUPAC, *Nomenclature of Organic Chemistry", Sections A, B, C, D, E, F and H, 1979 Edition*, Pergamon Press, Oxford (1979);
(a) rule B-1.1, p. 53; D-1.61, p. 334; Table I, Appendix, p. 459 – 460; (b) Spiro hydrocarbons, p. 37.

5. IUPAC, *A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993*, Blackwell Scientific Publications, Oxford (1993); http://www.acdlabs.com/iupac/nomenclature
(a) Table 3, rule R-2.3.3, p. 42; rule R-9.3, p. 182.

6. IUPAC, "Corrections to *A Guide to IUPAC Nomenclature of Organic Compounds*", *Pure Appl. Chem.* **71**, 1327 – 1330 (1999).

7. Y. Tezuka, H. Oike, *J. Am. Chem. Soc.* **123**, 11570 – 11576 (2001).

8. Y. Tezuka, *Chem. Rec.* **5**, 17 – 26 (2005)

9. (a) IUPAC, *Compendium of Chemical Terminology: IUPAC Recommendations* (The IUPAC 'Gold Book'); 2nd edition. Compiled by A.D. McNaught and A. Wilkinson, Blackwell Science, Oxford, UK (1997); (b) Gold Book online edition: www.iupac.org/publications/compendium/index.html.

10. IUPAC, "Glossary of Basic Terms in Polymer Science", *Pure Appl. Chem.* **68**, 2287 – 2311 (1996).

For Peer Review Only
IUPAC Provisional Recommendations

11. IUPAC, "Extension and revision of the von Baeyer system for naming polycyclic compounds (including bicyclic compounds)", *Pure Appl. Chem.* **71**, 513 – 529 (1999); http://www.chem.qmul.ac.uk/iupac/vonBaeyer/.

12. IUPAC, Nomenclature of rotaxanes (document in preparation)

13. IUPAC, "Extension and Revision of the Nomenclature for Spiro Compounds", *Pure Appl. Chem*. **71**, 531 – 558 (1999); http://www.chem.qmul.ac.uk/iupac/spiro/.

14. IUPAC, *Nomenclature of Inorganic Chemisty, Recommendations 1990*, rule I-2.15.4, p. 31; Table IV, appendix, p. 244; Table VI, appendix, p. 246.

15. IUPAC, "Nomenclature of fused and bridged fused ring systems", *Pure Appl. Chem*. **70**, 143 – 216 (1998); http://www.chem.qmul.ac.uk/iupac/.

16 A. Horbach, H. Vernaleken, K. Weirauch, *Makromol. Chem.* **181**, 111 – 124 (1980); H. R. Kricheldorf, S. Böhme, G. Schwarz, C.-L. Schultz, *Macromol. Rapid Commun.* **23**, 803 – 808 (2002).

17 C. W. Bielawski. D. Benitez, R. H. Grubbs, *Science* **297**, 2041 – 2044 (2002).

18 K. Ishizu, Y. Akiyama, *Polymer* **38**, 491 – 494 (1997).

19 H. R. Kricheldorf, L. Vakhtangishvili, G. Schwarz, G. Schulz, R.-P. Krüger, *Polymer*, **44**, 4471 – 4480 (2003).

20 Y. Tezuka, A. Tsuchitani, Y. Yoshioka, H. Oike, *Macromolecules* **36**, 65 – 70 (2003).

21. H. R. Kricheldorf, S. Rost, *Macromol. Chem. Phys.* **205**, 1031 – 1038 (2004).

22. H. Oike, M. Hamada, S. Eguchi, Y. Danda, Y. Tezuka, *Macromolecules* **34**, 2776 – 2782 (2001).

23. H. R. Kricheldorf, S. Rost, *Macromolecules*, **37**, 7955 – 7959 (2004).

Formatted: Bullets and Numbering

For Peer Review Only
IUPAC Provisional Recommendations