

# Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes (IUPAC Recommendations 2012)

Jiří Vohlídal<sup>1,‡</sup>, Edward S. Wilks<sup>2</sup>, Andrey Yerin<sup>3</sup>, Alain Fradet<sup>4</sup>, Karl-Heinz Hellwich<sup>5</sup>, Philip Hodge<sup>6</sup>, Jaroslav Kahovec<sup>7</sup>, Werner Mormann<sup>8</sup>, Robert Stepto<sup>9</sup>

<sup>1</sup>Charles University in Prague, Faculty of Sciences, Albertov 2030, CZ-128 40 Praha 2, Czech Republic; <sup>2</sup>113 Meriden Drive, Canterbury Hills, Hockessin, DE 19707, USA; <sup>3</sup>Advanced Chemistry Development, ul. Akademika Bakuleva 6, RF-117513 Moscow, Russia; <sup>4</sup>Laboratoire de Chimie des Polymères, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris, France; <sup>5</sup>Postfach 10 07 31, 63007 Offenbach, Germany; <sup>6</sup>School of Chemistry, The University of Manchester, Manchester M13 9PL, UK; <sup>7</sup>Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovsky Sq. 2, 162 06 Praha 6, Czech Republic; <sup>8</sup>Makromolekulare Chemie Universität-Gesamthochschule Siegen, Adolf-Reichwein-Straße, D-57068 Siegen, Germany; <sup>9</sup>School of Materials, The University of Manchester, Manchester M1 7HS, UK.

**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-molecular-weight rotaxanes and the nomenclature rules for macromolecules (both established in published IUPAC Recommendations) in such a way that the developed nomenclature system provides unambiguous names for macromolecular rotaxanes (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 pseudorotaxane; macromolecular rotaxane; nomenclature recommendations; polypseudorotaxane; polyrotaxane; pseudorotaxane polymer; rotaxane polymer; rules; source-based polymer names, structure-based polymer names.

## CONTENTS

MRO-0	INTRODUCTION
MRO-1	TERMINOLOGY FOR MACROMOLECULAR ROTAXANES

<sup>‡</sup>Corresponding author: E-mail: vohlidal@natur.cuni.cz; j.vohlidal@centrum.cz

*Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes***MRO-2 NOMENCLATURE FOR MACROMOLECULAR ROTAXANES**

- MRO-2.1 Names for macromolecular rotaxanes and macromolecular pseudorotaxanes
- MRO-2.2 Sources of the nomenclature for macromolecular rotaxanes
- MRO-2.3 Use of systematic and non-systematic names and abbreviations
- MRO-2.4 Generic types of and generic name formats for macromolecular rotaxanes
- MRO-2.5 Guideline for construction of names for macromolecular rotaxanes
- MRO-2.6 Isomerism of macromolecular rotaxanes
  - MRO-2.6.1 Isomerism – positions of various macrocyclic components threaded on several linear sections
  - MRO-2.6.2 Isomerism – positions of various threading components threaded through different threadable cycles
  - MRO-2.6.3 Isomerism – recognition sites

**MRO-3 EXAMPLES OF SYSTEMATIC NAMES FOR MACROMOLECULAR ROTAXANES**

- MRO-3.1 Type 1 – linear macromolecule threads one or more macrocyclic components
- MRO-3.2 Type 2 – normal macromolecule with rotaxane end unit(s)
- MRO-3.3 Type 3 – regular macromolecular rotaxanes
- MRO-3.4 Type 4 – irregular macromolecular rotaxanes
- MRO-3.5 Type 5 – rotaxane-interlocked macromolecules

**MEMBERSHIP OF SPONSORING BODIES****REFERENCES****ALPHABETICAL INDEX OF TERMS****LIST OF ABBREVIATIONS AND PREFIXES****MRO-0 INTRODUCTION**

Supramolecular assemblies consisting of macrocyclic molecules physically threaded by, but not chemically bonded to, a linear molecule chain 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 non-linear 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], in 1999 [4], in 2001 [5], in 2005 [6], in 2007 [7], in 2009 [8-10] and in 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 have to be identical.

The nomenclature recommendations for macromolecular rotaxanes and pseudorotaxanes presented in this document were developed by combining the nomenclature principles for low-molecular-weight 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

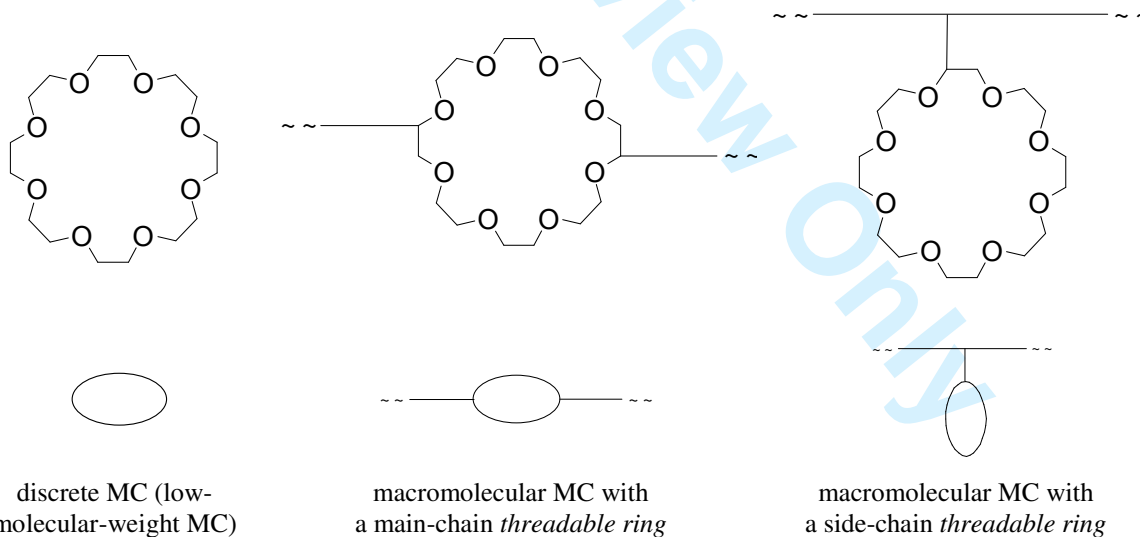
For ease of reference, the terms in this section are listed alphabetically and numbered sequentially. To assist the reader, cross-references to terms also defined in this chapter are denoted in *italic* typeface. If there are two terms in an entry on successive lines, the second is a synonym.

### MRO-1.1 macrocyclic component recommended abbreviation MC

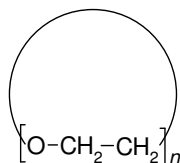
Molecule that has at least one ring (cycle) large enough to allow it to be threaded onto a linear subchain of another molecule.

*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:



*Note 3:* The literature on *rotaxanes* frequently cites the word “macrocycle” as a contraction of (and an abbreviation for) macrocyclic molecule. 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 Table 2.1).

### MRO-1.3 macromolecular pseudorotaxane

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

*Note 1:* Macromolecular pseudorotaxanes are a subclass of *macromolecular rotaxanes*.

*Note 2:* 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 these compound classes.

*Note 3:* Macromolecular pseudorotaxanes in which only one end of a *threading component* is capped with a stopper are sometimes called “macromolecular semirotaxanes”.

### 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 macrocyclic molecule threaded onto its linear section or at least one linear molecule threaded through its threadable cycle.

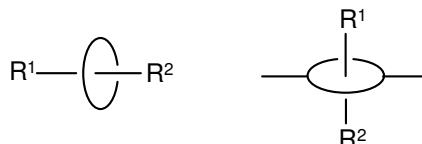
*Note 2:* *Rotaxane constitutional unit(s)* may be located within a specific part of a macromolecular rotaxane: (i) within end-group(s); (ii) within a main chain (*main-chain macromolecular rotaxane*); (iii) within side chains (*side-chain macromolecular rotaxane*).

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*.

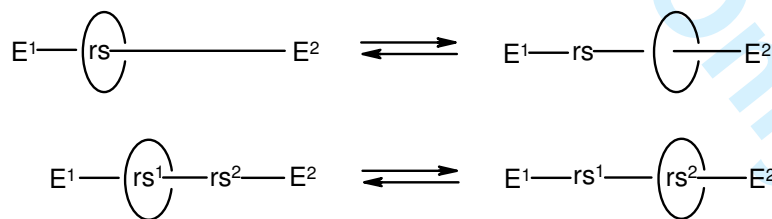
### MRO-1.6 main-chain rotaxane polymer (main-chain polyrotaxane)

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

Note: See Note 4 in entry MRO-1.9 and Note 2 in entry 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*; [see ref. 1, entry ROT-1.6].



Motion schemes for two basic types of molecular shuttles  
(rs, rs<sup>1</sup> and rs<sup>2</sup> stand for recognition sites, E<sup>1</sup> and E<sup>2</sup> 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).

*Note 1:* Pseudorotaxanes can be regarded as a subclass of *rotaxanes*.

*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:* Pseudorotaxane polymers are a subclass of *rotaxane polymers*.

*Note 3:* A pseudorotaxane polymer in molecule of which only one end of a *threading component* is capped with a stopper is sometimes called “semirotaxane polymer” or “polysemirotaxane”.

*Note 4:* Though the synonym “polypseudorotaxane” currently appears in literature, its use should be discouraged. This term, from purely semantic point of view, namely implies many threaded rings – polymer formed from a *pseudorotaxane*, while a molecule of a pseudorotaxane polymer can comprise a single threaded ring.

*Note 5:* 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**

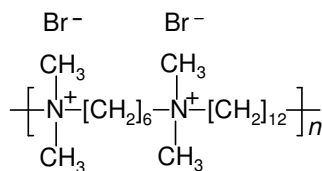
recommended abbreviation: rs

Part of the *threading component*, at which a *macrocyclic component* of a *rotaxane* prefers to locate.

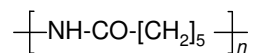
*Note 1:* A recognition site immobilizes a *macrocyclic component* (MC) on the basis of the host-guest non-covalent interactions typical of supramolecular chemistry, while a couple of *stoppers* sterically demarcate a region in which a *macrocyclic component* can more or less freely move.

*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:

## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

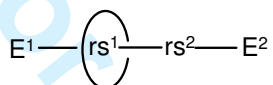


poly[(dimethyliminio)hexane-1,6-diyl  
(dimethyliminio)dodecane-1,12-diyl dibromide]

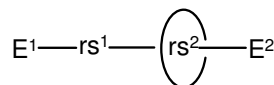


poly[imino(1-oxohexane-1,6-diyl)]  
poly(hexano-6-lactam)  
poly( $\epsilon$ -caprolactam)  
polyamide 6 (trivial name)

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



*rs*<sup>1</sup>-MC



*rs*<sup>2</sup>-MC

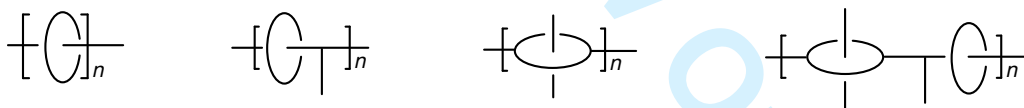
*Macrocyclic component (MC)* that can associate with various recognition sites ( $rs$ ) of the same *threading component*: principle of the *molecular shuttle*

The italicized abbreviation  $rs^i$  is used as a prefix assigning the actual position of a *macrocyclic component (MC)* on a particular *threading component*.

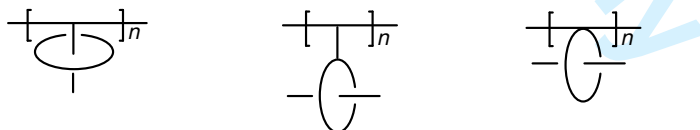
### MRO-1.11 regular macromolecular rotaxane

*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:

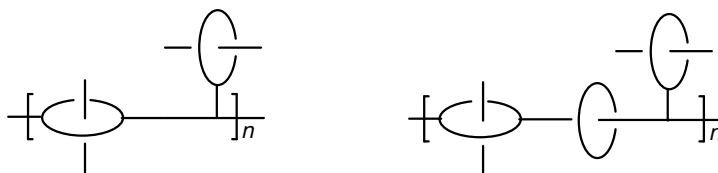


Schematic representations of some types of regular *main-chain macromolecular rotaxanes*



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

## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

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 that has a *rotaxane* structure.

*Note:* For a definition of constitutional repeating unit (CRU) see ref. [23].

**MRO-1.14 rotaxane constitutional unit  
rotaxane CU**

recommended abbreviation *rot*-CU

Constitutional unit that has a *rotaxane* structure.

*Note:* For a definition of constitutional unit (CU) see ref. [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 *threading* or *macrocyclic component*.

**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 literature, its use should be discouraged. This term, from purely semantic point of view, namely implies many threaded rings – 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 principle 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 entry MRO-1.9 and Note 2 in entry MRO-1.18.

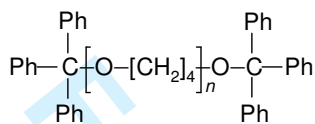
**MRO-1.21 stopper**

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*.

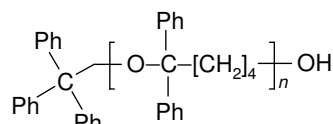
*Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes*

*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 (MC). Accordingly when stoppers are mentioned, the MC should also be mentioned. Examples of stoppers for  $\beta$ -cyclodextrine MC are  $-\text{CPh}_3$  end-groups or  $-\text{CPh}_2-$  groups included in constitutional repeating units:



Macromolecular threading component with end-group stoppers ( $-\text{CPh}_3$ )



Macromolecular *threading component* with internal stoppers ( $-\text{CPh}_2-$ ) 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 branching 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 *threading component*.

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

## 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*, *threading component* may be either a macromolecular chain with a linear section or a linear low-molecular-weight 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 a part of 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



for a rotaxane composed of independent TC and MC molecules and



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

$n = t + m$	the total number of independent components in a <i>rotaxane</i> species;
$t$	the number of threading components in a rotaxane species;
$m$	the number of macrocyclic components in a rotaxane species.

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



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



for the source-based systematic 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 which 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 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-molecular-weight 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 semisystematic and trivial names, or abbreviations, for low-molecular-weight and macromolecular components is permitted, provided no ambiguity is thereby introduced. However, note that such names are less preferred than systematic names.

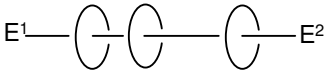
*Note 1:* The IUPAC preferred name for a macromolecular rotaxane is the name composed of the structure-based name for the macromolecule component and systematic IUPAC name for the low-MW component of the macromolecular rotaxane.

*Note 2:* As a rule, if the source-based name or a trivial name or an abbreviation is used for naming the macromolecule component it is combined with the semisystematic name of low-MW 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 2.1.

**Table 2.1 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<sup>i</sup> for end-group(s) of a macromolecular component and R<sup>i</sup> for end-group(s) of a low-molecular-weight 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	<p><u>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</u></p>  <p><math>E^1 - \text{---} \text{---} \text{---} \text{---} E^2</math></p> <p>[n]{[t][name of macromolecule]-rotaxa-[m][name(s) of MC(s)]}</p>	Position(s) of MC(s) is(are) not known or is(are) variable with time.
2	<p><u>Exclusively end unit(s) of macromolecule rotaxane possess(es) the rotaxane structure; generic name format is:</u></p> <p><math>\alpha</math>-(name of <i>rot</i>-EU<sup>1</sup> or E<sup>1</sup>)-<math>\omega</math>-(name of <i>rot</i>-EU<sup>2</sup> or E<sup>2</sup>)(name of the main part of macromolecule)</p>	

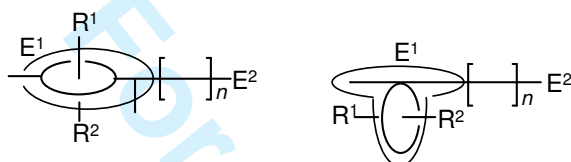
2a



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 (branching point of CRU).

$\alpha$ -[ $n$ ]{[(name of  $E^1$ )-rotaxa-[ $m$ ](name of MC)]}- $\omega$ -(name of  $E^2$ )(name of the main part of macromolecule)  
(the order of end-groups (end units) is given by the correct orientation of CRU)

2b



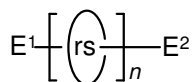
Macromolecular component contains at least one end-group with threadable cycle (MC), through which is threaded a short linear molecule (TC). Note that  $E^1$  includes the part of the macromolecular component demarcated by the dashed closed curve.

$\alpha$ -([ $n$ ]{[ $t$ ](name of TC)-rotaxa-[ $m$ ](name of  $E^1$ )}]- $\omega$ -(name of  $E^2$ )(name of the main part of 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)**

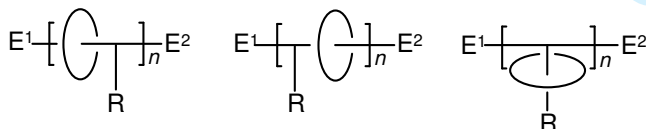
3a



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)})

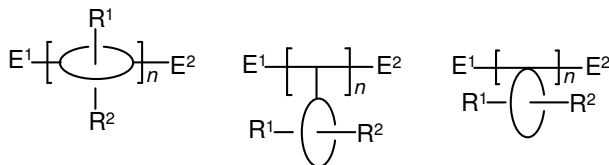
3b



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

## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

according to certain statistical law

- 4a 
$$\left( \left[ \text{rot-CRU} \right]_x / \left[ \text{CRU} \right]_y \right)_n$$

$$\left( \left[ \text{rot-MU} \right]_x / \left[ \text{MU} \right]_y \right)_n$$
 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).

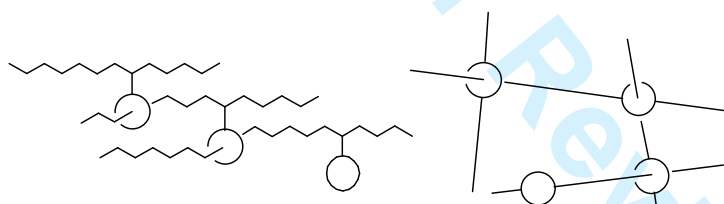
**poly{[name of *rot*-CRU]/[name of normal CRU]}**  
**poly{[name of *rot*-monomer]-co-[name of normal monomer]}**

- 4b 
$$\left( \left[ \text{rot-CRU}^1 \right]_x / \left[ \text{rot-CRU}^2 \right]_y / \left[ \text{rot-CRU}^3 \right]_z / \dots \right)_n$$

$$\left( \left[ \text{rot-MU}^1 \right]_x / \left[ \text{rot-MU}^2 \right]_y / \left[ \text{rot-MU}^3 \right]_z / \dots \right)_n$$
 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<sup>1</sup>]/[name of *rot*-CRU<sup>2</sup>]/ [name of *rot*-CRU<sup>3</sup>]/.....}**  
**poly{[name of *rot*-monomer<sup>1</sup>]-co-[name of *rot*-monomer<sup>2</sup>]-co-[name of *rot*-monomer<sup>3</sup>]/.....}**

- 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)]}**

*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*, as a partly indefinite prefix [*t+m*] (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-molecular-weight rotaxanes and several other compound classes).

**MRO-2.5 Guideline for construction of names for macromolecular rotaxanes**

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

- 1 Identify the threading (TC) and macrocyclic (MC) components and determine the structure type of the macromolecular rotaxane according to Table 2.1.
  - 2 Create the name(s) for the low-molecular-weight component(s) of the macromolecular rotaxane and enclose the name(s) in square brackets: [low-MW 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 macromolecule nomenclature system (structure-based 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-MW component] according to the relevant generic name format for *rot*-CRU:
 

$[n]\{\text{[CRU]-rotaxa-}[m]\text{[low-MW component]}\}$	if [CRU] is TC and [low-MW component] MC;
$[n]\{\text{[t][low-MW component]-rotaxa-[CRU]}\}$	if [low-MW component] is TC and [CRU] MC;
  - if a *rot*-CRU is of the Type 3b or 3c, create locants for low-MW component that are MCs (see MRO-2.6 and Examples 8 - 10);
  - create the name the macromolecular rotaxane according to the generic name format (Table 2.1) for the identified type of macromolecular rotaxane.
  - 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 2.1 for the Type 2 macromolecular rotaxanes.
- 7b) Source-based macromolecular nomenclature 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) 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-MW component] according to the generic name format for rotaxanes:
 

$[n]\{\text{[monomer]-rotaxa-}[m]\text{[low-MW component]}\}$	if [monomer] is TC and [low-MW component] MC;
$[n]\{\text{[t][low-MW component]-rotaxa-[monomer]}\}$	if [low-MW 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-MW component that is MC (see MRO-2.6);
  - create the name the macromolecular rotaxane according to the identified generic name format (Table 2.1);

- 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 2.1 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:

- positions of MCs at linear sections of a complex TC or positions of TCs at several macrocyclic parts of a complex MC, or both;
- the order in which several nonequivalent MCs are positioned at the same linear section of a TC;
- the position of an MC at different recognition sites within the same linear section of a TC;
- 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-MW rotaxanes [1].

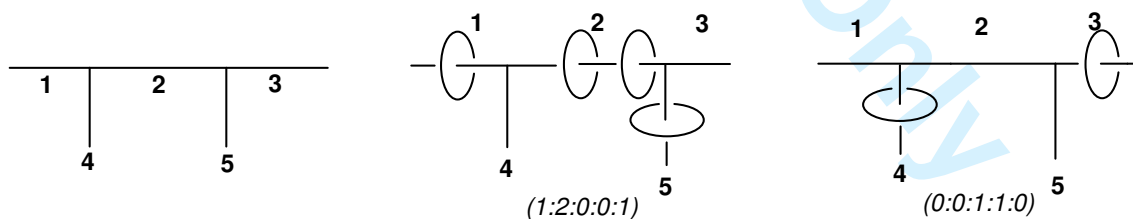
### MRO-2.6.1 Isomerism – positions of various macrocyclic components threaded on several linear sections.

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 macrocyclic components, MC, is addressed by a composed prefix generated in a manner similar to that described for low-molecular-weight 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 CRU (main chain of macromolecule) and then continuing by numbering side chains, again from the left to the right end of 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 number of MCs threaded onto particular linear section.

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



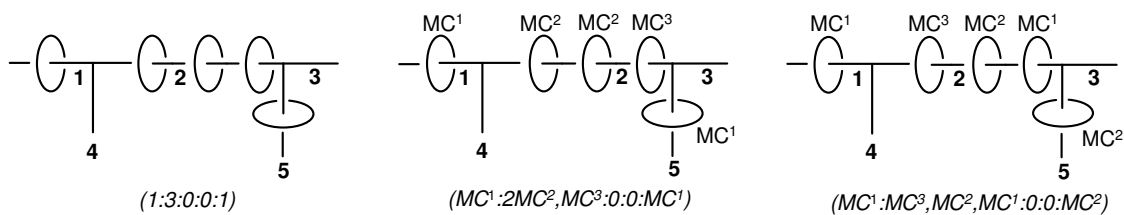
a) numbering of linear sections

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 ( $i = 1, 2, 3, \dots$ ) where the superscript  $i$  designates the order in which MCs are cited in the complete name of the macromolecular rotaxane:



## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

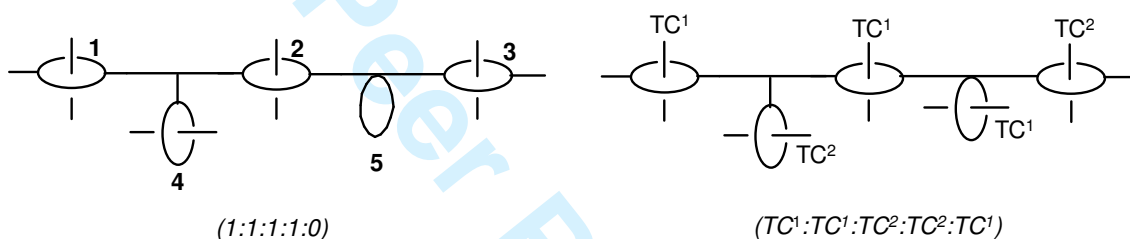


a) rotaxane locant for uniform MCs

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 threading components, TC, is addressed by a composed prefix generated in a manner analogous to that described in MRO-2.6.1. Some examples are:

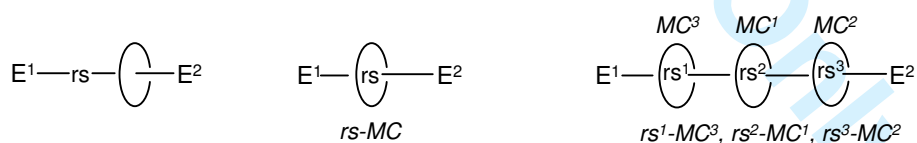


a) numbering of threadable rings and the rotaxane locant for uniform TCs

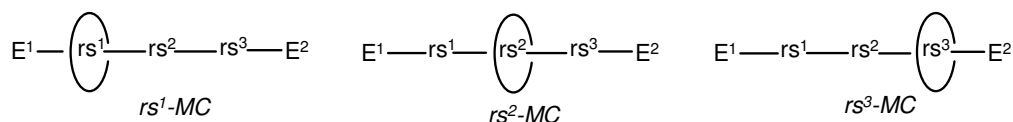
b) example of an isomer (scheme) and rotaxane locant if TCs are not uniform

**MRO-2.6.3 Isomerism – recognition sites**

If there are two or more recognition sites in a TC or a linear section of TC, the association of an MC with a specific recognition site is indicated by an italicized prefix  $rs^n$  ( $n = 1, 2, 3, \dots$ ) where  $n$  is the order number of particular recognition site starting from the beginning to 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 neededb) MC associated with  $rs$ ; prefix needed

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

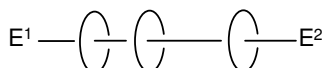


d) The same MC associated with various recognition sites of the same linear section - molecular shuttle

### 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 macromolecular rotaxanes and macromolecular pseudorotaxanes reported in the literature (see examples in refs. [3-11]). Unlike the generic names introduced in Table 2.1 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.

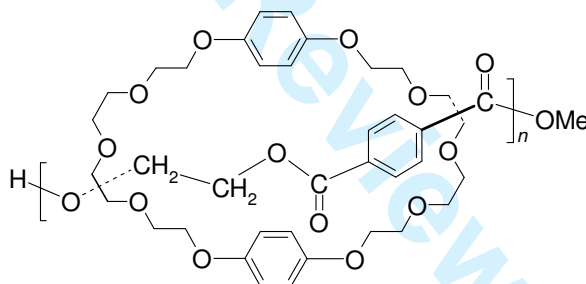
#### MRO-3.1 Type 1 - linear macromolecule threads one or more macrocyclic components



Generic name format for macromolecular rotaxanes of Type 1 (Table 2.1) is:



*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. [27]).



As the macromolecular threading component 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 (semisystematic) name of the MC is: bis(1,4-phenylene)[34]crown-10.

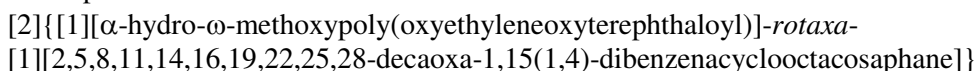
Structure-based name of the macromolecule is:  $\alpha$ -hydro- $\omega$ -methoxy-poly(oxyethyleneoxyterephthaloyl).

Source-based name of the macromolecule is:  $\alpha$ -hydro- $\omega$ -methoxy-poly(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:

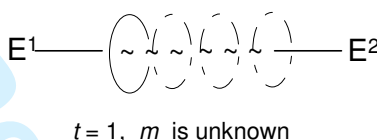


- Combination of the structure-based name for macromolecule and semisystematic name for MC:

[2]{[1][ $\alpha$ -hydro- $\omega$ -methoxypoly(oxyethyleneoxyterephthaloyl)]-rotaxa-[1][bis(1,4-phenylene)[34]crown-10]}

- Combination of the source-based name for macromolecule and semisystematic name for MC:  
[2]{[1][ $\alpha$ -hydro- $\omega$ -methoxypoly(ethylene terephthalate)]-rotaxa-[1][bis(1,4-phenylene)[34]crown-10]}
- Combination of the abbreviation for macromolecule and semisystematic name for MC:  
[2]{[1][ $\alpha$ -hydro- $\omega$ -methoxyPET]-rotaxa-[1][bis(*p*-phenylene)[34]crown-10]}

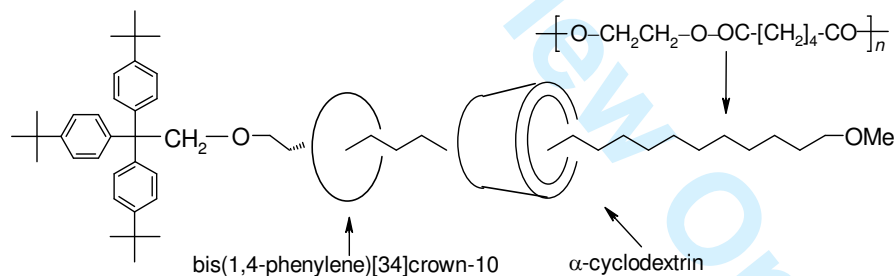
*Example 2* Poly(ethylene terephthalate) molecule threads an unknown number of bis(1,4-phenylene)[34]crown-10 rings. The schematic representation of such a macromolecular pseudorotaxane is:



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][ $\alpha$ -hydro- $\omega$ -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  $\alpha$ -cyclodextrin ring.



As the macromolecule threading component contains only one stopper, 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:  $\alpha$ -[2,2,2-tris(4-*tert*-butylphenyl)ethyl]- $\omega$ -methoxy-poly(oxyethyleneoxyadipoyl).

Source-based name of the macromolecule is:  $\alpha$ -[2,2,2-tris(4-*tert*-butylphenyl)ethyl]- $\omega$ -methoxy-poly(ethylene adipate).

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

## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

*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.

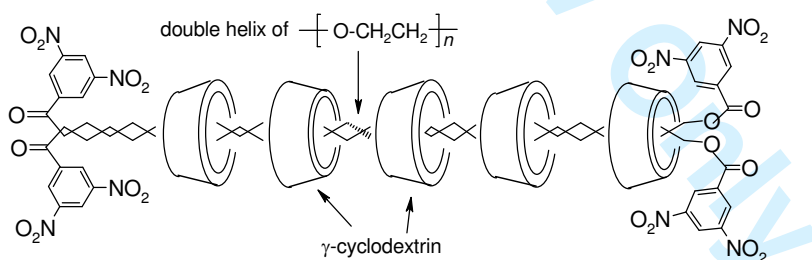
Possible names for this main-chain macromolecular pseudorotaxane are:

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

*Note:* If the order of 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 semisystematic name for the MC gives the following name:

[3]{[ $\alpha$ -[2,2,2-tris(4-*tert*-butylphenyl)ethyl]- $\omega$ -methoxypoly(ethylene adipate)]-rotaxa-[1][ $\alpha$ -cyclodextrin]-[1][bis(1,4-phenylene)[34]crown-10]}.

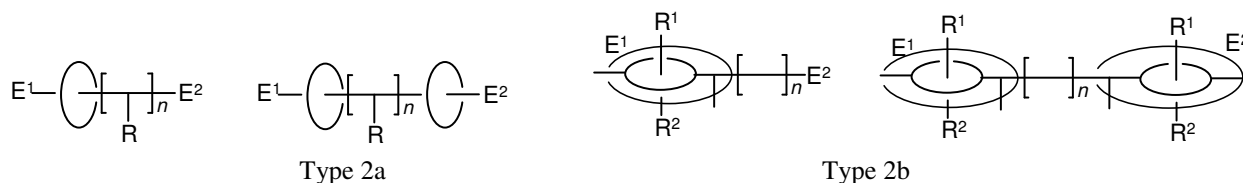
*Example 4* Double helix of two poly(oxyethylene) chains,  $t = 2$ , with 3,5-dinitrobenzoyl end-groups threads uncertain number of  $\gamma$ -cyclodextrin rings ( $m$  and thus also  $n$  are not known).



[2+m]{[2][ $\alpha$ -(3,5-dinitrobenzoyl)- $\omega$ -[(3,5-dinitrobenzoyl)oxy]poly(oxyethylene)]-rotaxa-[m][ $\gamma$ -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)

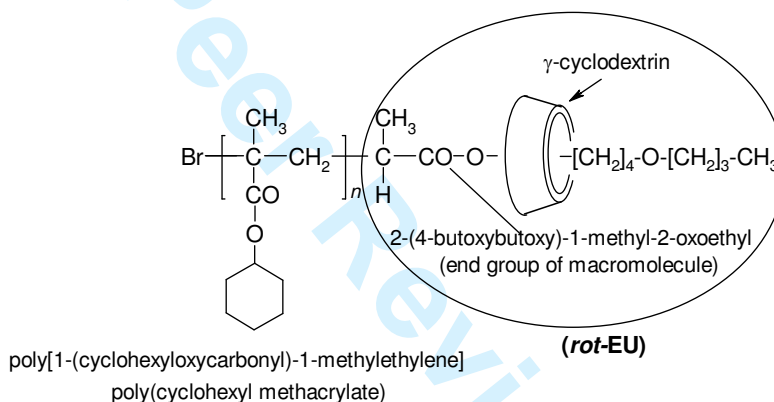


The generic name format for macromolecular rotaxanes of Type 2 (Table 2.1) is:

$\alpha$ -(name of *rot*-EU<sup>1</sup> or E<sup>1</sup>)- $\omega$ -(name of *rot*-EU<sup>2</sup> or E<sup>2</sup>)(name of the main part of macromolecule)

Note that the order of end-groups (E<sup>i</sup>) and rotaxane end units (*rot*-EU<sup>i</sup>) 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  $\gamma$ -cyclodextrin ring.

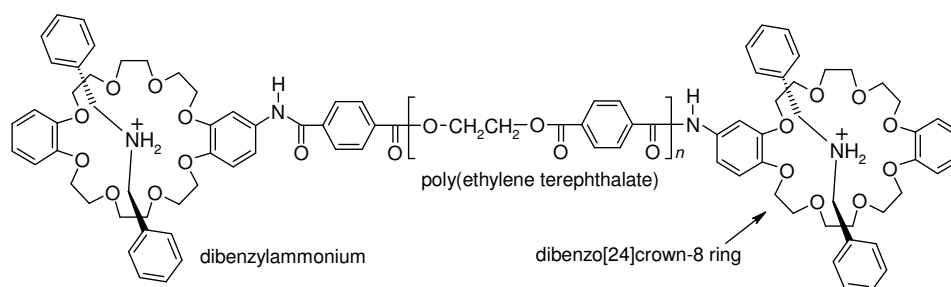


Structure-based and source-based names of the main part of macromolecule as well as the name of the threaded end-group are shown in the above formula. The other end-group is bromo. Possible names are:

$\alpha$ -bromo- $\omega$ -[2]{[2-(4-butoxybutoxy)-1-methyl-2-oxoethyl]-*rotaxa*-[ $\gamma$ -cyclodextrin]}poly[1-(cyclohexyloxycarbonyl)-1-methylethylene];

$\alpha$ -bromo- $\omega$ -[2]{[2-(4-butoxybutoxy)-1-methyl-2-oxoethyl]-*rotaxa*-[ $\gamma$ -cyclodextrin]}poly(cyclohexyl methacrylate).

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



## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

Systematic names of the end-groups are:

$\alpha$ -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

$\omega$ -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-ylamino.

Semisystematic names of the end-groups are:

$\alpha$ -group: 4-[[dibenzo[24]crown-8)-2-yl]carbamoyl]benzoyl

$\omega$ -group: (dibenzo[24]crown-8)-2-ylamino.

Systematic name of TC is: *N*-benzyl-1-phenylmethanamine

Semisystematic name of TC is: dibenzylammonium.

Semisystematic (usual) names of rotaxane EUs (*rot*-EU) are:

$\alpha$ -*rot*-EU: [2]{[dibenzylammonium]-*rotaxa*-[4-[[dibenzo[24]crown-8)-2-yl]carbamoyl]benzoyl}};

$\omega$ -*rot*-EU: [2]{[dibenzylammonium]-*rotaxa*-[(dibenzo[24]crown-8)-2-ylamino]}.

Structure-based name of the macromolecule main part is: poly(oxyethyleneoxyterephthaloyl).

Source-based name of macromolecule main part is: poly(ethylene terephthalate); its abbreviation is PET.

To highlight that the macrocyclic component is associated recognition sites of TCs the prefix (*rs-MC*) may be added before the name of rotaxane assembly.

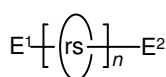
A combination of semisystematic names for *rot*-EUs with structure-based name for the macromolecule main part gives the name:

$\alpha$ -(*rs-MC*)[2]{[dibenzylammonium]-*rotaxa*-[4-[[dibenzo[24]crown-8)-2-yl]carbamoyl]benzoyl}- $\omega$ -(*rs-MC*)[2]{[dibenzylammonium]-*rotaxa*-[(dibenzo[24]crown-8)-2-ylamino]}poly(oxyethyleneoxyterephthaloyl).

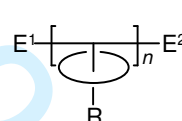
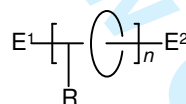
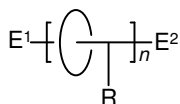
If a source-based name or abbreviation is used to name the macromolecule main part, the rigorous inclusion of the terephthaloyl MU into  $\alpha$ -*rot*-EU need not be expressed and a shortened name format can be used, for example:

$\alpha,\omega$ -bis((*rs-MC*)[2]{[dibenzylammonium]-*rotaxa*-[(dibenzo[24]crown-8)-2-ylamino]})PET.

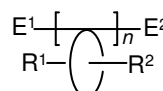
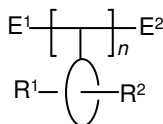
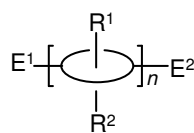
### MRO-3.3 Type 3 - regular macromolecular rotaxanes



Type 3a



Type 3b



Type 3c

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:

## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

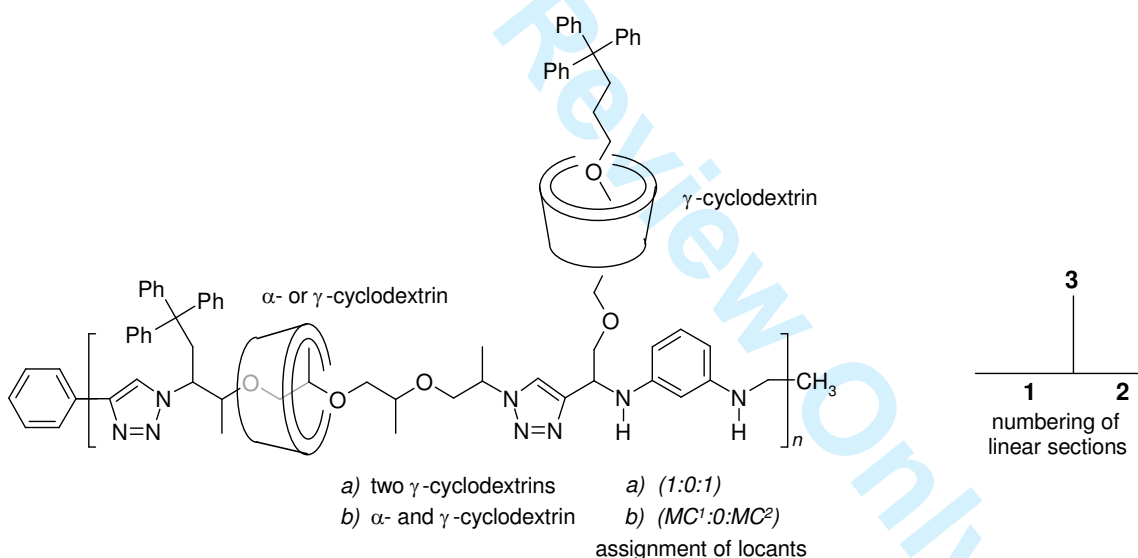


The IUPAC preferred structure-based name is: poly((*rs*-MC)-[2]{[(dimethyliminio)dodecane-1,12-diyl bromide]-rotaxa-[2,5,8,11,14,16,19,22,25,28-decaoxa-1,15(1,4)-dibenzenacyclooctacosaphane]}).

Combination of the structure-based name for macromolecule and semisystematic 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 - rotaxane CRU with a side chain as stopper; two of three linear sections of CRU are threaded:

- two identical MCs – each  $\gamma$ -cyclodextrin molecule;
- two different MCs – one  $\alpha$ -cyclodextrin molecule; another one  $\gamma$ -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-molecular-weight rotaxanes (see section MRO-2.6 and ref. [1], section ROT-5). The order numbers are assigned to the linear sections starting from the beginning to 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:

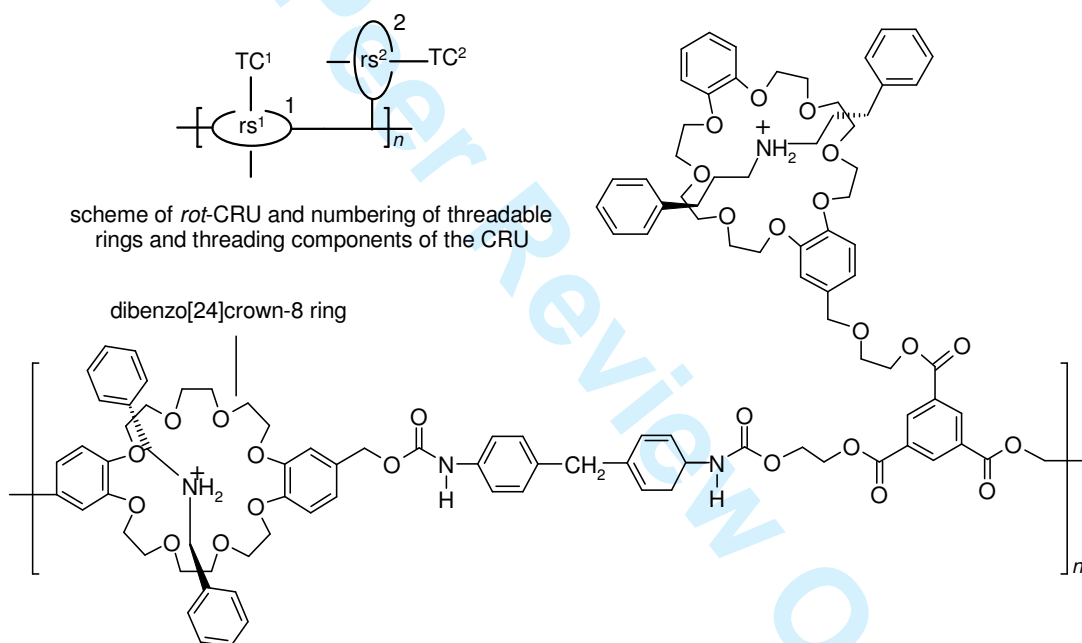
## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

- a)  $\alpha$ -phenyl- $\omega$ -methyl-poly[(1:0:1)-[3]{[1][(triazole-4,1-diyl)[1-(2,2,2-triphenylethyl)-2,5,8,11-tetramethyl-3,6,9-trioxaundecane-1,11-diyl](triazole-1,4-diyl)[(11,11,11-triphenyl-2,7-dioxaundecan-1-yl)methylene]imino(1,3-phenylene)iminomethylene]-rotaxa-[2][ $\gamma$ -cyclodextrin}}].

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

- b)  $\alpha$ -phenyl- $\omega$ -methyl-poly[( $MC^1:0:MC^2$ )-[3]{[(triazole-4,1-diyl)[1-(2,2,2-triphenylethyl)-2,5,8,11-tetramethyl-3,6,9-trioxaundecane-1,11-diyl](triazole-1,4-diyl)[(11,11,11-triphenyl-2,7-dioxaundecan-1-yl)methylene]imino(1,3-phenylene)iminomethylene]-rotaxa-[1][ $\alpha$ -cyclodextrin]-rotaxa-[1][ $\gamma$ -cyclodextrin}}].

**Example 9** Type 3c macromolecular rotaxanes - 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<sup>1</sup>:TC<sup>2</sup>)-[3]{[1]([dibenzylammonium]-[1][bis(3-phenylpropyl)ammonium]-rotaxa-[1]([dibenzo[24]crown-8)-2,12-diylmethyleneoxycarbonylimino(1,4-phenylene)methylene(1,4-phenylene)iminocarbonyloxyethyleneoxycarbonyl[5-(2-[(dibenzo[24]crown-8)-2-yl]methoxy}ethoxycarbonyl)-1,3-phenylene]carbonyloxymethylene}}].

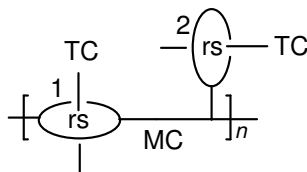
(Note that dibenzylammonium and bis(3-phenylpropyl)ammonium are both semisystematic names.)



## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

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 CRU of the macromolecular part of *rot*-CRU, possible name for such macromolecular rotaxane would be:

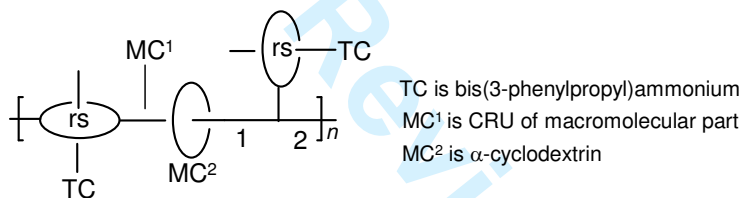
poly[(*rs*-*MC*)-(1:1)-[3]{[2][bis(3-phenylpropyl)ammonium]-*rotaxa*-[1][abbreviation for CRU]}].



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*<sup>1</sup>:*rs*-*MC*<sup>2</sup>) can be added to emphasize association of TCs with *MC*<sup>1</sup> and *MC*<sup>2</sup>.

**Example 10** Type 3 – a model complex macromolecular rotaxane that is a combination of types 3b and 3c - 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. Scheme of such macromolecular 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*<sup>1</sup>) 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*<sup>2</sup> is  $\alpha$ -cyclodextrin. Then a possible name for such a macromolecular rotaxane can be:

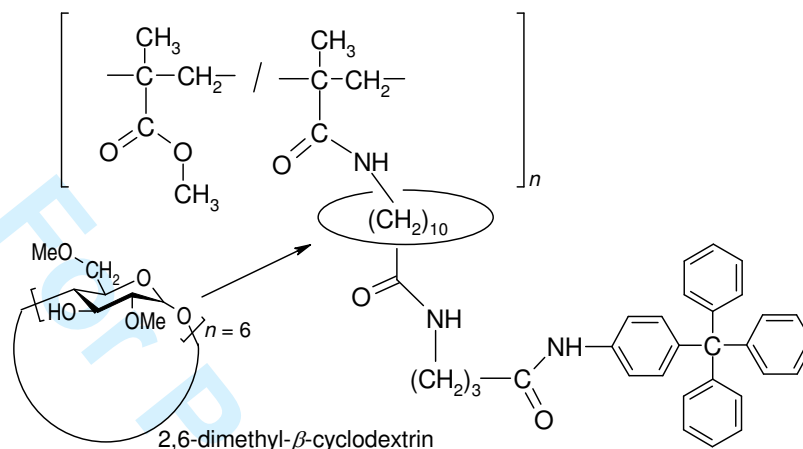
poly((*rs*-*MC*)-(1:1)-[4]{[2][bis(3-phenylpropyl)ammonium]-*rotaxa*-[(1:0)-[2]{[1][abbreviation for CRU]-*rotaxa*-[1][ $\alpha$ -cyclodextrin]}]}).

### MRO-3.4 Type 4 - irregular macromolecular rotaxanes

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

## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes

**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-dimethyl- $\beta$ -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:

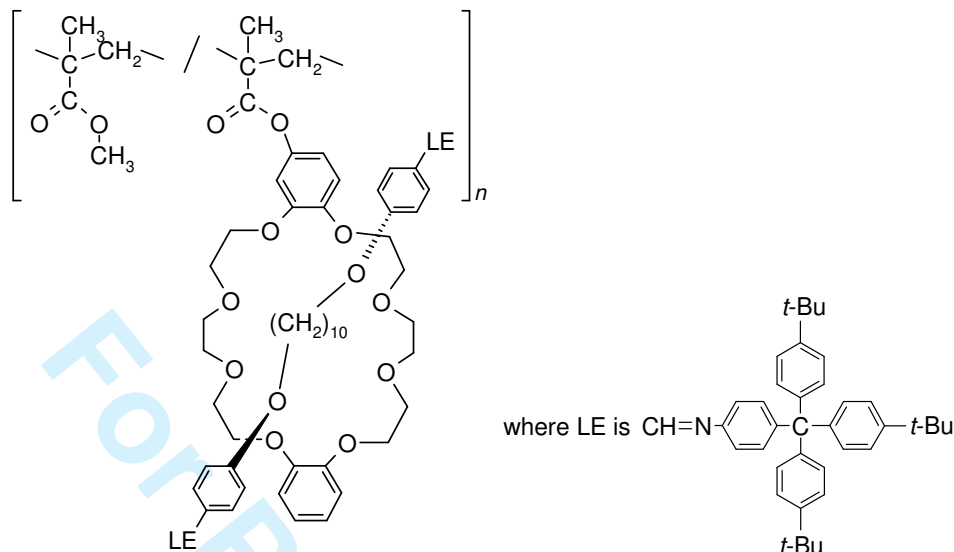
structure-based name:

poly([1-(methoxycarbonyl)-1-methylethylene]/(*0:1*)-[2]{[1-methyl-1-[[11-oxo-11-({4-oxo-4-[(4-tritylphenyl)amino]butyl}]amino)undecyl]carbonyl}ethylene]-*rotaxa*-[2,6-dimethyl- $\beta$ -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-dimethyl- $\beta$ -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-phenylenemethylidene)]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:

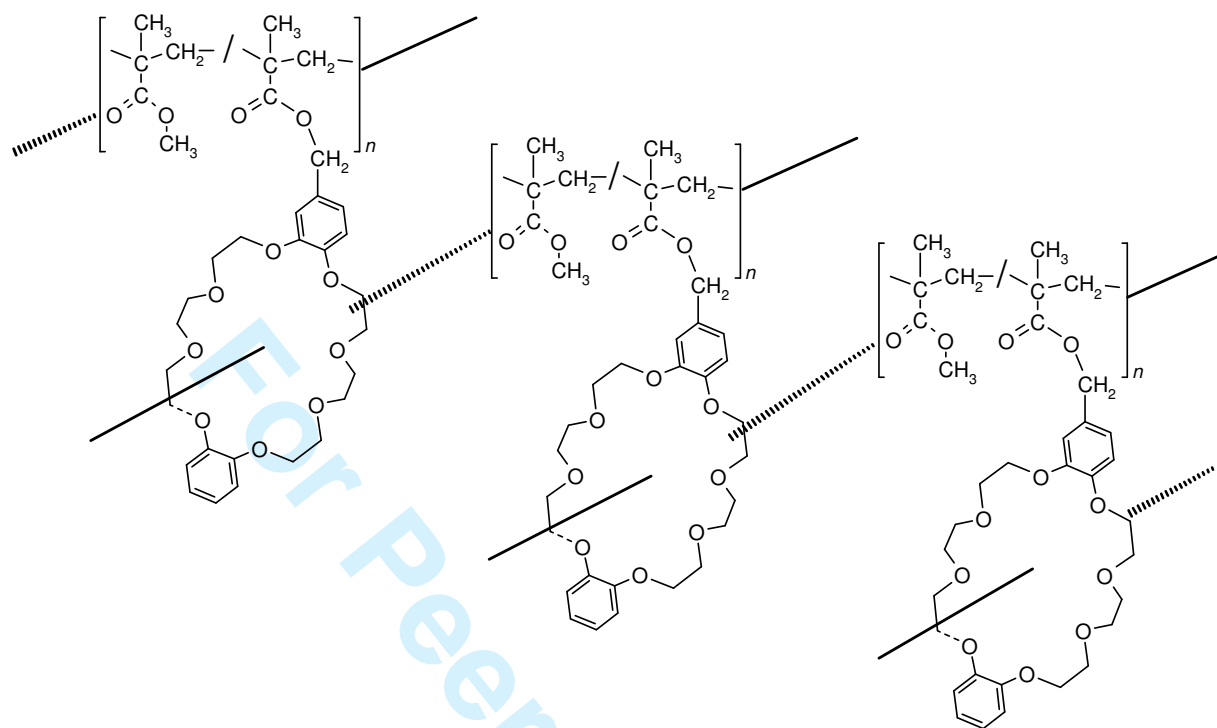
poly(methyl methacrylate-*co*-[2][[*N,N'*-(decane-1,10-diylbis(oxy-4,1-phenylenemethylidene)]bis{4-[tris(4-*tert*-butylphenyl)methyl]aniline}-rotaxa-(dibenzo[24]crown-8)-2-yl methacrylate]])

### 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 section(s) - threading component(s), and threadable ring(s) – macrocyclic component(s).

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

## Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes



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}].

## MEMBERSHIP OF SPONSORING BODIES

Membership of the IUPAC Chemical Nomenclature and Structure Representation Division for the period 2010–2011 was as follows:

**President:** R. M. Hartshorn (New Zealand); **Secretary:** T. Damhus (Denmark); **Past President:** G. P. Moss (UK); **Titular Members:** J. Brecher (USA); K. Degtyarenko (UK); P. Hodge (UK); A. T. Hutton (South Africa); L. G. Jeffery (UK); J. Wilson (USA), A. Yerin (Russia); **Associate Members:** K.-H. Hellwich (Germany); J. Kahovec (Czech Republic); E. Nordlander (Sweden); J. Nyitrai (Hungary); W. H. Powell (USA); J. Reedijk (Netherlands) **National Representatives:** S. Baskaran (India); M. A. J. Miah (Bangladesh); P. Moyna (Uruguay); H. Ogino (Japan); R. F. Pellón (Cuba); A. P. Rauter (Portugal); R. B. de Alencatro (Brasil).

Membership of the IUPAC Polymer Division Committee for the period 2010–2011 was as follows:

**President:** C. K. Ober (USA); **Vice President:** M. Buback (Germany); **Secretary:** M. Hess (Germany); **Past President:** J.-I. Jin (Korea); **Titular Members:** T. Chang (Korea); R. G. Jones (UK); S. Penczek (Poland); G. T. Russell (New Zealand); M. Sawamoto (Japan); R. F. T. Stepto (UK), J.-P. Vairon (France); **Associate Members:** S. C. Kim (Korea); T. Kitayama (Japan); P. Kubisa (Poland); W.

Mormann (Germany); J. Stejskal (Czech Republic); M. Vert (France); **National Representatives:** D. Berek (Slovakia); D. J. Dijkstra (Germany); G. Galli (Italy); J. K. Kallitsis (Greece); Z.-C. Li (China); G. Moad (Australia); M. Raza Shah (Pakistan); R. Prakesh Singh (India); M. Žigon (Slovenia).

Membership of the Subcommittee on Polymer Terminology (until 2005, the Subcommittee on Macromolecular Terminology) for the period 2009–2010 was as follows:

**Chair:** R. G. Jones (UK); **Secretary:** M. Hess (Germany); **Members:** G. Allegra (Italy); M. Barón (Argentina); T. Chang (Korea); C. dos Santos (Brazil); A. Fradet (France); J. He (China); K.-H. Hellwich (Germany); R. C. Hiorns (France); 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); S. V. Meille (Italy); I. Mita (Japan); G. Moad (Australia); W. Mormann (Germany); N. Nakabayashi (Japan); C. K. Ober (USA); S. Penczek (Poland); I. Schopov (Bulgaria); F. Schué (France); S. Slomkowski (Poland); R. F. T. Stepto (UK); D. Tabak (Brazil); J.-P. Vairon (France); M. Vert (France); J. Vohlídal (Czech Republic); W. J. Work (USA).

## REFERENCES

1. A. Yerin, E. S. Wilks, G. P. Moss, A. Harada. *Pure Appl. Chem.* **80**, 2041 (2008).
2. M. Barón, K.-H. Hellwich, M. Hess, K. Horie, A. D. Jenkins, R. G. Jones, J. Kahovec, P. Kratochvíl, W. V. Metanomski, W. Mormann, R. F. T. Stepto, J. Vohlídal, E. S. Wilks. *Pure Appl. Chem.* **81**, 1131 (2009).
3. H. W. Gibson, M. C. Bheda, P. T. Engen. *Prog. Polym. Sci.* **19**, 843 (1994).
4. J.-P. Sauvage, C. Dietrich-Buchecker, (Eds.). *Molecular Catenanes, Rotaxanes and Knots*. Wiley-VCH, Weinheim 1999. See Chapter 11: "Polyrotaxanes - Syntheses and Properties" (pp. 277-321).
5. I. G. Panova, I. N. Topchieva. *Russian Chemical Reviews* **70**, 23 (2001).
6. F. H. Huang, H. W. Gibson. *Prog. Polym. Sci.* **30**, 982 (2005).
7. J. Araki, K. Ito. *Soft Mat.* **3**, 1456 (2007).
8. A. Harada, A. Hashidzume, H. Yamaguchi, Y. Takashima. *Chem. Rev.* **109**, 5974 (2009).
9. A. Harada, Y. Takashima, H. Yamaguchi. *Chem. Soc. Rev.* **38**, 875 (2009).
10. H. W. Gibson, A. Farcas, J. W. Jones, Z. X. Ge, F. H. Huang, M. Vergne, D. M. Hercules. *J. Polym. Sci. Polym. Chem.* **47**, 3518 (2009).
11. L. Fang, M. A. Olson, D. Benitez, E. Tkatchouk, W. A. Goddard, J. F. Stoddart. *Chem. Soc. Rev.* **39**, 17 (2010).
12. *Compendium of Polymer Terminology and Nomenclature*. IUPAC Recommendations 2008. Edited by R. G. Jones, J. Kahovec, R. Stepto, E. S. Wilks, M. Hess, T. Kitayama, W. V. Metanomski, with advice from A. Jenkins and P. Kratochvíl, RSC Publishing, Cambridge, UK (2008).
13. W. Ring, I. Mita, A. D. Jenkins, N. M. Bikales. *Pure Appl. Chem.* **57**, 1427 (1985). (Reprinted as Chapter 19 in ref. 12.).
14. J. Kahovec, P. Kratochvíl, A. D. Jenkins, I. Mita, I. M. Papisov, L. H. Sperling, R. F. T. Stepto. *Pure Appl. Chem.* **69**, 2511 (1997). (Reprinted as Chapter 20 in ref. 12.).
15. R. E. Bareiss, R. B. Fox, K. Hatada, K. Horie, A. D. Jenkins, J. Kahovec, P. Kubisa, E. Maréchal, I. Meisel, W. V. Metanomski, I. Mita, R. F. T. Stepto, E. S. Wilks. *Pure Appl. Chem.* **73**, 1511 (2001). (Reprinted as Chapter 21 in ref. 12.).
16. R. B. Fox, N. M. Bikales, K. Hatada, J. Kahovec. *Pure Appl. Chem.* **66**, 873 (1994). (Reprinted as Chapter 17 in ref. 12.).
17. J. Kahovec, R. B. Fox, K. Hatada. *Pure Appl. Chem.* **74**, 1921 (2002). (Reprinted as Chapter 15 in ref. 12.).

*Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes*

18. W. V. Metanowski, R. E. Bareiss, J. Kahovec, K. L. Loening, L. Shi, V. P. Shibaev. *Pure Appl. Chem.* **65**, 1561 (1993). (Reprinted as Chapter 16 in ref. 12.).
19. M. Barón, R. B. Fox, A. Fradet, K.-H. Hellwich, P. Hodge, K. Horie, J. Kahovec, P. Kubisa, E. Maréchal, W. Mormann, R. F. T. Stepto, J. L. Schultz, E. S. Wilks. *Pure Appl. Chem.* **80**, 201 (2008).
20. *IUPAC. Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H*, Pergamon Press, Oxford (1979).
21. *A Guide to IUPAC Nomenclature of Organic Compounds*, R. Panico, W. H. Powell, J.-C. Richer (eds.), Blackwell Scientific Publications, Oxford, 1993. Errata: H. A. Favre, K.-H. Hellwich, G. P. Moss, W. H. Powell, J. G. Traynham. *Pure Appl. Chem.* **71**, 1327 (1999).
22. *IUPAC. Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005* (the “Red Book”), N. G. Connelly, T. Damhus, R. M. Hartshorn, A. T. Hutton (eds.), RSC Publishing, Cambridge (2005).
23. A. D. Jenkins, P. Kratochvíl, R. F. T. Stepto, U. W. Suter. *Pure Appl. Chem.*, **68**, 2287 (1996). (Reprinted as Chapter 1 in ref. 12.).
24. K. Horie, M. Barón, R. B. Fox, J. He, M. Hess, J. Kahovec, T. Kitayama, P. Kubisa, E. Maréchal, W. Mormann, R. F. T. Stepto, D. Tabak, J. Vohlídal, E. S. Wilks, W. J. Work. *Pure Appl. Chem.* **76**, 889 (2004).
25. S. Brovelli, F. Cacialli. *SMALL* **6**, 2796 (2010).
26. M. Hess, R. G. Jones, J. Kahovec, T. Kitayama, P. Kratochvíl, P. Kubisa, W. Mormann, R. F. T. Stepto, D. Tabak, J. Vohlídal, E. S. Wilks. *Pure Appl. Chem.* **78**, 2067 (2006). (Reprinted as Chapter 10 in ref. 12.).
27. C. J. Pedersen and H. K. Frensdorff. *Angew. Chem.* **84**, 16 (1972); *Angew. Chem. Int. Ed. Engl.* **11**, 16 (1972).

**ALPHABETICAL INDEX OF TERMS**

(prefixes MRO- are omitted)

(bold characters refer to **main entries**)**TERMINOLOGY FOR MACROMOLECULAR****ROTAXANES 1**

cyclic macromolecule 1.1

end-group 1.15, 1.21, 2.4

end-group stopper 1.21

**EXAMPLES OF SYSTEMATIC NAMES FOR****MACROMOLECULAR ROTAXANES 3**Generic types of and generic name formats for macromolecular rotaxanes **2.4**Guideline for a construction of the names for macromolecular rotaxanes **2.5**

half-capped pseudorotaxane 1.8

internal stopper 1.21

irregular macromolecular rotaxane 2.4, 3.4

Isomerism of macromolecular rotaxanes **2.6**

Isomerism – positions of various macrocyclic components

threaded on several linear sections **2.6.1**

Isomerism – positions of various threading components

threaded through different threadable cycles **2.6.2**Isomerism – recognition sites **2.6.3**

Isomerism – positions of various macrocyclic components

threaded on several linear sections **2.6.1**

macrocyclic 1.1

macrocyclic component **1.1** and almost each entry

macrocyclic molecule 1.1

macromolecular component **1.2**macromolecular pseudorotaxane **1.3**, 1.9, 2.1macromolecular rotaxane **1.4** and almost each entry

macromolecular semirotaxane 1.3

main-chain macromolecular rotaxane 1.4, **1.5**, 1.6, 1.11

main-chain polyrotaxane 1.6

main-chain rotaxane polymer **1.6**

main-chain threadable ring 1.1

molecular shuttle **1.7**, 1.10, 2.6.3

Names for macromolecular rotaxanes and

macromolecular pseudorotaxanes **2.1****NOMENCLATURE FOR MACROMOLECULAR****ROTAXANES 2**

non-threadable cycle 1.22

polymeric rotaxane **1.18**

polypseudorotaxane 1.9

polyrotaxane 1.18

polysemirotaxane 1.9

pseudopolyrotaxane 1.9

pseudorotaxane 1.3, 1.7, **1.8**, 1.9pseudorotaxane polymer 1.8, **1.9**recognition site 1.7, **1.10**, 2.4, 2.6.3regular macromolecular rotaxane 1.3, **1.11**, 2.4, 3.3rotaxane **1.12** and almost each entryrotaxane constitutional repeating unit 1.4, 1.14, **1.13**, 1.21, 2.4, 2.5rotaxane constitutional unit 1.4, 1.5, **1.14**, 1.19rotaxane end unit **1.15**, 2.4, 2.5

rotaxane isomer locant 2.6.1, 2.6.2, 2.6.3

rotaxane monomer **1.16**, 2.4, 2.5rotaxane monomer unit **1.17**, 2.4, 2.5rotaxane monomeric unit **1.17**, 2.4, 2.5rotaxane polymer **1.18**, 2.4

semirotaxane 1.8, 1.9

semirotaxane polymer 1.9

side-chain macromolecular rotaxane 1.4, 1.5, 1.11, **1.19**, 1.20

side-chain polyrotaxane 1.20

side-chain rotaxane polymer **1.20**

side-chain threadable ring 1.1

source-based systematic names for macromolecules 2.2, 2.4, 2.5

Sources of the nomenclature for macromolecular rotaxanes **2.2**stopper 1.11, **1.21**, 2.1, 2.4

structure-based systematic names for macromolecules 2.2, 2.4, 2.5

systematic name formats for rotaxanes, generic **2.4**threadable cycle 1.3, **1.22**, 1.23threadable ring 1.1, **1.22**, 1.23threading component **1.23** and almost each entry

topologic isomerism 2.6

Type 1 - linear macromolecule threads one or more macrocyclic components **3.1**Type 2 – normal macromolecule with rotaxane end unit(s) **3.2**Type 3 - regular macromolecular rotaxanes **3.3**Type 3 - irregular macromolecular rotaxanes **3.4**Type 5 - interlocked macromolecules **3.5**types of rotaxanes, generic **2.4**Use of systematic and non-systematic names and abbreviations **2.3**

1  
2  
3  
4 **LIST OF ABBREVIATIONS AND PREFIXES**  
5

6 -*co*- connective to join names of monomers in the  
7 source-based name of a copolymer  
8 CRU constitutional repeating unit  
9 CU constitutional unit  
10 *m* number of macrocyclic components in a  
11 rotaxane species  
12 MC macrocyclic component (of rotaxane)  
13 *MC<sup>i</sup>* locant for *i*-th macrocyclic component  
14 MRO IUPAC identifier of this nomenclature  
15 document on macromolecular rotaxanes  
16 MU monomeric unit  
17 *n* total number of independent components in a  
18 rotaxane species;  $n = t + m$   
19 ROT IUPAC identifier of the nomenclature  
20 document on rotaxanes, ref. [1]  
21 -*rotaxa*- connective to join the names of the threading  
22 and macrocyclic components in the name of a  
23 rotaxane  
24 *rot*-CRU rotaxane CRU  
25 *rot*-CU rotaxane CU  
26 *rot*-EU rotaxane end unit  
27 *rot*-MU rotaxane MU  
28 *rs* recognition site  
29 *rs<sup>i</sup>* locant for *i*-th recognition site  
30 *t* number of threading components in a  
31 rotaxane species  
32 TC threading component  
33 *TC<sup>i</sup>* locant for *i*-th threading component  
34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60