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Terminology and nomenclature for macromolecular rotaxanes and pseudorotaxanes (IUPAC Recommendations 2012)*

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Abstract: This document provides (i) definitions of terms related to macromolecular rotaxanes and macromolecular pseudorotaxanes and (ii) recommendations for naming these macromolecular assemblies. The nomenclature recommendations presented here have been developed by combining the nomenclature rules for the low-molar-mass (low-M) rotaxanes and those for macromolecules (both established in published IUPAC recommendations) in such a way that the developed nomenclature system provides unambiguous names for macromolecular rotaxanes (and pseudorotaxanes), including differentiation among various isomers of these supramolecular assemblies. Application of the nomenclature recommendations is illustrated using examples covering a wide range of structure types of macromolecular rotaxanes and pseudorotaxanes. An Alphabetical Index of Terms and a List of Abbreviations and Prefixes are included.

Keywords: IUPAC Chemical Nomenclature and Structure Representation Division; IUPAC Polymer Division; macromolecular pseudorotaxanes; macromolecular rotaxanes; nomenclature recommendations; polypseudorotaxanes; polyrotaxanes; pseudorotaxane polymers; rotaxane polymers; rules; source-based polymer names; structure-based polymer names.

*Sponsoring bodies: IUPAC Chemical Nomenclature and Structure Representation Division; IUPAC Polymer Division: see more details on p. 2161.

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MRO-0 INTRODUCTION

Supramolecular assemblies consisting of macrocyclic molecules physically threaded by, but not chemically bonded to, a linear molecule or a linear subchain of a molecule capped with bulky end-groups (referred to as "stoppers"), which prevent dethreading of cyclic molecules, are known as "rotaxanes"; similar assemblies, in which one or both stoppers are missing, are referred to as "pseudorotaxanes" [1]. Analogous supramolecular assemblies in which the threading linear chain(s) consist(s) of a linear macromolecule or a linear subchain of a nonlinear macromolecule (knotted structures are excluded) as well as assemblies in which the threaded macrocyclic component(s) are part(s) of a macromolecule are as a class called "macromolecular rotaxanes" or "macromolecular pseudorotaxanes". Materials composed of these assemblies are known as "rotaxane polymers" and "pseudorotaxane polymers" or, shortly but ambiguously (see further, MRO-1.9 and MRO-1.18), "polyrotaxanes" and "polypseudorotaxanes" [2–7]. These polymeric counterparts of rotaxanes and pseudorotaxanes have been reviewed, particularly in 1994 [3], 1999 [4], 2001 [5], 2005 [6], 2007 [7], 2009 [8–10], and 2010 [11].

From the nomenclature point of view, structural differences between macromolecular rotaxanes and macromolecular pseudorotaxanes are not substantial; they consist only in the presence or absence of stopper(s) that is(are) part of the structure of the linear (threading) component(s) of the assembly. Therefore, differentiation between macromolecular rotaxanes and pseudorotaxanes can be used only in a general terminological sense but not as part of a systematic name. Hence, the nomenclature principles for both types of these complex macromolecular assemblies are identical.

The nomenclature recommendations for macromolecular rotaxanes and pseudorotaxanes presented in this document were developed by combining the nomenclature principles for low-molar-mass (low-M) rotaxanes [1] and the nomenclature principles for macromolecules (polymers) established in published IUPAC recommendations [12–19]. Low-molar-mass components of rotaxanes are named according to IUPAC recommendations on organic and inorganic nomenclature [20–22]. These recommendations have been combined in such a way that the developed nomenclature system provides unambiguous names for macromolecular rotaxanes. This has been achieved by specifying their composition as well as location (or the distribution of sites) of threaded rings in these supramolecular assemblies, and through differentiation of the various isomers as precisely as macromolecular nomenclature allows given the structural non-uniformity of polymer molecules. Application of the nomenclature recommendations is illustrated by a series of examples covering a wide range of structure types of macromolecular rotaxanes and pseudorotaxanes.

MRO-1 TERMINOLOGY FOR MACROMOLECULAR ROTAXANES

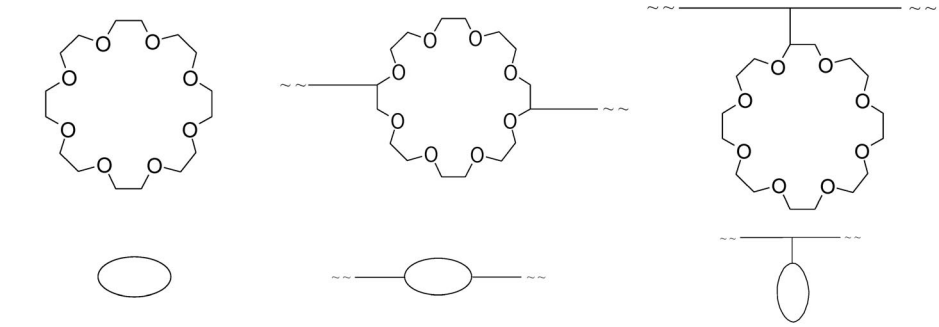
For ease of reference, the terms in this section are listed alphabetically and numbered sequentially. To assist the reader, cross-references to terms also defined in this chapter are denoted in italic typeface. If there are two terms in an entry on successive lines, the second is a synonym.

MRO-1.1 macrocyclic component
recommended abbreviation: MC

Molecule that has at least one ring (cycle) large enough to allow it to be threaded onto a linear subchain of another molecule.

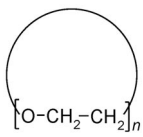
Note 1: To thread a simple hydrocarbon chain such as a polyethylene chain, at least a 24-membered ring is needed.

Note 2: In a *macromolecular rotaxane*, a macrocyclic component can be a discrete macrocyclic molecule or a macromolecule that includes one or more *threadable ring*(*s*). Examples and structure representations of both are shown:



discrete MC (low-molar-mass MC) | macromolecular MC with a main-chain *threadable ring* | macromolecular MC with a side-chain *threadable ring*

Note 3: The literature on *rotaxanes* frequently cites the word "macrocycle" as a contraction of (and an abbreviation for) macrocyclic component. A use of the word "macrocycle" in rotaxane terminology is incompatible with the IUPAC definition of a macrocycle [19,23], which is "a cyclic macromolecule or a macromolecular cyclic portion of a macromolecule":



Such a macrocycle is virtually never used as a macrocyclic component in a rotaxane assembly. Therefore, since the term "macrocycle" is ambiguous, its use should be avoided in the macromolecular rotaxane literature.

Note 4: See also threading component.

MRO-1.2 macromolecular component (of a rotaxane)

Macromolecule that is part of a rotaxane assembly.

Note: A macromolecular component can be a *macrocyclic component* or a *threading component* of a *rotaxane* or both (see MRO-2.4).

MRO-1.3 macromolecular pseudorotaxane

Pseudorotaxane, at least one component of which is a macromolecule.

Note 1: Structural differences between macromolecular pseudorotaxanes and *macromolecular rotaxanes* are neither substantial nor always obvious; macromolecular rotaxanes from which macromolecular component(s) can be dethreaded (i.e., the macromolecular rotaxane becomes a macromolecular pseudorotaxane) under some specific conditions are known [8]. Therefore, the overwhelming majority of definitions concerning macromolecular rotaxanes are fully applicable also to macromolecular pseudorotaxanes after

replacing the word "rotaxane" with the word "pseudorotaxane"; also, nomenclature rules are the same for both of these compound classes.

Note 2: A macromolecular pseudorotaxane in which only one end of a *threading component* is capped with a stopper is sometimes called a "macromolecular semirotaxane".

MRO-1.4 macromolecular rotaxane

Rotaxane, at least one component of which is a macromolecule.

Note 1: A macromolecular rotaxane is composed of a macromolecular chain with either at least one cyclic molecule threaded onto its linear section or at least one linear molecule threaded through its threadable cycle.

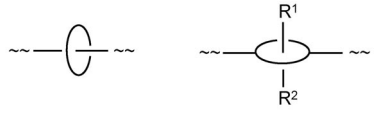
Note 2: *Rotaxane constitutional unit*(*s*) may be located within a specific part of a macromolecular rotaxane: (i) within end-group(s); (ii) within a main chain (see *main-chain macromolecular rotaxane*); (iii) within side chains (see *side-chain macromolecular rotaxane*).

Note 3: See also *regular macromolecular rotaxane* and *rotaxane constitutional repeating unit*.

MRO-1.5 main-chain macromolecular rotaxane

Macromolecular rotaxane in which *rotaxane constitutional units* are exclusively located within the main macromolecular chain.

Note 1: Structure representations of basic constitutional units of main-chain macromolecular rotaxanes are as follows:



where R^1 and R^2 are end-groups of a threading component.

Note 2: See also *side-chain macromolecular rotaxane*.

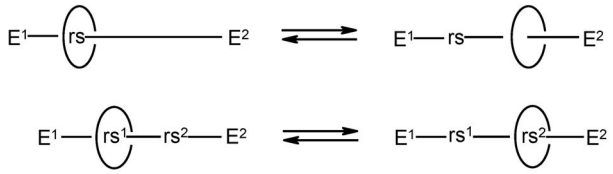
MRO-1.6 main-chain rotaxane polymer (main-chain polyrotaxane)

Polymer composed of macromolecular assemblies that are *main-chain macromolecular rotaxanes*.

Note: See *Note 4* in MRO-1.9 and *Note 2* in MRO-1.18.

MRO-1.7 molecular shuttle

Rotaxane or *pseudorotaxane* comprising a *threading component* upon which is threaded a macrocyclic component that, depending on the conditions, can reside at either a specific *recognition site* on the threading component or away from any recognition site (ROT-1.6 [1]).



Motion schemes for two basic types of molecular shuttles
(rs, rs^1 and rs^2 stand for recognition sites, E^1 and E^2 for end-groups of the macromolecular threading component)

Note: *Rotaxane polymers* composed of molecules that contain units of the molecular shuttle type are a special class of functional polymers [24,25].

MRO-1.8 pseudorotaxane

Rotaxane-like molecular assembly in which the *threading component*(*s*) has(have) ends small enough to permit threading or dethreading of the *macrocyclic component*(*s*) (ROT-1.4 [1]).

Note 1: The stability of a pseudorotaxane may arise not only from spatially hindered dethreading of its components, but also from interaction between threading and macrocyclic components, e.g., donor–acceptor or electrostatic or coordination (see *recognition site*).

Note 2: Pseudorotaxanes in which only one end of a threading component is capped with a stopper are sometimes called "semirotaxanes" or "half-capped pseudorotaxanes".

MRO-1.9 pseudorotaxane polymer (polypseudorotaxane)

Polymer composed of macromolecules that are *macromolecular pseudorotaxanes*.

Note 1: A narrower definition of pseudorotaxane polymer as a *rotaxane polymer* without bulky end-groups preventing dethreading of cyclic molecules has been published in ref. [2].

Note 2: A pseudorotaxane polymer in the molecule of which only one end of a *threading component* is capped with a stopper is sometimes called "semirotaxane polymer" or "polysemirotaxane".

Note 3: Though the synonym "polypseudorotaxane" currently appears in the literature, its use is discouraged. This term, from a purely semantic point of view, implies many threaded rings, a polymer formed from a *pseudorotaxane*, while a molecule of a pseudorotaxane polymer can comprise a single threaded ring.

Note 4: Pseudorotaxane polymers are sometimes referred to in the literature as "pseudopolyrotaxanes". Use of this term is strongly discouraged owing to possible misinterpretation as "pseudopolymeric" or "pseudomacromolecular" *rotaxane*.

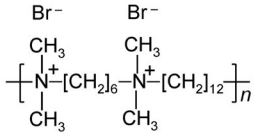
MRO-1.10 recognition site
recommended abbreviation: rs

Part of the *threading component*, at which a *macrocyclic component* of a rotaxane prefers to locate (revised ROT-1.5 [1]).

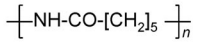
Note 1: A recognition site immobilizes a macrocyclic component on the basis of the host–guest noncovalent interactions typical of supramolecular chemistry, while a couple of *stop-*

pers sterically demarcate a region in which a macrocyclic component can more or less freely move.

Note 2: Typical examples of recognition sites in a *macromolecular rotaxane* are ionic or polar main-chain groups together with neighboring hydrophobic segments acting synergically in the molecular recognition, such as quaternary ammonium groups and amide groups in the main chains of ionenes [2,26] and polyamides [2], respectively:

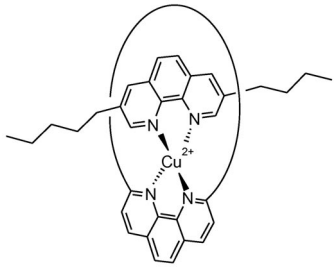


poly[(dimethyliminio)hexane-1,6-diyl-(dimethyliminio)dodecane-1,12-diyl dibromide]



poly[imino(1-oxohexane-1,6-diyl)]
poly(hexano-6-lactam)
poly(ε-caprolactam)
polyamide 6 (trivial name)

Another example is a coordination recognition site in which binding between macrocyclic and threading components is mediated by a metal ion [27]:



Note 3: In the schematic representation of a *macromolecular rotaxane*, different recognition sites are distinguished by rs^i where i = 1, 2, ... is the order number of the rs counting from the beginning to the end of the oriented threading component:

rs¹-MC *rs²-MC*

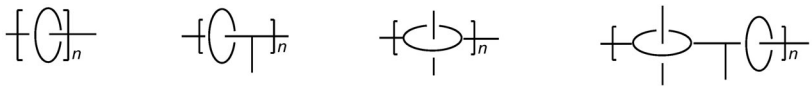
Macrocyclic component (MC) that can associate with various recognition sites (rs) of the same *threading component*: principle of the *molecular shuttle*

The italicized abbreviation rs^i is used as a prefix assigning the actual position of a macrocyclic component on a particular threading component. In this structural descriptor, the superscript numerals are also italic.

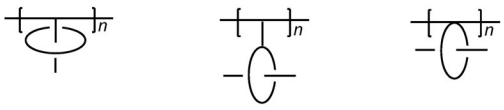
MRO-1.11 regular macromolecular rotaxane

Macromolecular rotaxane, the structure of which essentially comprises the repetition of a single constitutional unit of the *rotaxane* type, referred to as the *rotaxane constitutional repeating unit*, *rot-CRU*, with all units connected identically with respect to directional sense.

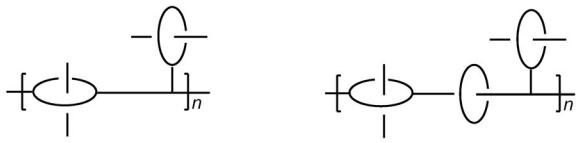
Note: Structure representations of typical regular macromolecular rotaxanes are:



Schematic representations of some types of regular *main-chain macromolecular rotaxanes*



Schematic representations of some types of regular *side-chain macromolecular rotaxanes*



Schematic representations of mixed types (*main-chain*/*side-chain*) of *macromolecular rotaxanes*

MRO-1.12 rotaxane

Complex molecular assembly comprising at least one molecule with a linear section threaded through at least one macrocyclic part of another or the same molecule, and having end-groups large enough to prevent dethreading of the *macrocyclic component* [1].

MRO-1.13 rotaxane constitutional repeating unit
rotaxane CRU
recommended abbreviation: *rot*-CRU

Constitutional repeating unit (CRU) that has a *rotaxane* structure.

Note: Constitutional repeating unit is the smallest constitutional unit the repetition of which constitutes a regular macromolecule, a regular oligomer molecule, a regular block, or a regular chain [23].

MRO-1.14 rotaxane constitutional unit
rotaxane CU
recommended abbreviation: *rot*-CU

Constitutional unit (CU) that has a *rotaxane* structure.

Note: Constitutional unit is an atom or group of atoms (with pendant atoms or groups, if any) comprising a part of the essential structure of a macromolecule, an oligomer molecule, a block, or a chain [23].

MRO-1.15 rotaxane end-unit
recommended abbreviation: *rot*-EU

Constitutional unit of a *macromolecular rotaxane* consisting of an end-group of its macromolecular component and a complementary *threading* or *macrocyclic component*.

Note: End-group is a constitutional unit that is an extremity of a macromolecule or oligomer molecule. An end-group is attached to only one constitutional unit of a macromolecule or oligomer molecule [23].

MRO-1.16 rotaxane monomer

Monomer that is a *rotaxane*.

Note: For a definition of monomer, see ref. [23].

MRO-1.17 rotaxane monomeric unit
rotaxane monomer unit
rotaxane MU
recommended abbreviation: *rot*-MU

Monomeric unit (monomer unit, mer) that has a *rotaxane* structure.

Note: For a definition of monomeric unit (MU), see ref. [23].

MRO-1.18 rotaxane polymer
polymeric rotaxane
(polyrotaxane)

Polymer composed of macromolecules that are *macromolecular rotaxanes*.

Note 1: A narrower definition of rotaxane polymer: "Polymer composed of macromolecules consisting of cyclic molecules threaded by a linear macromolecule that is eventually capped with bulky end-units preventing dethreading of cyclic molecules" has been published in ref. [2].

Note 2: Though the synonym "polyrotaxane" currently appears in the literature, its use is discouraged. This term, from a purely semantic point of view, namely, implies many threaded rings, i.e., a polymer formed from a *rotaxane*, while a molecule of a rotaxane polymer can comprise a single threaded ring.

MRO-1.19 side-chain macromolecular rotaxane

Macromolecular rotaxane in which *rotaxane constitutional units* are located exclusively in side chains of the macromolecule.

Note: Typical structure representations of the most common side-chain rotaxane constitutional units are as follows:

where R^1 and R^2 are end-groups of a *threading component* and R is a capping group of a side chain.

MRO-1.20 side-chain rotaxane polymer
(side-chain polyrotaxane)

Polymer composed of macromolecular assemblies that are *side-chain macromolecular rotaxanes*.

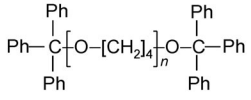
Note: See *Note 4* in MRO-1.9 and *Note 2* in MRO-1.18.

MRO-1.21 stopper

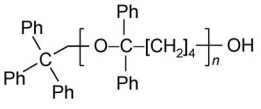
Group bulky enough to prevent dethreading of a given *macrocyclic component* from a *threading component* or its translocation to another linear section of the threading component.

Note 1: A stopper can be positioned at the end of the whole chain: end-group stopper, or along it: internal stopper. The latter is often a part of a *rotaxane constitutional repeating unit*.

Note 2: Whether a group functions as a stopper or not depends on the size of the macrocyclic component. Accordingly, when stoppers are mentioned, the macrocyclic component should also be mentioned. Examples of stoppers for β-cyclodextrin macrocyclic component are $–CPh_3$ end-groups or $–CPh_2–$ groups included in constitutional repeating units:



Macromolecular threading component with end-group stoppers (-CPh_3)



Macromolecular *threading component* with internal *stoppers* (-CPh_2-) that are each a part of a CRU and an end-group *stopper*

Note 3: A more complex threading component may contain several linear sections due to the presence of branch points or internal large groups that prevent movement of macrocyclic components from one linear section to another.

MRO-1.22 threadable ring
threadable cycle

Key part of a *macrocyclic component*: molecular ring (cycle) large enough to be threaded onto a linear subchain of a *threading component*.

Note: A threadable ring (cycle) should be distinguished from other smaller, non-threadable rings within a complex macrocyclic component, such as benzene, cyclooctane, or similar rings.

MRO-1.23 threading component
recommended abbreviation: TC

Molecule with at least one linear section onto which at least one *macrocyclic component* is threaded.

Note 1: In the context of *macromolecular rotaxanes*, a threading component may be either a macromolecular chain with a linear section or a linear low-M molecule if a macromolecular component includes *threadable ring*(*s*).

Note 2: For a *rotaxane*, the word "linear" is to be interpreted broadly. The linear section of a threading component can be either an unbranched chain or a linear subchain of a

branched chain or a network chain, or it can be a linear chain or subchain that includes small cyclic parts that do not prevent threading through a macrocyclic component.

MRO-2 NOMENCLATURE FOR MACROMOLECULAR ROTAXANES

MRO-2.1 Names for macromolecular rotaxanes and macromolecular pseudorotaxanes

Macromolecular rotaxanes and macromolecular pseudorotaxanes are named according to the same nomenclature principles using the same connective *-rotaxa-* to join the names of the threading and macrocyclic components.

Structural differences between macromolecular rotaxanes and pseudorotaxanes are not substantial; they differ only in the presence or absence of stopper(s). Therefore, the term "macromolecular pseudorotaxane" can be used exclusively in general terminological sense and not as part of a systematic name.

MRO-2.2 Sources of the nomenclature for macromolecular rotaxanes

Since macromolecular rotaxanes possess structural features of both macromolecules and rotaxanes, the nomenclature for macromolecular rotaxanes is a combination of the nomenclatures for rotaxanes [1] and macromolecules [12–18].

- IUPAC nomenclature for rotaxanes [1] recommends that the name(s) of the threading component(s), TC(s), should precede the name(s) of the macrocyclic component(s), MC(s). Basic **generic formats of systematic names for rotaxanes** are

  [*n*]{[*t*][name for TC]-*rotaxa*-[*m*][name for MC]}

  for a rotaxane composed of independent TC and MC molecules and

  [*n*]{*rotaxa*-[name of molecule(s)]}

  for a rotaxane composed of molecule(s), each possessing both TCs and MCs, wherein n, t, and m are positive integers that define:

$n = t + m$	the total number of independent components in a rotaxane species;
t	the number of TCs in a rotaxane species;
m	the number of MCs in a rotaxane species.

- IUPAC nomenclature for macromolecules [12–18] recommends two basic **generic formats of systematic names for macromolecules:**

  α-(name for E^1)-ω-(name for E^2)-poly(name of CRU^1/name of CRU^2/...)

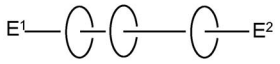
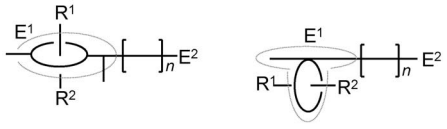
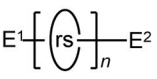
  for the *structure-based name* of a macromolecule (CRU^i stands for *i*-th constitutional repeating unit and E^1 and E^2 for end-groups [12,23]) and

  α-(name for E^1)-ω-(name for E^2)-poly(name of monomer^1-*conn*-monomer^2-*conn*-...)

  for the **source-based names** of a macromolecule (*-conn-* is connective such as *-co-*, *-alt-*, *-stat-*, *-ran-* [13] characterizing the type of the distribution of monomeric units [23] along the chain of a copolymeric macromolecule).

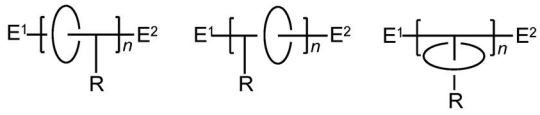
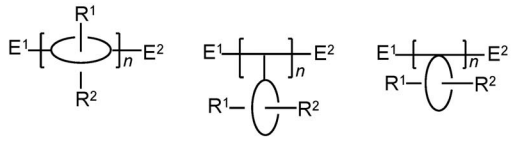
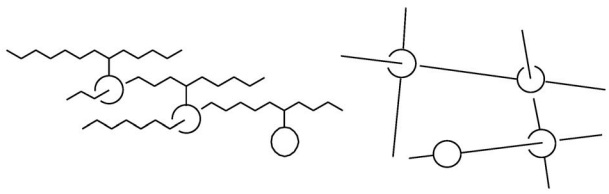
In the present nomenclature for macromolecular rotaxanes the above two nomenclature systems are combined in such a way that the new nomenclature provides unambiguous names for macromolecular rotaxanes that specify the composition, number, and location or type of distribution of rotaxane units in these supramolecular assemblies as precisely as it allows the macromolecular nomenclature that

Table 1 Generic Types of macromolecular rotaxanes and corresponding **Generic Name Formats** (end-units are omitted in the formats except for Type 2 macromolecular rotaxanes); MC stands for macrocyclic component, TC for threading component; E^i for end-group(s) of a macromolecular component and R^i for end-group(s) of a low-M TC and capping group of a side chain; *rot*-EU for rotaxane end-unit, CRU for constitutional repeating unit, *rot*-CRU for rotaxane constitutional repeating unit; MU for monomeric unit and *rot*-MU for rotaxane monomeric unit.

Type	Generic structure	Key structural features
1	*Macromolecular rotaxane consists of a single linear macromolecule(s) (TC) without an internal stopper threaded through one or more MC(s) distributed in an unknown way along the macromolecule*	
		Position(s) of MC(s) is(are) not known or is(are) variable with time.
	[*n*]{[*t*][name of macromolecule]-*rotaxa*-[*m*][name(s) of MC(s)]}	
2	*Exclusively end unit(s) of macromolecular rotaxane possess(es) the rotaxane structure; generic name format is:* **α-(name of *rot*-EU^1 or E^1)-ω-(name of *rot*-EU^2 or E^2)(name of the main part of the macromolecule)**	
2a		Macromolecular component contains end-group(s) with at least one linear segment (TC); at least one is threaded through an MC. Note that E^1 includes the linear end segment up to brackets (branch point of CRU).
	α-[*n*]{[(name of E^1)-*rotaxa*-[*m*](name of MC)]}-ω-(name of E^2)(name of the main part of the macromolecule) (the order of end-groups (end units) is given by the correct orientation of CRU)	
2b		Macromolecular component contains at least one end-group with threadable ring (MC), through which is threaded a short linear molecule (TC). Note that E^1 includes the part of the macromolecular component demarcated by the grey dashed curve.
	α-([*n*]{[*t*][name of TC]-*rotaxa*-[*m*][name of E^1]})-ω-(name of E^2)(name of the main part of the macromolecule) (the order of end-groups (end units) is given by the orientation of CRU)	
3	*Regular macromolecular rotaxane that is fully described by a rotaxane CRU, rot-CRU; general name format is:* **poly(name of *rot*-CRU) or poly(name of *rotaxane monomer*)**	
3a		Macromolecular part of the rotaxane CRU is a linear segment (TC) comprising recognition site(s), rs, with non-covalently bound MC(s) threaded onto the segment.
	poly([*n*]{[name of macromolecular part of *rot*-CRU]-*rotaxa*-[*m*][name of MC]}) *t* = 1 by default **poly([*n*]{[name of monomer]-*rotaxa*-[*m*][name of MC]})**	

(*continues on next page*)

Table 1 (*Continued*).

Type	Generic structure	Key structural features
3b		Macromolecular part of the rotaxane CRU contains linear segments (TC) demarcated by stopper(s); MC(s) is(are) uniformly threaded onto given linear segment(s) of the CRU.
	poly[(*locants for MC*)-[*n*]{[name of macromolecular part of *rot*-CRU]-*rotaxa*-[*m*][name of MC]}] **poly[(*locants for MC*)-[*n*]{[name of monomer]-*rotaxa*-[*m*][name of MC]}]**	
3c		Macromolecular part of the rotaxane CRU contains main-chain, or side-chain, or cardo-side-chain threadable cycle(s) (MC), through which is(are) threaded short linear molecule(s) (TC).
	poly([*n*]{[*t*][name of TC]-*rotaxa*-[name of macromolecular part of CRU]}) **poly([*n*]{[*t*][name of TC]-*rotaxa*-[name of monomer]})**	
4	*Macromolecular rotaxane chain comprises at least two types of CRUs (or monomeric units, MUs), of which at least one has the rotaxane structure; CRUs (MUs) are distributed along the chain irregularly according to a certain statistical law*	
4a	$\left(\left[rot\text{-CRU}\right]_x / \left[\text{CRU}\right]_y\right)_n$ $\left(\left[rot\text{-MU}\right]_x / \left[\text{MU}\right]_y\right)_n$	Macromolecular rotaxane comprises one type of rotaxane CRU (*rot*-CRU) (e.g., any of the structures **3a** to **3c**) or rotaxane MU (*rot*-MU) and one type of normal (non-rotaxane) CRU (MU).
	poly[(name of *rot*-CRU)/(name of normal CRU)] **poly[(name of *rot*-monomer)-*co*-(name of normal monomer)]**	
4b	$\left(\left[rot\text{-CRU}^1\right]_x / \left[rot\text{-CRU}^2\right]_y / \left[rot\text{-CRU}^3\right]_z / \cdots\cdots\right)_n$ $\left(\left[rot\text{-MU}^1\right]_x / \left[rot\text{-MU}^2\right]_y / \left[rot\text{-MU}^3\right]_z / \cdots\cdots\right)_n$	Macromolecular rotaxane comprises two or more kinds of rotaxane CRUs (*rot*-CRU) or two or more kinds of rotaxane monomeric units (*rot*-MU).
	poly[(name of *rot*-CRU^1)/(name of *rot*-CRU^2)/(name of *rot*-CRU^3)/.....] **poly[(name of *rot*-monomer^1)-*co*-(name of *rot*-monomer^2)-*co*-(name of *rot*-monomer^3)/.....]**	
5	*Macromolecular rotaxane consists exclusively of macromolecules each comprising at least one threadable ring (MC) and at least one linear segment (TC) capable of threading through an MC*	
		Each macromolecule is locked within a rotaxane assembly by its linear section threaded through a threadable ring of another macromolecule, or by its threadable ring threaded onto a linear section of another macromolecule, or by both.
	[*n*]{*rotaxa*-[name(s) of macromolecule(s)]}	

is almost always burdened with some uncertainty owing to molecular non-uniformity of macromolecules.

MRO-2.3 Use of systematic and non-systematic names and abbreviations

(a) Low-molar-mass threading and macrocyclic components of macromolecular rotaxanes should each be named according to IUPAC recommendations for the naming of organic or other corresponding classes of chemical structures [1,20–22].

(b) Macromolecular threading and macrocyclic components may be named by either source-based [12–15] or structure-based [16–19] nomenclature systems. Structure-based nomenclature is preferred, but source-based nomenclature is acceptable.

(c) Systematic names for macromolecular rotaxanes are usually long, complex, or both. Therefore, the use of short and trivial names, or abbreviations, for low-molar-mass and macromolecular components is permitted, provided no ambiguity is thereby introduced. However, note that such names are less preferred than systematic names.

Note 1: The IUPAC-preferred name for a macromolecular rotaxane is the name composed of the structure-based name for the macromolecular component and preferred IUPAC name for the low-molar-mass component of the macromolecular rotaxane.

Note 2: As a rule, if the source-based name or a trivial name or an abbreviation is used for naming the macromolecular component, it is combined with a short name of the low-molar-mass component.

MRO-2.4 Generic types of and generic name formats for macromolecular rotaxanes

A summary of fundamental generic types of macromolecular rotaxanes and the corresponding generic name formats is presented in Table 1.

Note 1: For a macromolecular rotaxane, the specified numbers (t or m or both) of components must usually be treated as a statistical ratio if another is not explicitly stated or can be deduced from the specific structure of components. This is not the case for macromolecular rotaxanes in which rotaxane constitutional unit(s) is(are) the end-unit(s) only.

Note 2: If the number t or $m = 1$, it may (but need not) be omitted.

Note 3: If the numbers t or m, and thus also $n = t + m$, are unknown, they should be cited as indefinite prefixes [t] or [m], or n should be cited as a partly indefinite prefix, e.g., [1 + m] or [t + 1], see Section MRO-3.1, Examples 2 and 4.

Note 4: IUPAC [18, R-0.1.5.1] recommends the nesting order of enclosing marks—parentheses, square brackets, or braces—in chemical names as follows: {[( )]}. However, because rotaxane names are often complex, fixed types of enclosing marks for names of rotaxane components and for the entire rotaxane name are recommended here (like for low-M rotaxanes and several other compound classes). Note that the system of enclosing marks presented in this document is specific to the nomenclature of rotaxanes.

MRO-2.5 Guidelines for the construction of names for macromolecular rotaxanes

The complete name of a macromolecular rotaxane is generated by the following steps:

1. Identify the TCs and MCs and determine the structure type of the macromolecular rotaxane according to Table 1.

2. Create the name(s) for the low-molar-mass component(s) of the macromolecular rotaxane and enclose the name(s) in square brackets: [low-M component].
3. Create the name(s) for the end-groups of the macromolecular component (if known). These names are almost always structure-based names.
4. If the end-group is a part of the rotaxane end-unit, enclose its name in square brackets: [end-group].
5. Create the name(s) of the rotaxane end-unit(s) according to one of the generic name formats.
6. Select the macromolecular nomenclature system (structure- or source-based).

7a. *Structure-based macromolecular nomenclature selected*:

- create the name(s) for constitutional repeating unit(s) (CRU(s)) of the macromolecular component;
- enclose in square brackets names of CRU(s) that is(are) part(s) of the rotaxane CRU(s): [CRU];
- create names of rotaxane CRU(s) by assembling integers [*t*], [*m*], and [*n*] and names of the relevant [CRU] and [low-M component] according to the relevant generic name format for the *rot*-CRU:

  [*n*]{[CRU]-*rotaxa*-[*m*][low-M component]} if [CRU] is TC and [low-M component] MC;

  [*n*]{[*t*][low-M component]-*rotaxa*-[CRU]} if [low-M component] is TC and [CRU] MC;

- if a *rot*-CRU is of the Type 3b or 3c, create locants for low-M components that are MCs (see MRO-2.6 and Examples 8–10);
- create the name of the macromolecular rotaxane according to the generic name format (Table 1) for the identified type of macromolecular rotaxane; and
- if possible or needed, complete the obtained name with the names of end-groups or rotaxane end-units or with both using the format shown in Table 1 for the Type 2 macromolecular rotaxanes.

7b. *Source-based macromolecular nomeclature selected*:

- create the name(s) for monomer(s) from which the macromolecular part of macromolecular rotaxane was or can be prepared;
- enclose in square brackets name(s) of the monomer(s) that is(are) part(s) of rotaxane monomer(s): [monomer];
- create names of rotaxane monomer(s) by assembling integers [*t*], [*m*], and [*n*] and names of the relevant [monomer] and [low-M component] according to the generic name format for rotaxanes:

  [*n*]{[monomer]-*rotaxa*-[*m*][low-M component]} if [monomer] is TC and [low-M component] MC;

  [*n*]{[*t*][low-M component]-*rotaxa*-[monomer]} if [low-M component] is TC and [monomer] MC;

- if a rotaxane monomer is, upon polymerization, transformed into *rot*-MU of the structure Type 3b, determine locants for low-M component that is MC (see MRO-2.6);
- create the name of the macromolecular rotaxane according to the identified generic name format (Table 1); and
- if possible or needed, complete the obtained name with the names of end-groups or rotaxane end-units or with both using the format shown in Table 1 for the Type 2 macromolecular rotaxanes.

MRO-2.6 Isomerism of macromolecular rotaxanes

Isomerism of rotaxanes, including macromolecular rotaxanes, exclusively describes different arrangements that can be formed by assembling the same rotaxane components; it does not deal with isomerism of the components, which is included implicitly (see [1], Section ROT-5). The rotaxane isomers can differ in:

a) positions of MCs at linear sections of a complex TC or positions of TCs at several macrocyclic parts of a complex MC, or both;
b) the order in which several nonequivalent MCs are positioned at the same linear section of a TC;
c) the position of an MC at different recognition sites within the same linear section of a TC; and
d) the arrangement of unsymmetrical rotaxane components with respect to each other (topologic isomerism).

Recommendations concerning the topologic isomerism of macromolecular rotaxanes are not presented in this document because these rules are still under preparation for low-molar-mass rotaxanes [1].

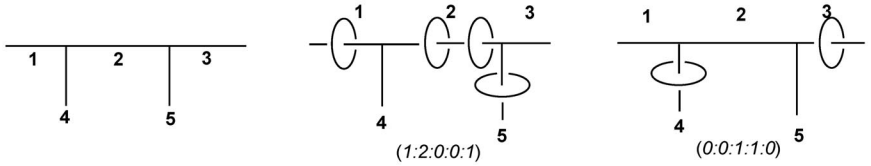
MRO-2.6.1 Isomerism: Positions of various macrocyclic components threaded on several linear sections

If an irregular macromolecule [12,23] component or CRU of a macromolecular component has several linear potentially threadable sections, the occupancy of the sections with MCs is addressed by a composed prefix generated in a manner similar to that described for low-M rotaxanes [1]. For this purpose, it is necessary to assign the order numbers to the linear sections starting from the left end of the correctly oriented CRU (or macromolecule) first going along the main-chain part of the CRU (main chain of macromolecule) and then continuing by numbering side chains, again from the left to the right end of the CRU (macromolecule) as shown below.

The rotaxane-isomer locant for the species with uniform MCs consists of a series of numbers separated by colons:

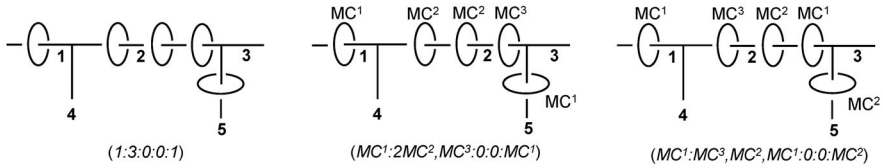
- the position of the number in the series specifies the order number of the linear section;
- the number value specifies the number of MCs threaded onto the particular linear section.

The systems of numbering the linear sections and examples of rotaxane prefixes for species with uniform MCs are:



a) numbering of linear sections *b)* examples of assignments of rotaxane locants

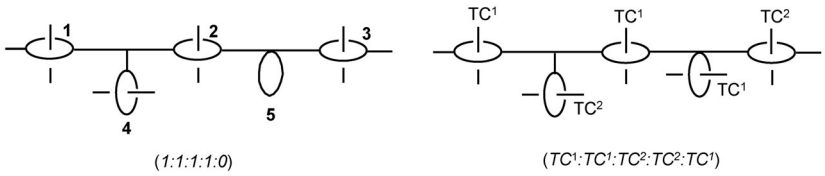
The rotaxane isomer locant for a species threaded with MCs of two or more kinds is constructed similarly but the numbers, except for 0 (zero), are replaced with MC^i terms (i = 1, 2, 3, ...) where the superscript i designates the order in which MCs are cited in the complete name of the macromolecular rotaxane:



a) rotaxane locant for uniform MCs *b)* examples of isomers and rotaxane locants if MCs are not uniform

MRO-2.6.2 Isomerism: Positions of various threading components threaded through different threadable cycles

If an irregular macromolecule [12,23] component or CRU of a macromolecular component has several threadable rings, the occupancy of the rings with TCs is addressed by a composed prefix generated in a manner analogous to that described in MRO-2.6.1. Some examples are:

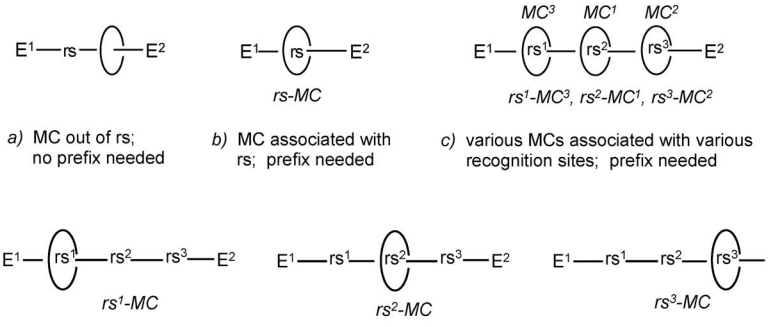


a) numbering of threadable rings and the rotaxane locant for uniform TCs

b) example of an isomer (scheme) and rotaxane locant if TCs are not uniform

MRO-2.6.3 Isomerism: Recognition sites

If there are two or more recognition sites in a TC or a linear section of a TC, the association of an MC with a specific recognition site is indicated by an italicized prefix rs^n (n = 1, 2, 3, ...) where n is the order number of particular recognition site starting from the beginning to the end of the oriented linear section (ref. [1], Section ROT-5.5.3). Note that order numbers of recognition sites and MCs are independent. Examples are:



a) MC out of rs; no prefix needed

b) MC associated with rs; prefix needed

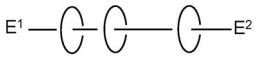
c) various MCs associated with various recognition sites; prefix needed

d) The same MC associated with various recognition sites of the same linear section - molecular shuttle

MRO-3 EXAMPLES OF SYSTEMATIC NAMES FOR MACROMOLECULAR ROTAXANES

This section illustrates the application of the above-stated principles of the macromolecular-rotaxane nomenclature for systematic naming of macromolecular rotaxanes and macromolecular pseudorotaxanes reported in the literature (see examples in refs. [3–11]). Unlike the generic names introduced in Table 1, the names presented in this section are complete names including the names of end-groups of the macromolecular components, and they demonstrate the applicability of the nomenclature rules given in this document for highly complex macromolecular rotaxane assemblies.

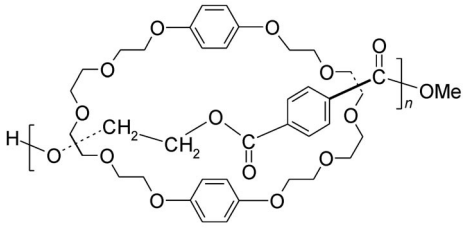
MRO-3.1 Type 1: Linear macromolecule threads one or more macrocyclic components



The generic name format for macromolecular rotaxanes of Type 1 (Table 1) is:

[*n*]{[*t*][name of macromolecule]-*rotaxa*-[*m*][name of MC]}

Example 1: Poly(ethylene terephthalate) molecule with known end-groups threads one bis(1,4-phenylene)[34]crown-10 ring. (For short names of crown ethers, see ref. [28].)



As the macromolecular TC does not contain a stopper, the above rotaxane assembly should be classified as a main-chain macromolecular pseudorotaxane.

IUPAC name of the MC is: 2,5,8,11,14,16,19,22,25,28-decaoxa-1,15(1,4)-dibenzenacyclooctacosaphane.

Short name of the MC is: bis(1,4-phenylene)[34]crown-10.

Structure-based name of the macromolecule is: α-hydro-ω-methoxypoly(oxyethyleneoxyterephthaloyl).

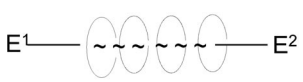
Source-based name of the macromolecule is: α-hydro-ω-methoxypoly(ethylene terephthalate).

Abbreviation of the name of the macromolecule (without end-units) is: PET [12].

Possible names for this main-chain macromolecular pseudorotaxane are:

- IUPAC-preferred structure-based name:
  [2]{[1][α-hydro-ω-methoxypoly(oxyethyleneoxyterephthaloyl)]-*rotaxa*-[1][2,5,8,11,14,16,19,22,25,28-decaoxa-1,15(1,4)-dibenzenacyclooctacosaphane]}
- Combination of the structure-based name for macromolecule and short name for MC:
  [2]{[1][α-hydro-ω-methoxypoly(oxyethyleneoxyterephthaloyl)]-*rotaxa*-[1][bis(1,4-phenylene)[34]crown-10]}
- Combination of the source-based name for macromolecule and short name for MC:
  [2]{[1][α-hydro-ω-methoxypoly(ethylene terephthalate)]-*rotaxa*-[1][bis(1,4-phenylene)[34]crown-10]}
- Combination of the abbreviation for macromolecule and short name for MC:
  [2]{[1][α-hydro-ω-methoxyPET]-*rotaxa*-[1][bis(*p*-phenylene)[34]crown-10]}

Example 2: Poly(ethylene terephthalate) molecule threads an unknown number of bis(1,4-phenylene)[34]crown-10 rings. The schematic representation of such a macromolecular pseudorotaxane is:

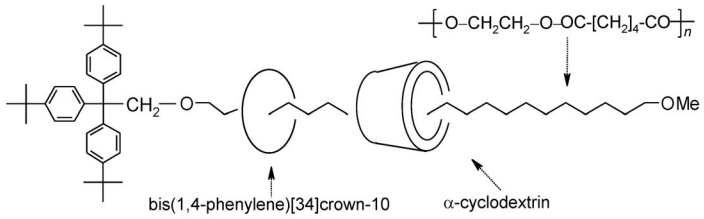


t = 1, *m* is unknown

Possible names for this main-chain macromolecular pseudorotaxane are in principle the same as those shown in Example 1 except for number prefixes in the name: indefinite prefix [*m*] is placed before the name of MC and indefinite prefix [1 + *m*] at the beginning of the name, for example:

[1 + *m*]{[1][α-hydro-ω-methoxyPET]-*rotaxa*-[*m*][bis(*p*-phenylene)[34]crown-10]}

Example 3: Poly(ethylene adipate) with one end-group stopper threads one bis(1,4-phenylene)-[34]crown-10 ring and one α-cyclodextrin ring.



As the macromolecule TC contains only one stopper, the MC can be dethreaded and thus the above rotaxane assembly should be classified as a main-chain macromolecular pseudorotaxane.

Names of MCs are given in Example 1 and the above figure.

Structure-based name of the macromolecule is: α-[2,2,2-tris(4-*tert*-butylphenyl)ethyl]-ω-methoxypoly(oxyethyleneoxyadipoyl).

Source-based name of the macromolecule is: α-[2,2,2-tris(4-*tert*-butylphenyl)ethyl]-ω-methoxypoly(ethylene adipate).

Abbreviation of the macromolecule (without end-units) can be: PEA [12].

Note: A problem with all cyclodextrins is that they are not symmetrical and so they can be threaded in two ways. This is a question of the topological isomerism (MRO-2.6) that is not solved within this document.

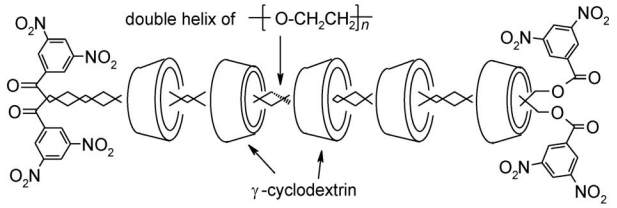
Possible names for this main-chain macromolecular pseudorotaxane are:

- IUPAC-preferred structure-based name:
  [3]{[α-[2,2,2-tris(4-*tert*-butylphenyl)ethyl]-ω-methoxypoly(oxyethyleneoxyadipoyl)]-*rotaxa*-[1][2,5,8,11,14,16,19,22,25,28-decaoxa-1,15(1,4)-dibenzenacyclooctacosaphane]-[1][α-cyclodextrin]}
- Combination of the structure-based name for macromolecule and short name for MC:
  [3]{[α-[2,2,2-tris(4-*tert*-butylphenyl)ethyl]-ω-methoxypoly(oxyethyleneoxyadipoyl)]-*rotaxa*-[1][bis(1,4-phenylene)[34]crown-10]-[1][α-cyclodextrin]}
- Combination of the source-based name for macromolecule and short name for MC:
  [3]{[α-[2,2,2-tris(4-*tert*-butylphenyl)ethyl]-ω-methoxypoly(ethylene adipate)]-*rotaxa*-[1][bis(1,4-phenylene)[34]crown-10]-[1][α-cyclodextrin]}
- Combination of the abbreviation for macromolecule and short name for MC:
  [3]{[α-[2,2,2-tris(4-*tert*-butylphenyl)ethyl]-ω-methoxyPEA]-*rotaxa*-[1][bis(*p*-phenylene)[34]crown-10]-[1][α-cyclodextrin]}

Note: If the order of the MC threaded on the macromolecular chain is reversed, it will be reflected in the name of the macromolecular rotaxane, because its macromolecular component has two different end-groups! For example, the combination of the source-based name for the macromolecule and short name for the MC gives the following name:

[3]{[α-[2,2,2-tris(4-*tert*-butylphenyl)ethyl]-ω-methoxypoly(ethylene adipate)]-*rotaxa*-[1][α-cyclodextrin]-[1][bis(1,4-phenylene)[34]crown-10]}

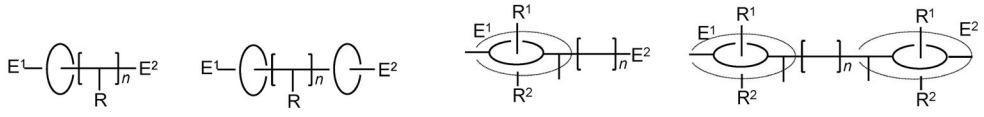
Example 4: Double helix of two poly(oxyethylene) chains, $t = 2$, with 3,5-dinitrobenzoyl end-groups threads uncertain number of γ-cyclodextrin rings (m and thus also n are not known).



[2 + *m*]{[2][α-(3,5-dinitrobenzoyl)-ω-[(3,5-dinitrobenzoyl)oxy]poly(oxyethylene)]-*rotaxa*-[*m*]-[γ-cyclodextrin]}

Because end-groups are not stoppers in this case, the rotaxane assembly should be classified as a main-chain macromolecular pseudorotaxane. The above IUPAC name might be shortened by using an IUPAC-recommended abbreviation for the polymer main chain: POE instead of poly(oxyethylene) or abbreviation PEO or PEG standing for trivial names poly(ethylene oxide) and poly(ethylene glycol), respectively.

MRO-3.2 Type 2: Normal macromolecule with rotaxane end-unit(s)



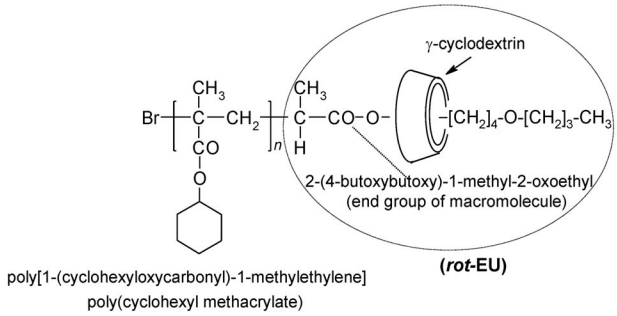
Type 2a Type 2b

The generic name format for macromolecular rotaxanes of Type 2 (Table 1) is:

α-(name of *rot*-EU[1] or E[1])-ω-(name of *rot*-EU[2] or E[2])(name of the main part of macromolecule)

Note that the order of end-groups (E^i) and rotaxane end-units (*rot*-EU^i) is given by the correct orientation of CRU.

Example 5: Type 2a. Poly(cyclohexyl methacrylate) molecule prepared by ATRP has one 2-(4-butoxybutoxy)-1-methyl-2-oxoethyl end-group onto which is threaded, on average, one γ-cyclodextrin ring.

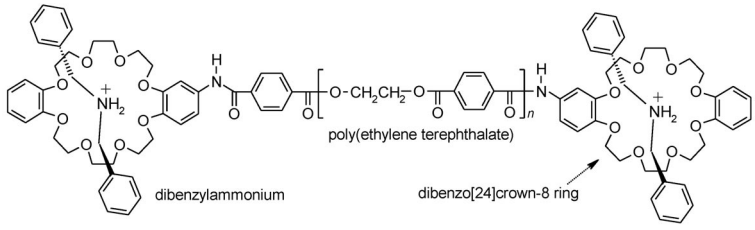


Structure- and source-based names of the main part of the macromolecule as well as the name of the threaded end-group are shown in the above formula. The other end-group is bromo. Possible names are:

α-bromo-ω-([2]{[2-(4-butoxybutoxy)-1-methyl-2-oxoethyl]-*rotaxa*-[γ-cyclodextrin]})poly[1-(cyclohexyloxycarbonyl)-1-methylethylene]

α-bromo-ω-([2]{[2-(4-butoxybutoxy)-1-methyl-2-oxoethyl]-*rotaxa*-[γ-cyclodextrin]})poly(cyclohexyl methacrylate)

Example 6: Type 2b. Poly(ethylene terephthalate) molecule has crown-ether end-groups; through each is threaded a dibenzylammonium chain.



Systematic names of the end-groups are:

α-group: 4-[(6,7,9,10,12,13,20,21,23,24,26,27-dodecahydrodibenzo[*b,n*][1,4,7,10,13,16,19,22]-octaoxacyclotetracosin-2-yl)carbamoyl]benzoyl

ω-group: (6,7,9,10,12,13,20,21,23,24,26,27-dodecahydrodibenzo[*b,n*][1,4,7,10,13,16,19,22]-octaoxacyclotetracosin-2-yl)amino

Short names of the end-groups are:

α-group: 4-{[(dibenzo[24]crown-8)-2-yl]carbamoyl}benzoyl
ω-group: [(dibenzo[24]crown-8)-2-yl]amino

Systematic name of the TC is: *N*-benzyl-1-phenylmethanammonium.
Short name of the TC is: dibenzylammonium.
Short (usual) names of rotaxane EUs (*rot*-EU) are:

α-*rot*-EU: [2]{[dibenzylammonium]-*rotaxa*-[4-{[(dibenzo[24]crown-8)-2-yl]carbamoyl}benzoyl]}

ω-*rot*-EU: [2]{[dibenzylammonium]-*rotaxa*-[[(dibenzo[24]crown-8)-2-yl]amino]}

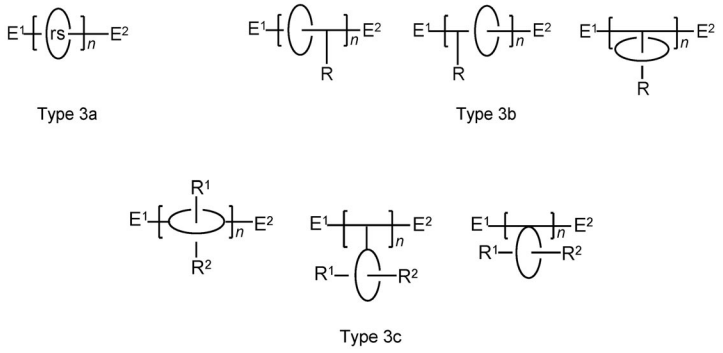
Structure-based name of the macromolecule main part is: poly(oxyethyleneoxyterephthaloyl).
Source-based name of the macromolecule main part is: poly(ethylene terephthalate); its abbreviation is PET.
To highlight that the MC is associated with recognition sites of TCs, the prefix (*rs-MC*) may be added before the name of the rotaxane assembly.
A combination of short names for *rot*-EUs with structure-based name for the macromolecule main part gives the name:

α-[(*rs-MC*)[2]{[dibenzylammonium]-*rotaxa*-[4-{[(dibenzo[24]crown-8)-2-yl]carbamoyl}benzoyl]]-ω-[(*rs-MC*)[2]{[dibenzylammonium]-*rotaxa*-[(dibenzo[24]crown-8)-2-ylamino]}]poly(oxyethyleneoxyterephthaloyl)

If a source-based name or abbreviation is used to name the macromolecule main part, the rigorous inclusion of the terephthaloyl MU into α-*rot*-EU need not be expressed and a shortened name format can be used, for example:

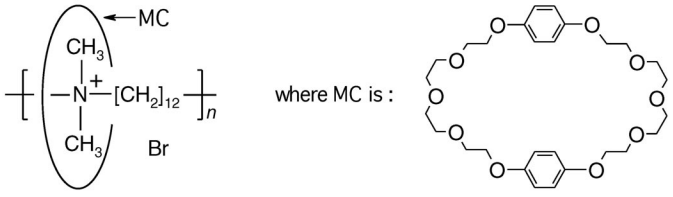
α,ω-bis((*rs-MC*)[2]{[dibenzylammonium]-*rotaxa*-[[(dibenzo[24]crown-8)-2-yl]amino]})PET

MRO-3.3 Type 3: Regular macromolecular rotaxanes



General generic name formats for Type 3 macromolecular rotaxanes are: **poly(name of *rot*-CRU)** or **poly(name of rotaxane monomer)**, both completed with end-groups or *rot*-EUs if known.

Example 7: Type 3a macromolecular rotaxane consisting of rotaxane CRUs with a recognition site:

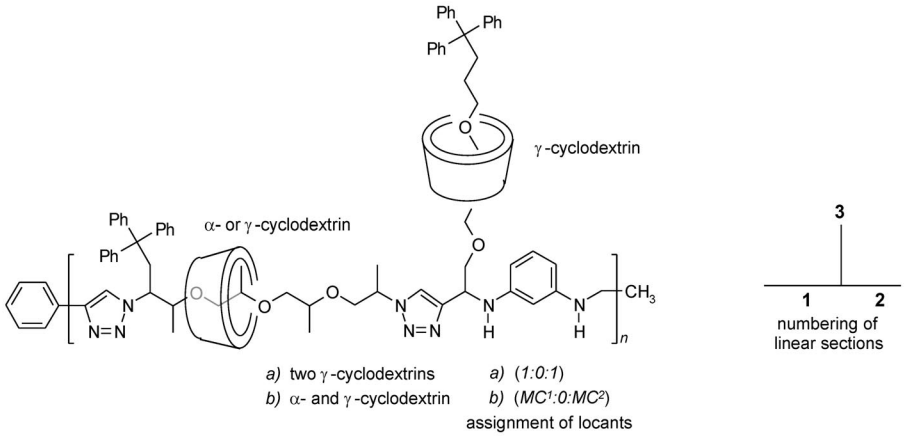


The IUPAC-preferred structure-based name is: poly((*rs-MC*)-[2]{[(dimethyliminio)dodecane-1,12-diyl bromide]-*rotaxa*-[2,5,8,11,14,16,19,22,25,28-decaoxa-1,15(1,4)-dibenzenacyclooctacosaphane]}).

Combination of the structure-based name for macromolecule and short name for MC is: poly((*rs-MC*)[2]{[(dimethyliminio)dodecane-1,12-diyl bromide]-*rotaxa*-[bis(1,4-phenylene)[34]crown-10]}).

Example 8: Type 3b macromolecular rotaxanes: the rotaxane CRU with a side chain as stopper; two of three linear sections of CRU are threaded:

- two identical MCs: each γ-cyclodextrin molecule;
- two different MCs: one α-cyclodextrin molecule; another one γ-cyclodextrin molecule.



In this case, the CRU of the macromolecular component has three linear, potentially threadable sections the occupancy of which should be addressed by number prefixes as established for low-M rotaxanes (see MRO-2.6 and ref. [1], section ROT-5). The order numbers are assigned to the linear sections starting from the beginning to the end of oriented CRU first numbering the main-chain sections and after all branches starting from the beginning (see MRO-2.6.1).

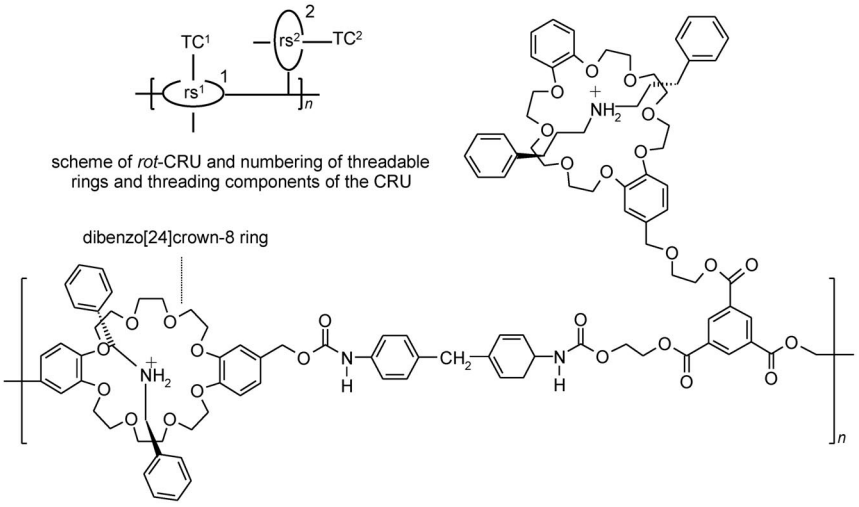
In the case of macromolecular rotaxane a, the MCs are uniform and so the prefix consists of only numbers:

a) α-phenyl-ω-methylpoly[(*1:0:1*)-[3]{[1][(1,2,3-triazole-4,1-diyl)[1-(2,2,2-triphenylethyl)-2,5,8,11-tetramethyl-3,6,9-trioxaundecane-1,11-diyl]-1,2,3-triazole-1,4-diyl[(11,11,11-triphenyl-2,7-dioxaundecan-1-yl)methylene]imino-1,3-phenyleneiminomethylene]-*rotaxa*-[2][γ-cyclodextrin]}].

In the case of macromolecular rotaxane b, the MCs are different and so the prefix also includes MC^i terms (i = 1, 2, 3, ...) where the superscript i designates the order in which MCs are cited in the complete name of the macromolecular rotaxane:

b) α-phenyl-ω-methylpoly[(MC^1*:0:*MC^2)-[3]{[(1,2,3-triazole-4,1-diyl)[1-(2,2,2-triphenylethyl)-2,5,8,11-tetramethyl-3,6,9-trioxaundecane-1,11-diyl]-1,2,3-triazole-1,4-diyl[(11,11,11-triphenyl-2,7-dioxaundecan-1-yl)methylene]imino-1,3-phenyleneiminomethylene]-*rotaxa*-[1][α-cyclodextrin]-*rotaxa*-[1][γ-cyclodextrin]}].

Example 9: Type 3c macromolecular rotaxanes: a rotaxane CRU with two threadable cycles each threaded with different TC:

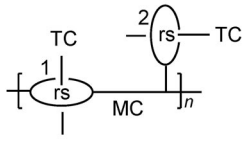


In this case, the threadable rings as well as TCs and their recognition sites are assigned by the superscript order numbers starting from the beginning to end of oriented CRU, first numbering the main-chain cycles and after all cycles in branches starting from the beginning, the same as in the case of macromolecules with threadable sections (see MRO-6.1, Example 8 and the inset in the above scheme). This approach provides the following possible name:

poly[(*rs*^{1}-*MC*^{1}:*rs*^{2}-*MC*^{2})-(*TC*^{1}:*TC*^{2})-[3]{[1][dibenzylammonium]-[1][bis(3-phenylpropyl)ammonium]-*rotaxa*-[1][(dibenzo[24]crown-8)-2,12-diylmethyleneoxycarbonylimino-1,4-phenylenemethylene-1,4-phenyleneiminocarbonyloxyethyleneoxycarbonyl[5-(2-{[(dibenzo[24]crown-8)-2-yl]methoxy}ethoxycarbonyl)-1,3-phenylene]carbonyloxymethylene]}]

If the same regular macromolecular component is threaded with uniform TCs (see scheme below), for example, with bis(3-phenylpropyl)ammonium, and an abbreviation is introduced for the CRU of the macromolecular part of *rot*-CRU, a possible name for such a macromolecular rotaxane would be:

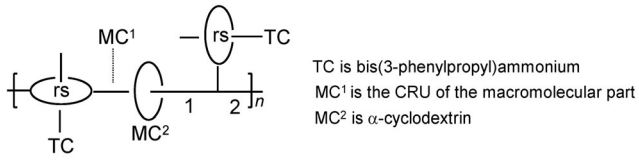
poly[(*rs-MC*)-(*1:1*)-[3]{[2][bis(3-phenylpropyl)ammonium]-*rotaxa*-[1][abbreviation for CRU]}]



Scheme of *rot*-CRU with two threadable rings each threaded with the same threading component comprising a recognition site

Since there is no ambiguity possible, simple prefix (*rs-MC*) instead of the more complex one: (*rs-MC*^{1}:*rs-MC*^{2}) can be added to emphasize association of TCs with MC^1 and MC^2.

Example 10: A model complex macromolecular rotaxane of the type 3 that is a combination of types 3b and 3c: a rotaxane CRU with two linear sections, onto one of which is threaded an MC, and two threadable cycles threaded with uniform TCs. The macromolecular part can be similar to that shown in the preceding Example 9. The scheme of such a macromoleular rotaxane is as follows:



Scheme of *rot*-CRU with two threadable rings threaded with uniform TCs and two linear sections onto one of which is threaded an MC

As can be seen, TCs are threaded through macromolecular MC (MC^1) that by itself possesses rotaxane structure. Therefore, the macromolecular MC shall be named using the rotaxane nomenclature for Type 3b macromolecular rotaxanes.

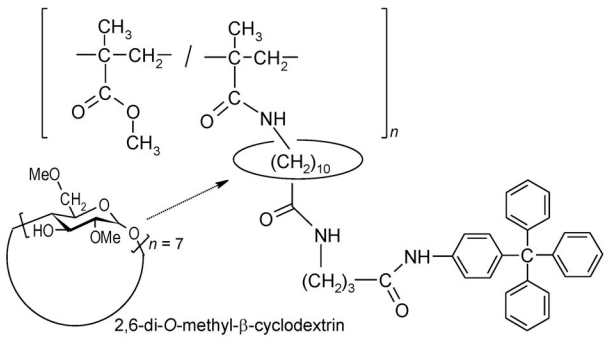
Let us assume that we have an abbreviation introduced for CRU of the macromolecular part of *rot*-CRU, that both TCs are bis(3-phenylpropyl)ammonium molecules and that the MC^2 is α-cyclodextrin. Then a possible name for such a macromolecular rotaxane can be:

poly((*rs-MC*)-(*1:1*)-[4]{[2][bis(3-phenylpropyl)ammonium]-*rotaxa*-[(*1:0*)-[2]{[1][abbreviation for CRU]-*rotaxa*-[1][α-cyclodextrin]}]})

MRO-3.4 Type 4: Irregular macromolecular rotaxanes

Names for irregular macromolecular rotaxanes are derived by combining the nomneclature for copolymers and irregular polymers [12–19] and the nomenclature rules used for naming *rot*-CRUs of regular macromolecular rotaxanes (MRO-3.3).

Example 11: Copolymer of methyl methacrylate and *N*-substituted methacrylamide with a threadable side chain capped with a stopper onto which is threaded 2,6-di-*O*-methyl-β-cyclodextrin ring as MC:



Though the main-chain part of *rot*-CRU is short, it neighbors with potentially threadable linear sections of methyl methacrylate MUs; therefore, its threading with an MC should be included using the prefix (*0:1*) (see MRO-3.3) addressing MC threaded on the pendant chain. Possible names for the above macromolecular rotaxane are:

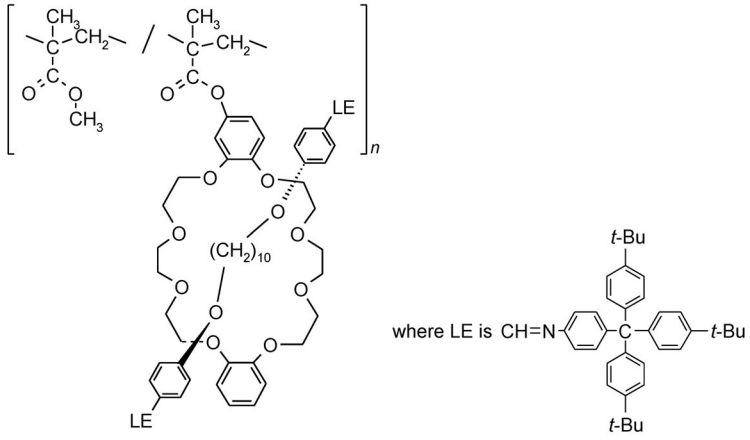
Structure-based name:

poly([1-(methoxycarbonyl)-1-methylethylene]/[(*0:1*)-[2]{[1-methyl-1-{[11-oxo-11-({4-oxo-4-[(4-tritylphenyl)amino]butyl}amino)undecyl]carbamoyl}ethylene]-*rotaxa*-[2,6-di-*O*-methyl-β-cyclodextrin]}])

Source-based name:

poly[(methyl methacrylate)-*co*-(*0:1*)-[2]{[11-[(2-methylacryloyl)amino]-*N*-{4-oxo-4-[(4-tritylphenyl)amino]butyl}undecanamide]-*rotaxa*-[2,6-di-*O*-methyl-β-cyclodextrin]}]

Example 12: Copolymer of methyl methacrylate and the methacrylate with a threadable (dibenzo[24]crown-8)-2-yl side ring which is threaded with linear molecule capped with stoppers:



Some names for the macromolecular rotaxane shown in the above figure are as follows:
Structure-based name:

poly{[1-(methoxycarbonyl)-1-methylethylene]/([2]{[*N*,*N*′-[decane-1,10-diylbis(oxy-4,1-phenylenemethylylidene)]bis{4-[tris(4-*tert*-butylphenyl)methyl]aniline}-*rotaxa*-[1-{[(6,7,9,10,12,13,20,21,23,24,26,27-dodecahydrodibenzo[*b*,*n*][1,4,7,10,13,16,19,22]-octaoxacyclotetracosin-2-yl)oxy]carbonyl}-1-methylethylene]})}

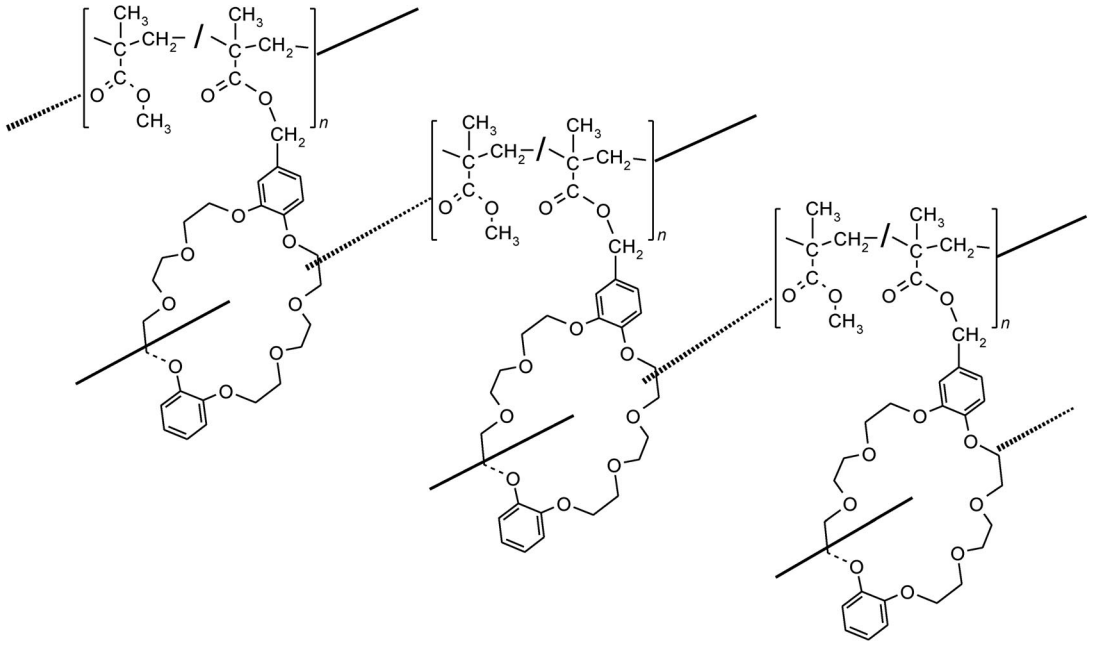
Source-based name:

poly(methyl methacrylate-*co*-[2]{[*N*,*N*′-[decane-1,10-diylbis(oxy-4,1-phenylenemethylylidene)]bis{4-[tris(4-*tert*-butylphenyl)methyl]aniline}]-*rotaxa*-[(dibenzo[24]crown-8)-2-yl methacrylate]})

MRO-3.5 Type 5: Interlocked macromolecules

In this type of macromolecular rotaxane, macromolecules spontaneously interweave or interlock through pendent or main-chain rings of other macromolecules. Nomenclature for this type of macromolecular rotaxane is necessarily different from that recommended for the other types because there is only one type of constituent(s) (macromolecular) and each component possesses both linear sections [threading component(s) and threadable rings(s)] and macrocyclic component(s).

Example 13: Copolymer of methyl methacrylate and [(dibenzo[24]crown-8)-2-yl]methyl methacrylate with threadable side rings (chains interlocks during copolymerization):



Some names for the above macromolecular rotaxane are as follows:
Structure-based name:

rotaxa-poly([1-(methoxycarbonyl)-1-methylethylene]/{1-[(6,7,9,10,12,13,20,21,23,24,26,27-dodecahydrodibenzo[*b*,*n*][1,4,7,10,13,16,19,22]octaoxacyclotetracosin-2-yl)methoxycarbonyl]-1-methylethylene})

Source-based name:

rotaxa-poly[(methyl methacrylate)-*co*-{[(dibenzo[24]crown-8)-2-yl]methyl methacrylate}]

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ALPHABETICAL INDEX OF TERMS

(prefixes MRO- are omitted)
(bold characters refer to **main entries**)

LIST OF ABBREVIATIONS AND PREFIXES

-co-	connective to join names of monomers in the source-based name of a copolymer
CRU	constitutional repeating unit
CU	constitutional unit
m	number of macrocyclic components in a rotaxane species
MC	macrocyclic component (of rotaxane)
MC^i	locant for *i*-th macrocyclic component
MRO	IUPAC identifier of this nomenclature document on macromolecular rotaxanes
MU	monomeric unit
n	total number of independent components in a rotaxane species; $n = t + m$
ROT	IUPAC identifier of the nomenclature document on rotaxanes [1]
-rotaxa-	connective to join the names of the threading and macrocyclic components in the name of a rotaxane
rot-CRU	rotaxane CRU
rot-CU	rotaxane CU
rot-EU	rotaxane end-unit
rot-MU	rotaxane MU
rs	recognition site
rs^i	locant for *i*-th recognition site
t	number of threading components in a rotaxane species
TC	threading component
TC^i	locant for *i*-th threading component

