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Nomenclature for Rotaxanes

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Complete List of Authors:	Yerin, Andrey; Advanced Chemistry Development Metanomski, W. Val; Chemical Abstracts Service Moss, Gerard; Queen Mary College, University of London, Department of Chemistry Wilks, Edward S.; N/A Harada, Aika; Osaka University, Graduate School of Science
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INTRODUCTORY NOTES
for IUPAC Provisional Recommendations
"NOMENCLATURE FOR ROTAXANES"

The first IUPAC recommendations for naming of rotaxanes provide a method for unambiguous description of composition and structure of various types of rotaxanes and include the following main parts:

1. Definitions of terms used in rotaxanes:
    a. rotaxane itself,
    b. rotaxane components,
        i. threading component and linear section,
        ii. macrocyclic component and threadable ring,
    c. molecular shuttles and recognition sites.
2. History of the nomenclature of rotaxanes.
3. Classification of rotaxane types.
4. Generic name format for rotaxanes.
5. Types of rotaxane isomerism and description of the location of simple macrocyclic components at different linear sections of a complex threading component and location of simple threading components in macrocyclic components with several threadable rings.
6. Types and specification of rotaxane stereoisomerism – orientation of rotaxane components in relation to each other.
7. Examples of rotaxanes and recommended names.

The recommended generic name format is:

$$\textbf{\textit{prefix}}\text{-}[\textit{v}]\{[\textit{w}_1](\mathrm{TC}_1)\text{-}[\textit{w}_2](\mathrm{TC}_2)\text{-}\ldots\text{-}\textbf{\textit{rotaxa}}\text{-}[\textit{x}_1](\mathrm{MC}_1)\text{-}[\textit{x}_2](\mathrm{MC}_2)\text{-}\ldots\}$$

where:

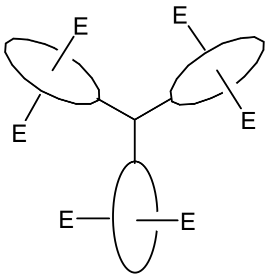
TC$_n$ – names of threading components,
rotaxa - a connector to join the names of the threading and macrocyclic components,
MC$_n$ – names of macrocyclic components,
w$_n$ and **x$_n$** – numbers of specific threading and macrocyclic components respectively,
v – total number of rotaxane components – sum of **w$_n$** and **x$_n$**,
prefix – description of position and orientation of rotaxane components with respect to each other if variants are possible.

The recommended name format allows use of retained names and abbreviations for components in rotaxane names for general use, but chemical names created according to IUPAC nomenclature recommendations are preferred in systematic nomenclature.

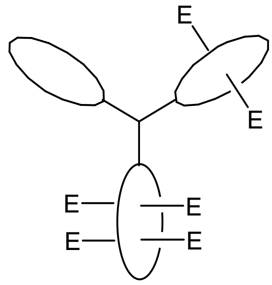
The recommendations provide principles to specify isomerism for the following basic types of rotaxanes:

- rotaxanes composed of simple threading components and simple macrocyclic components,
- rotaxanes composed of several simple macrocyclic components and a single threading component with several linear sections,
- rotaxanes composed of a single complex macrocyclic component with several threadable rings and several simple threading components
- molecular shuttles.

For specification of positional isomerism in rotaxanes that include macrocyclic components with several threading rings, the prefix includes the number of threading components positioned in each threadable ring. For example, the following two isomeric [4]rotaxanes will have the following generic names:

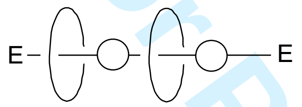


***1:1:1*-[4]{[3](TC)-*rotaxa*-(MC)}**

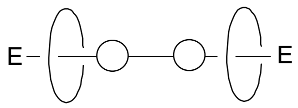


***2:1:0*-[4]{[3](TC)-*rotaxa*-(MC)}**

Rotaxanes composed of several macrocyclic components and one threading component with several threading sections are named according to the same principles:



***1:1:0*-[3][(TC)-*rotaxa*-[2](MC)]**

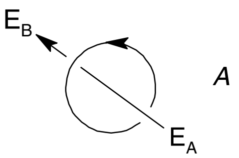


***1:0:1*-[3][(TC)-*rotaxa*-[2](MC)]**

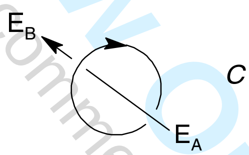
To define stereoisomers of rotaxanes, the following types of asymmetry of rotaxane components are taken into account:

- threading component direction,
- threadable ring direction, and
- nonequivalence of threadable ring sides.

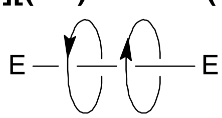
Several types of stereoisomerism and the procedures to define specific stereoisomers in a rotaxane name are recommended. For example, the reported cases of "cyclochirality" are unambiguously defined by means of *A* and *C* descriptors that correspond to anticlockwise and clockwise orientation of a macrocyclic component in relation to unsymmetrical threading components or to another macrocyclic component.



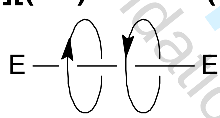
***A*-[2][(TC)-*rotaxa*-(MC)]**



***C*-[2][(TC)-*rotaxa*-(MC)]**



***C,A*-[3][(TC)-*rotaxa*-[2](MC)]**



***A,C*-[3][(TC)-*rotaxa*-[2](MC)]**

The procedures to assign direction in threading and macrocyclic components are based on Cahn-Ingold-Prelog sequence rules.

The recommended procedures are defined for many reported types of rotaxanes and can be expanded to more complex types.

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INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION

NOMENCLATURE FOR ROTAXANES

(IUPAC Recommendations 2005)

Prepared by a Working Group Consisting of

A. HARADA (Japan), W. V. METANOMSKI (USA), G. P. MOSS (UK), E. S. WILKS (USA), and A. YERIN (Russia)

CONTENTS

Abstract: Expanded definitions of rotaxanes, their components, and other terms concerning rotaxanes are given. The classification of rotaxanes and nomenclature principles for naming of different types of rotaxanes are described and illustrated with examples. Recommendations are provided for unambiguous description of rotaxane isomerism with special descriptors that include information about position and orientation of rotaxane components.

INTRODUCTION

Rotaxanes were first represented pictorially in 1958 [1] as in-situ intermediates in the synthesis of [2]catenanes. Rotaxanes were proposed as a new type of species (though not referred to as pseudorotaxanes or rotaxanes) in 1961 [2], and shown to exist in 1967 [3-5]. However, it was not until 1971 that Schill [6] introduced a nomenclature system for rotaxanes. In 2000, Vögtle and co-workers [7] proposed a generic nomenclature system in which Schill's description was extended to include information about mechanical or covalent linkages within the components of the rotaxane to distinguish between intermolecular and intramolecular rotaxanes. Nevertheless the proposed nomenclature cannot unambiguously describe the whole range of rotaxane structures reported in the literature. The current document specifies a systematic nomenclature for rotaxanes that includes the composition, structure, and isomerism of rotaxanes.

This document discusses only rotaxanes in which none of the components is a macromolecule, but the naming principles specified in this document can also be used to name macromolecular rotaxanes. Specific recommendations for naming rotaxanes with at least one polymeric component will be published in a separate document.

Because the structures of rotaxanes are often large, in most cases throughout this document schematic presentations of rotaxanes and their components are used. Full chemical structures of rotaxanes and their systematic names are given in the Section ROT-7 of this document.

The rotaxane literature has been extensively reviewed [8-19].

ROT-1. GLOSSARY

ROT-1.1. Rotaxane (generic)

A substance comprising a molecule with at least one structurally linear section onto which is threaded at least one **macrocyclic molecule** or a cyclic part of the molecule with a linear section.

The term rotaxane describes a molecular arrangement stabilized by some means, such as large end-groups attached to the linear component(s), specific interaction between the macrocyclic and linear components, or both. More particularly, a rotaxane is a molecular complex in which a linear molecule has ends (terminal groups) large enough to prevent a cyclic component from dethreading.

An example of a rotaxane is given in Figure 1.1.1

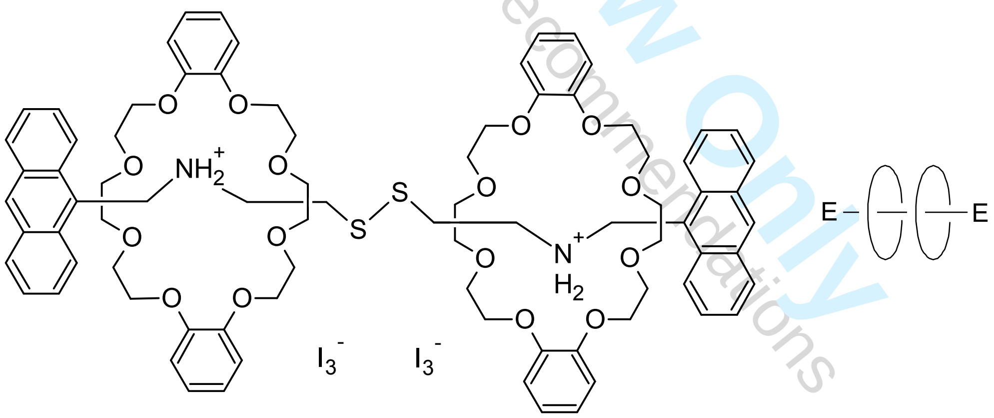


Figure 1.1.1. [3]Rotaxane and its schematic representation; E represents end-groups of threading molecule(s).

Note 1.1.1. The IUPAC Compendium of Chemical Terminology defines rotaxanes as molecules in which a ring encloses another, rod-like molecule having end groups too large to pass through the ring opening, and thus holds the rod-like molecule in position without covalent bonding [20]. The definition given in this document is more general to accommodate the wide variety of reported rotaxane compounds.

ROT-1.2. Macrocyclic molecule

A cyclic molecule of low molar mass that has at least one large ring and is not a macromolecule. In the rotaxane context, the term large ring means a ring size that allows it to be threaded onto a linear section of another molecule. Such large rings can be called threadable to distinguish them from the other smaller cycles within a complex macrocyclic component. Examples of macrocyclic molecules are shown in Figure 1.2.1.

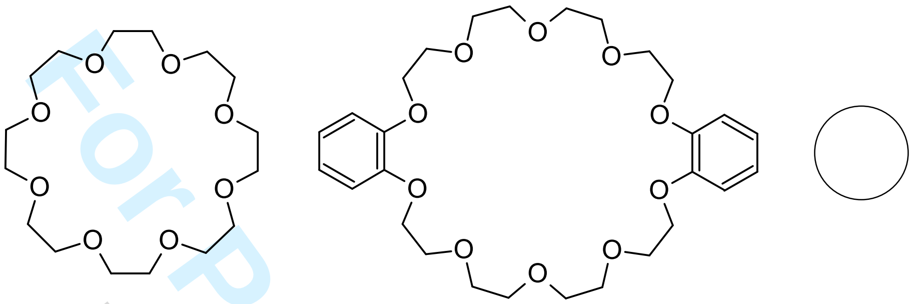


Figure 1.2.1. Macrocyclic molecules and their schematic representation

In addition to simple macrocyclic components that include only one threadable ring, more complex macrocyclic components may contain several such rings connected with each other. Several generic types of such macrocyclic components are described in sections ROT-3 and ROT-5, and specific examples are shown in section ROT-7.

Note 1.2.1. The literature on rotaxanes frequently cites the word “macrocycle”, which is, in rotaxanes, a contraction of (and an abbreviation for) macrocyclic molecule, rather than cyclic macromolecule; the latter are virtually never used as cyclic components in rotaxane assemblies. Use of the word “macrocycle” in rotaxane terminology is incompatible with the IUPAC definition of a macrocycle, which is “a cyclic macromolecule or a macromolecular cyclic portion of a macromolecule”. IUPAC recommendations for nomenclature of cyclic macromolecules are discussed elsewhere [21]. Figure 1.2.2 shows an example of a cyclic macromolecule.

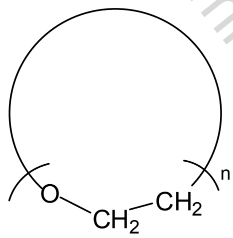


Figure 1.2.2. Cyclic macromolecule

Therefore, because the term “macrocycle” is ambiguous, its use in the rotaxane literature is not recommended.

ROT-1.3. Threading component (generic)

A component of a rotaxane assembly comprising at least one structurally linear section onto which at least one macrocyclic molecule is threaded.

The simplest threading component consists of one linear section and end-groups large enough to prevent dethreading of macrocyclic components; this is often called a dumbbell or sometimes an axle.

Note 1.3.1. For rotaxanes, the word "linear" is to be interpreted broadly. The linear section of the threading component can be either an unbranched chain or include small cyclic fragments that do not prevent threading through a macrocyclic molecule.

More complex threading components may contain several linear sections formed by branching points or internal large groups, often called stoppers, that prevent movement of macrocyclic components from one linear section to another. Threading components with several linear sections, such as "Y", "X", or "H"-shaped components that include three, four, or five linear sections respectively, are discussed in sections ROT-3 and ROT-5. Specific examples can be found in section ROT-7.

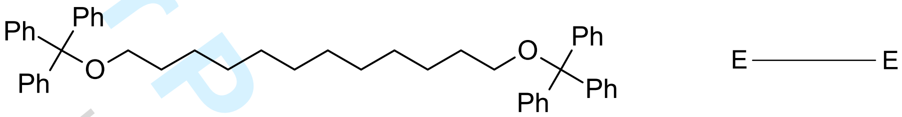


Figure 1.3.1. Example of threading component and its schematic representation

ROT-1.4. Pseudorotaxane (generic)

A rotaxane assembly in which threading component(s) has(have) ends small enough to permit threading or dethreading of the macrocyclic molecule(s).

The stability of such rotaxanes arises not from the spatially hindered dethreading of its components but by an interaction between threading and macrocyclic components, e.g., donor-acceptor or electrostatic.

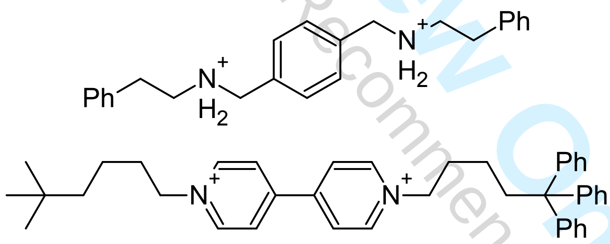


Figure 1.4.1. Examples of threading components; the first has two small end-groups and the second has one small and one large end-group.

Pseudorotaxanes in which only one end of a linear section is small enough to allow threading and dethreading of a macrocyclic component are sometimes called semirotaxanes or half-capped pseudorotaxanes.

The terms pseudorotaxane and semirotaxane are often used in the rotaxane literature, but from the nomenclature point of view it is immaterial whether the ends of a threading component are large enough to prevent dethreading or not. Also, the structural differences between pseudorotaxanes, semirotaxanes, and rotaxanes are not always obvious. It is possible to synthesize rotaxanes with ends that permit dethreading under some specific conditions (e.g., temperature, solvent, or both) but not others. Thus, differentiation between rotaxanes, pseudorotaxanes, and semirotaxanes is not the role of nomenclature. Systematic nomenclature names each specific structural component of the rotaxane, and the relationship of the structural components to each other, not the relative stability of the rotaxane assembly.

ROT-1.5. Recognition site

A recognition site is a part of a threading component with which a macrocyclic component prefers to associate.

Note 1.5.1. Examples of recognition sites in threading components of rotaxane assemblies are -N^+H_2- and [4,4′-bipyridinium]-1,1′-diyl. For threading components possessing more than one recognition site, the sites may be either identical with, or different from, each other.

ROT-1.6. Molecular shuttle

A molecular shuttle is a rotaxane assembly comprising a threading component, upon which is threaded a macrocyclic component that can reside at the specific recognition site (see ROT-1.5) on the threading component. Depending on the specific structural features and conditions such rotaxanes can exist either in a form in which macrocyclic components are associated with a specific fragment of threading component or in non-associated form where the macrocyclic component can move along a linear section . Figure 1.6.1 shows the representations of typical molecular shuttles. *E* represents an end-group and 'rs' represents a recognition site; the two recognition sites may be either identical or different.

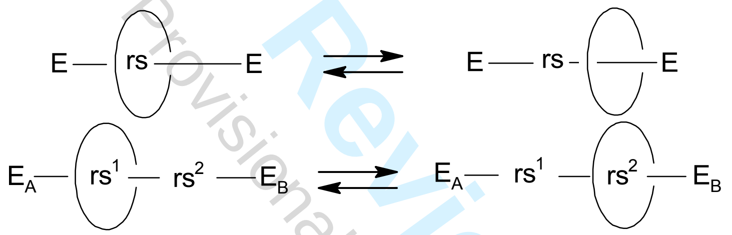


Figure 1.6.1. [2]Rotaxanes that function as a molecular shuttle.

ROT-2. HISTORY OF THE NOMENCLATURE OF ROTAXANES

The first nomenclature system for rotaxanes was proposed by Schill in 1971 [6]. According to this system the name of a rotaxane includes four parts:

(a) a prefix in the form of a bracketed integer that indicates the total number of components in the rotaxane
(b) the name of the threading component
(c) the name of each macrocyclic molecule, regardless of whether it is chemically identical with, or different from, other macrocyclic molecules present
(d) the unitalicized suffix 'rotaxane'.

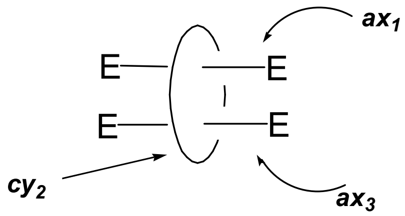
The following generic example summarizes Schill's nomenclature principle:

[*x*]-[name of threading component]-[name of macrocyclic molecule$_1$]-[name of macrocyclic molecule$_2$]-[name of macrocyclic molecule$_3$]-...-rotaxane

Note 2.1. In the prefix [*x*], the integer *x* represents the total number of threading and macrocyclic components; macrocyclic molecule$_1$, macrocyclic molecule$_2$, macrocyclic molecule$_3$, etc. represent structurally identical or different macrocyclic molecules.

In 2000, Vögtle and co-workers [7] proposed a generic nomenclature system in which Schill's prefix was extended to include information about mechanical (mec) or covalent (cov) linkage within the components of the rotaxane to distinguish between intermolecular and intramolecular rotaxanes.

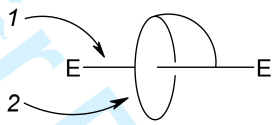
For example, for [3]rotaxanes of Type 2.1 (see Table 3.1), Vögtle's system leads to the prefix $[3^{ax1meccy2,cy2mecax3}]$.



ax_1, ax_3 = axles (components 1 and 3); cy_2 = macrocyclic molecule (component 2)

Figure 2.1. [3]Rotaxane of Type 2.1 (from Table 3.1)

For [1]rotaxanes of Type 9 (see Table 3.1), Vögtle and co-workers proposed the generic nomenclature system $[2^{1cov2,1mec2}]$rotaxane – see Figure 2.2.



ax = 1; *cy* = 2

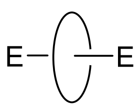
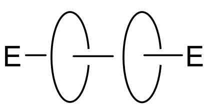
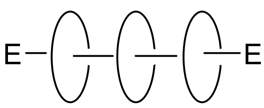
Figure 2.2. [1]Rotaxane of Type 9

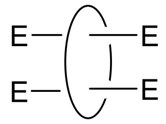
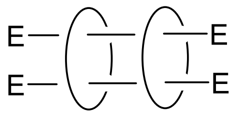
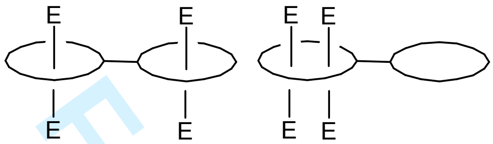
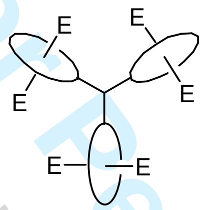
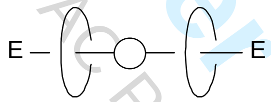
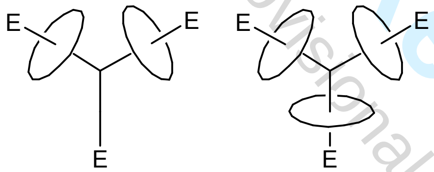
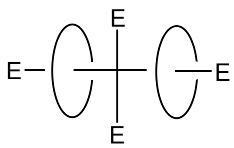
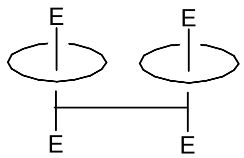
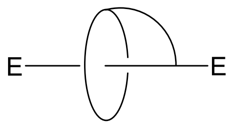
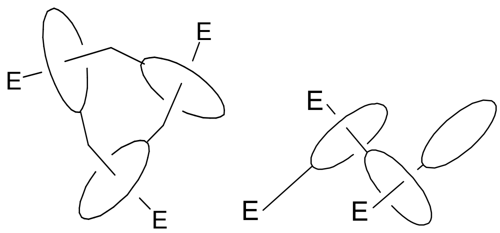
The nomenclature system described in this document is based on modifications of Schill's description of the rotaxane composition and Vögtle and co-workers' idea of the prefix that describes a specific arrangement of rotaxane components for each generic type of rotaxane.

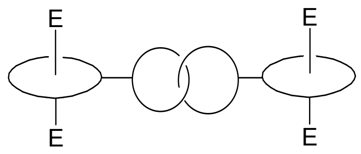
ROT-3. TYPES OF ROTAXANES

Schematic representations of eleven generic types of rotaxanes described since the earliest-known pictorial representation of a pseudorotaxane [1] in 1958 are given in Table 3.1.

Table 3.1. Idealized Representations of Eleven Generic Types of Rotaxanes.

Type	Generic Structure	Key Structural Features
1.1		[2]Rotaxane: a single linear molecule, upon which is threaded a single macrocyclic molecule.
1.2		[3]Rotaxane: a linear molecule, upon which are threaded two macrocyclic molecules.
1.3		[4]Rotaxane: a linear molecule, upon which are threaded three macrocyclic molecules.

2.1		[3]Rotaxane: two linear molecules, upon which are threaded a macrocyclic molecule.
2.2		[4]Rotaxane; two linear molecules, upon which are threaded two macrocyclic molecules.
3		Two covalently linked macrocyclic molecules that can be threaded by linear molecules. Two possible [3]Rotaxanes are shown [a]
4		Three macrocyclic molecules are covalently linked to form a Y-shaped molecule; each macrocyclic fragment may be threaded with a linear molecule. [4]Rotaxane is shown.
5		Threading component with two linear sections separated by a group large enough to prevent cyclic components from moving between the two linear sections. [3]Rotaxane is shown.
6		Y-shaped molecule with three linear sections; macrocyclic molecules can be situated at any linear section. [3] and [4]rotaxanes are shown.
7		X-shaped molecule with four linear sections; the macrocyclic molecules may be situated at any linear section. [3]Rotaxane is shown [a]
8		H-shaped threading component with five linear sections at which macrocyclic components may be situated. [3]Rotaxane is shown [b]
9		[1]Rotaxane: a linear part of a molecule threaded through a macrocyclic part of the same molecule.
10		Cyclic and acyclic "daisy chain": each molecule contains a linear moiety and a macrocyclic moiety. The linear moiety of one molecule is threaded through the macrocyclic moiety of another.

11		Catenarotaxane: Two components each composed of two covalently linked macrocyclic rings form a catenane; one or two macrocyclic rings not involved in the catenane junction are threaded with a linear molecule [c]

[a] In this table and throughout the document differences in length of representations of linear sections do not imply that they are structurally different.
[b] The designation [2-2]rotaxane may be used according to the nomenclature system of Vögtle *et al* [7].
[b] Catenarotaxanes [7] were formerly called catrotanes or rotacatenanes. The designation [2rot-2cat-2rot]catenane was proposed according to the nomenclature system of Vögtle *et al* [7].

Sections from ROT-4 to ROT-6 present the IUPAC recommendations for systematic nomenclature for the 11 types of rotaxanes listed in Table 3.1. Section ROT-7 illustrates these principles for real examples of rotaxanes from the published literature.

ROT-4. GENERAL PRINCIPLES OF ROTAXANE NOMENCLATURE

Because each of the types listed in Table 3.1 is structurally different from the others, a single recommendation for naming rotaxanes cannot be given. On the other hand, names for all types of rotaxanes can be created according to the same basic principles with small variations for specific types of rotaxanes.

ROT-4.1. Name styles

ROT-4.1.1. Use of systematic nomenclature

The name of a rotaxane should be constructed according to the IUPAC recommendations described in this document. The macrocyclic and threading components of rotaxanes should each be named according to IUPAC recommendations for the naming of organic or other corresponding classes of chemical structures [20].

ROT-4.1.2. Use of semi-systematic or trivial names

Systematic names for most macrocyclic and threading components of rotaxanes are usually long, complex, or both. The use of semi-systematic and trivial names, or acronyms, for components is therefore permitted, provided no ambiguity is thereby introduced.
Note that such names are less preferred than systematic names generated according to IUPAC nomenclature recommendations.

ROT-4.2. Name generation

ROT-4.2.1. Order of citation of component names in the complete name

It is recommended that in the complete name of the rotaxane the name(s) of the threading component(s) should precede the name(s) of the macrocyclic component(s). While there is no precedence for assigning seniority to threading components over macrocyclic components, adherence to this recommendation wherever possible will add consistency to names generated for rotaxanes.

Where several threading or macrocyclic components are to be listed they are preferably cited in descending seniority of compound classes and within an each class as defined by IUPAC recommendations for the naming of organic compounds [22]. The order of citation does not depend on the number and position of a component in a rotaxane.

ROT-4.2.2. Generic Names for Rotaxanes of Types 1 to 8

Systematic names for all rotaxane types listed in Table 3.1 are generated according to the same principles and include the names of rotaxane components and the number of each component in a rotaxane assembly. If different arrangements of rotaxane components are possible, the name also includes a prefix that describes the arrangement of the components and is specific for each type of rotaxane.

Systematic names for rotaxanes of Types 1 to 8 are constructed according to the following generic format:

***prefix*-[*v*]{[*w*][name(s) for threading component(s)]-*rotaxa*-[*x*][name(s) for macrocyclic component(s)]}**

wherein *prefix* indicates the position and orientation of rotaxane components with respect to each other if variants are possible and thus specifies the rotaxane isomer as described in sections ROT-5 and ROT-6. If only the composition of a rotaxane is known or isomers are not possible the prefix part is omitted.

The main part of the name describes the structures of rotaxane components and the rotaxane composition. This name part is generated in the same way for most types of rotaxanes:

- *-rotaxa-* is a connector that is used to join the names of the threading and macrocyclic components
- *v*, *w*, and *x* are integers that define the total number of rotaxane components, the number of threading components and the number of macrocyclic components, respectively, as described in more detail below.

If a rotaxane contains several different threading or macrocyclic components, each component is cited in the name only once and the number of such components is specified by enclosing it in brackets before each component. If only one component of a kind is present in a rotaxane the citation of [1] may be omitted.

For example, if a rotaxane contains one threading component and several macrocyclic components of different kinds, the generic name will be as follows:

[v]{(name of threading component)-*rotaxa*-[x_1](name of macrocyclic component ^{1})-[x_2](name of macrocyclic component ^{2})-…}

For a rotaxane composed of several threading components and one macrocyclic component, the generic name will be:

[v]{[w_1](name of threading component^1)-[w_2](name of threading component ^{2})-…-*rotaxa*-(name of macrocyclic component)}

The total number of rotaxane components v in the examples above is the following sum: $v = 1 + x_1 + x_2 + \ldots$ or $v = w_1 + w_2 + \ldots + 1$ correspondingly.

Names for rotaxanes of Types 1-8 are generated by following steps 1-10 in descending order:

1. Select the name for the threading component(s).

2. Enclose, within parentheses, square brackets, or braces, as appropriate, the name generated in step 1.

   Note 4.2.2.1. IUPAC [22, R-0.1.5.1] recommends the use of enclosing parentheses, square brackets, or braces in chemical names as follows: {[( )]}; if an extension is needed: {[({[( )]})]}, etc.

3. Enclose, within square brackets, an integer, *w*, that precedes the name generated in step 2 for the threading component(s); this indicates how many there are in the rotaxane.

4. Add the italicized connective -*rotaxa*- after the name generated in step 3.

5. Add the name for the macrocyclic component(s) after the italicized connective -*rotaxa*-.

6. Enclose, within parentheses, square brackets, or braces, as appropriate, the name(s) generated in step 5.

7. Enclose, within square brackets, an integer, *x*, that precedes the name(s) generated in step 6 for the macrocyclic component(s); this indicates how many there are in the rotaxane.

8. Enclose, within parentheses, square brackets, or braces, as appropriate, the entire name generated in steps 1–7.

9. Enclose, within square brackets, an integer, *v*, that precedes the name generated in steps 1–8; this indicates the total number of components present in the rotaxane.

10. Add the *prefix* part that describes the arrangement of rotaxane components and is generated as described in corresponding sections for each specific type of rotaxane.

This generic format is used to name rotaxanes of types 1 through 8. The generic name formats for rotaxanes of types 9, 10, and 11 are described in sections ROT-4.2.3 and ROT-4.2.4. The systematic names for specific examples are given in Section ROT-7.

ROT-4.2.3. Generic names for rotaxanes of Types 9 and 10

The rotaxanes of type 9 are composed of a component that contains a macrocyclic part and a linear section connected to each other. The general name format specified in the section ROT-4.2.2 is modified since there is no logical place within the complete name at which to insert -*rotaxa*- as a connector. Addition of *rotaxa*- as a prefix is therefore recommended.

Systematic names for rotaxanes of Type 9 are written according to the generic format:

[1][*rotaxa*-(name of the component)]

The prefix [1] cannot be omitted for rotaxanes of Type 9 because components that contain both a macrocyclic and a linear section can form other rotaxane arrangements, for example, Type 10 rotaxanes (“daisy chains”).

The names for rotaxanes of Type 10 are created in a similar way. Several components that consist of both a linear section and a threadable ring can form either acyclic or cyclic arrangements in which the linear section of one component is threaded through the macrocyclic part of another component to form so called “daisy chains”.

Systematic names for rotaxanes of Type 10 are written according to the following generic format:

[*n*][*rotaxa*-(name of the component)])

for an acyclic arrangement;

and

[*cyclo*-*n*][*rotaxa*-(name of the component)]

for a cyclic arrangement.

In both cases, *n* is the number of rotaxane components.

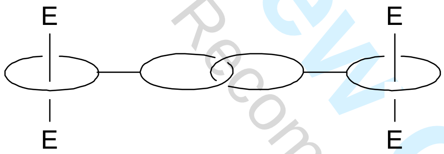
Figure 4.2.3.1 shows examples of acyclic and cyclic [4]rotaxanes of Type 10.

[4] [*cyclo*-4]

Figure 4.2.3.1. Acyclic and cyclic [4]rotaxanes of Type 10.

ROT-4.2.4. Generic names for catenarotaxanes of Type 11

Rotaxanes of Type 11 shown below include a two-component catenane, each macrocyclic ring of which has attached to it a macrocyclic ring that can enclose a threading component or components.



Note 4.2.4.1. The IUPAC Compendium of Chemical Terminology defines catenanes or catena-compounds as molecules having two or more rings connected in the manner of links of a chain, without a covalent bond [20]

The whole catenane component can be treated as a complex macrocyclic component. Thus, catenarotaxanes of Type 11 that include two threading components and one macrocyclic catena component can be named according to the following generic format:

[3]{[2](name of threading component)-*rotaxa*-(name of the [2]catenane)}

Several nomenclature systems for catenanes have been proposed, but there is no universally recommended system. Use of -*catena*- as an italicized connective for the [2]catenane component of the generic name format is recommended because it would be in accord with IUPAC recommendations for italicized connectives used in polymer nomenclature [23]. In contrast, the principles recommended in section ROT-4.2.3 for "daisy-chain" rotaxanes can be followed to create names of catenanes. Thus the [2]catenane composed of two equal components can be named according to the following generic format:

[2][*catena*-(name of the catena component)]

Thus the generic name for [3]rotaxanes of Type 11 can be constructed according to the following format:

[3]([2](name of threading component)-*rotaxa*-{[2][*catena*-(name of the catena component)]})

This generic name unambiguously describes all components and the composition of catenarotaxanes of Type 11. A specification of possible isomers of catenarotaxanes of Type 11 with prefixes is described in section ROT-5.4.

Note 4.2.4.2. Because the systematic nomenclature of catenanes is not developed yet, the name format proposed here for [2]catenane and thus [3]rotaxanes of Type 11 should be considered to be provisional.

ROT-5. SPECIFICATION OF ISOMERISM OF ROTAXANES

ROT-5.1. Types of isomerism in rotaxanes

Whereas the main part of the rotaxane name unambiguously describes the compositions of rotaxanes and isomerism of rotaxane components, the prefix describes the isomerism specific to each rotaxane. Thus the term 'isomerism of rotaxanes' does not include isomerism of rotaxane components and describes different arrangements that can be formed by the same components.

The isomers of rotaxanes can differ in:

a. positions of macrocyclic components at linear sections of complex threading components and/or positions of threading components at several macrocyclic parts of complex macrocyclic components,
b. the order in which several nonequivalent macrocyclic components are positioned at the same linear section of a threading component,
c. the position of a macrocyclic component at different recognition sites within the same linear section,
d. the arrangement of asymmetric rotaxane components with respect to each other.

Figure 5.1.1 shows examples of isomerism in rotaxanes.

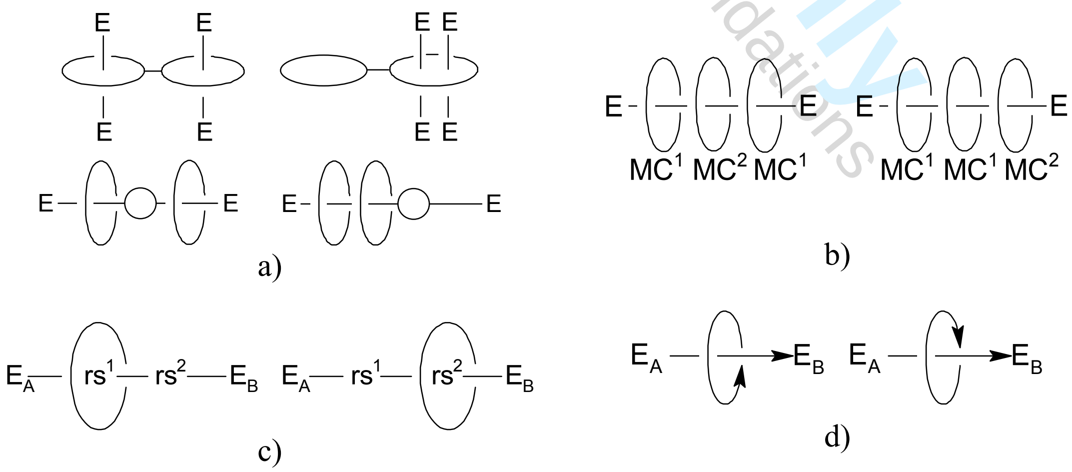
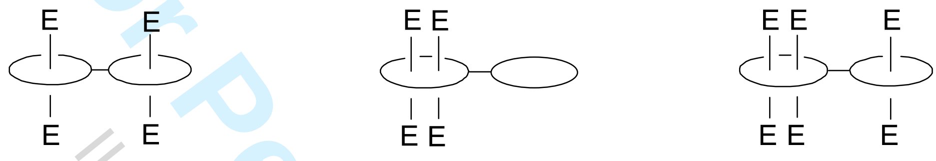


Figure 5.1.1. Types of rotaxane isomerism (E_A and E_B designate nonequivalent ends and arrows define the asymmetry of a component).

Isomers of types a, b, and c can exist for rotaxanes with both symmetrical and unsymmetrical components. The naming conventions for these types of isomers are described in the section below for the corresponding classes of rotaxanes. The asymmetry of rotaxane components and the specification of possible isomers of type d are described in the section ROT-6.

ROT-5.2. Position of threading components in several threadable rings (Types 3 and 4)

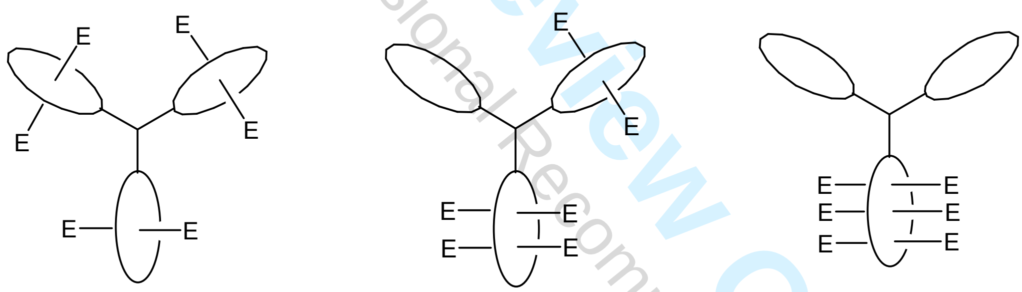
For rotaxanes of Type 3, isomers that differ in position of threading components in different threadable rings are possible. The position of threadable components, which can be unambiguously specified by the prefix part of the name, is designated by two numbers cited in decreasing order that indicate the number of threading components in each ring of the macrocyclic component. Examples of rotaxanes of Type 3 and their corresponding prefixes are shown in Figure 5.2.1.



1:1 *2:0* *2:1*

Figure 5.2.1. Isomeric rotaxanes of Type 3 and their corresponding prefixes.

The isomers of rotaxanes of Type 4 that differ in positions of threading components in three rings are defined in the same way; a minor difference is that the prefix in this case is composed of three numbers that indicate the number of threading components in each threadable ring. Figure 5.2.2 shows examples of [4]rotaxanes of Type 4 and their corresponding prefixes.



1:1:1 *2:1:0* *3:0:0*

Figure 5.2.2. Isomeric [4]rotaxanes of Type 4 and their corresponding prefixes.

The prefixes for more complex macrocyclic components can be created according to the principles specified above and in the section ROT-5.3.2 for rotaxanes with complex threading components.

Note 5.2.1. The numbers of threading components are cited in decreasing order if the threadable rings are structurally identical. If the threadable rings are not identical the numbers of components are cited in decreasing order of seniority of threadable rings. Thus, for [3]rotaxanes of Type 3 with identical symmetrical threading components three isomers with prefixes 2:0-, 0:2-, and 1:1- are possible. The procedure to establish the seniority of threadable rings should be based on principles specified in sections ROT-6.1.1 and ROT-6.1.2.

Note 5.2.2. For citation of nonequivalent threading components see section ROT-5.5.2; for indication of mutual orientation of unsymmetrical threading components see sections ROT-6.2.4 and ROT-6.2.5.

ROT-5.3. Position of Macrocyclic Components on Several Linear Sections (Types 5-8)

The positions of simple macrocyclic components on threading components with several linear sections are specified in a manner similar to that given in section ROT-5.2. The prefix in this case indicates the number of components threaded on each linear section.

ROT-5.3.1. Specification of the position of macrocyclic components for rotaxanes of Type 5

Type 5 rotaxanes have an unbranched threading component with two or more linear sections separated from each other by large groups preventing movement of a macrocyclic component from one section to another. In rotaxanes of Type 5 the sections are cited successively starting from one terminal linear section and proceeding through all internal sections, finally to the other terminal section. Sections containing the greatest number of components should be cited as early as possible. Examples of [3]rotaxanes of Type 5 are shown in Figure 5.3.1.1.

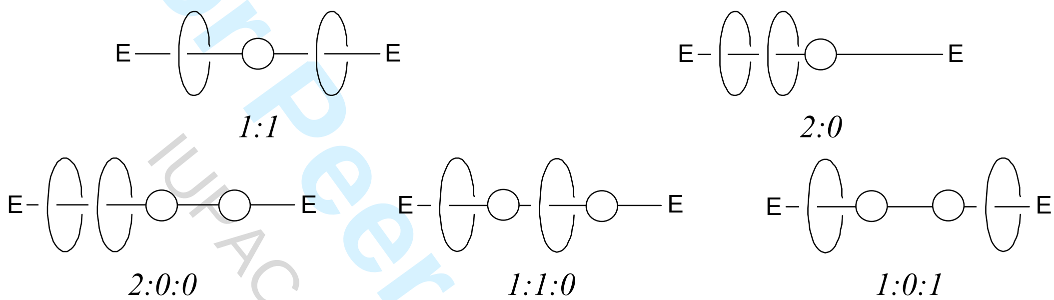


Figure 5.3.1.1. [3]Rotaxanes of Type 5 and their corresponding prefixes.

ROT-5.3.2. Specification of the position of macrocyclic components for rotaxanes with branched threading components (Types 6 to 8)

The isomers for rotaxanes of Type 6 with a Y-shaped threading component are specified in a manner similar to that described above for Type 5. Providing that the linear sections are equivalent, the prefix consists of three numbers that are cited in descending order. Examples of isomeric [4]rotaxanes of Type 6 and their corresponding prefixes are shown in Figure 5.3.2.1.

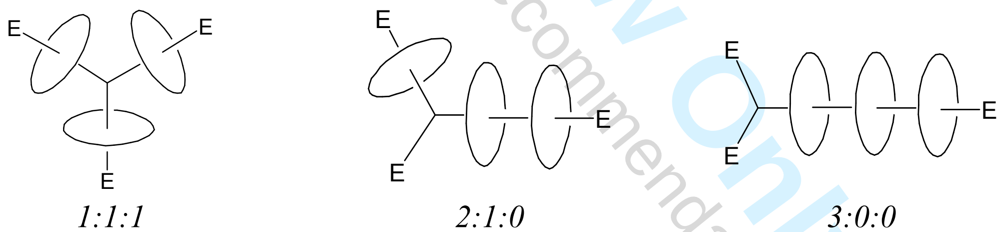


Figure 5.3.2.1. Isomeric [4]rotaxanes of Type 6 and their corresponding prefixes.

In rotaxanes of Type 7 with X-shaped threading components containing four topologically equivalent linear sections, the prefix consists of four numbers that indicate the number of macrocyclic components in each section. The order of citation of numbers for X-shaped threading components depends on the spatial structure of the X-shaped component. For tetrahedral X-shaped components, the numbers are cited simply in decreasing order, but for X-shaped components with square-planar configuration, the sections are listed successively clockwise or counterclockwise. Sections with the greatest number of components should be cited as early as possible. Figure 5.3.2.2 shows examples of [3]rotaxanes of Type 7 and their corresponding prefixes.

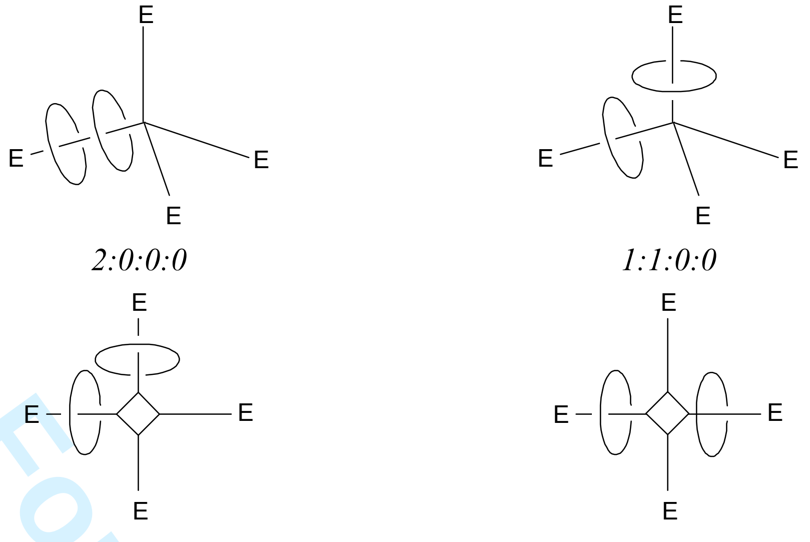
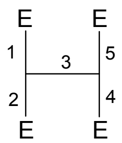


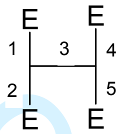
Figure 5.3.2.2. [3]Rotaxanes of Type 7 and their corresponding prefixes (the square in the center of the X-shaped component is added to indicate the square-planar configuration).

If rotaxanes of Types 5 to 7 with equivalent threading sections contain a single macrocyclic component, the prefixes *1:0, 1:0:0*, and *1:0:0:0* correspondingly are not cited, unless isomers are possible.

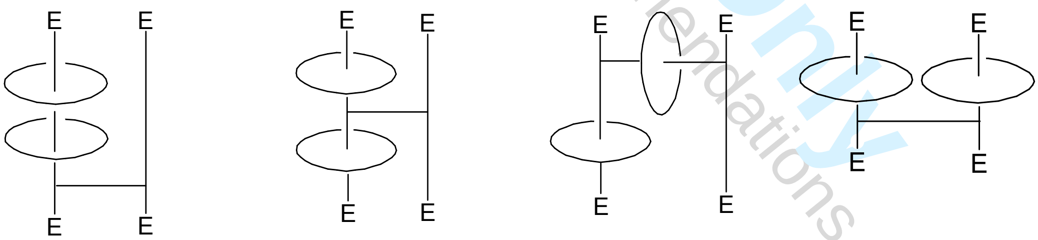
The prefix for rotaxanes of Type 8 that include an H-shaped threading component with five topologically nonequivalent linear sections is composed of five numbers. For unambiguous specification of isomers, the numbers of macrocyclic components are cited in a fixed order: (1) the two adjacent terminal sections; (2) the internal section; (3) the remaining two adjacent terminal sections. Among several possible prefixes the one that cites the most populated terminal section earliest is chosen. Figure 5.3.2.3 shows the order of sections with numbers placed near the corresponding section and examples of isomeric [3]rotaxanes of Type 8 with their prefixes.



(if free rotation is possible is equivalent to



)



2:0:0:0:0 *1:1:0:0:0* *1:0:1:0:0* *1:0:0:1:0* [a]

Figure 5.3.2.3. Order of citation of linear sections in an H-shaped threading component and Type 8 isomeric [3]rotaxanes with corresponding prefixes.

[a] The prefix *1:0:0:1:0* given for the last structure implies free rotation along the internal linear section. If such rotation is not possible the prefix will be *1:0:0:0:1* in accordance with the order of citation of the linear section

Note 5.3.1.1. The principles specified in this section imply that topologically equivalent sections are also structurally equivalent. For rotaxanes of Types 5–8 with structurally nonequivalent linear sections the numbers of components are cited first with respect to the topological order stated here, and then in decreasing order of seniority of linear sections. The principles for establishing the seniority of structurally nonequivalent sections should be based on the procedures specified in section ROT-6.1.1.

Note 5.3.1.2. For citation of nonequivalent macrocyclic components, see section ROT-5.5.1; for indication of orientation of asymmetrical components, see section ROT-6.2.3.

ROT-5.4. Position of threading components for catenarotaxanes of Type 11

Catenarotaxanes of Type 11 contain a catena macrocyclic component that includes four large rings that can be potentially threaded with linear components. To specify the structure, the prefix for rotaxanes of Type 11 consists of four numbers that indicate how many threading components are positioned in each macrocyclic ring. Figure 5.4.1 shows two examples of isomeric [3]rotaxanes of Type 11 and their corresponding prefixes.

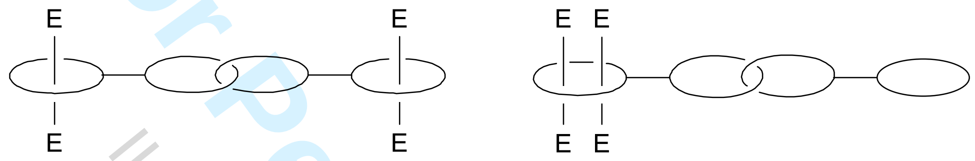


Figure 5.4.1. [3]Rotaxanes of Type 11 and their corresponding prefixes.

Each catena component of a rotaxane of Type 11 contains two large rings; thus, two different isomeric catenanes are possible. To indicate that only one large ring of each component forms a catena junction, the prefix *(1-1)* can be added in front of the catenane name. This prefix indicates that the first ring of one component forms a catena junction with the first ring of another component. Thus the whole name of a [2]catenane will be:

(*1-1*)-[2][*catena*-(name of the catena component with two large rings)]

Thus, the generic name for the first isomer of [3]rotaxanes of Type 11 shown in Figure 5.4.1 will be:

***1:0:0:1*-[3]([2](name of threading component)-*rotaxa*-{(*1-1*)-[2][*catena*-(name of the catena component with two large rings)]})**

Note 5.4.1. For catena components with two equivalent rings this generic name unambiguously indicates the structure of a catenane. The principles used to define senior ends in asymmetric threading components specified in section ROT-6.1.1 can be used to define the seniority of rings for catena components.

Note 5.4.2. Because the systematic nomenclature of catenanes is not developed yet, the name format proposed here for [2]catenane and thus for [3]rotaxanes of Type 11 should be considered to be provisional.

ROT-5.5. Positions and an order of nonequivalent components of the same type

For rotaxanes with different components of the same type, isomers that differ in position or order of components are possible. For an unambiguous description of positions of rotaxane components, the prefix part of the rotaxane name includes designations of specific rotaxane components in accordance with the order in which they are cited in the name as described below.

ROT-5.5.1. Specification of arrangement of nonequivalent macrocyclic components

For rotaxanes of Type 1 with more than one type of macrocyclic components, isomers differing in the order of macrocyclic components are possible. To define an arrangement of macrocyclic components, they are indicated by MC^n designations that define different macrocyclic components. *MC* is an abbreviation of "macrocyclic component" and *n* is the position of this component name in the whole name of the rotaxane. Thus, the macrocyclic component cited first in the name is designated in the prefix part by MC^1, the second by MC^2, and so on.

For the [4]rotaxane of Type 1.3 composed of two equal macrocyclic components cited earlier in the name, and a third, different macrocyclic component, and having the generic name

[3][(name of threading component)-*rotaxa*-[2](name of macrocyclic component $_1$)-[1](name of macrocyclic component $_2$)]

two isomers are possible. Figure 5.5.1.1 shows two possible isomers and their corresponding prefixes for this type of rotaxane.

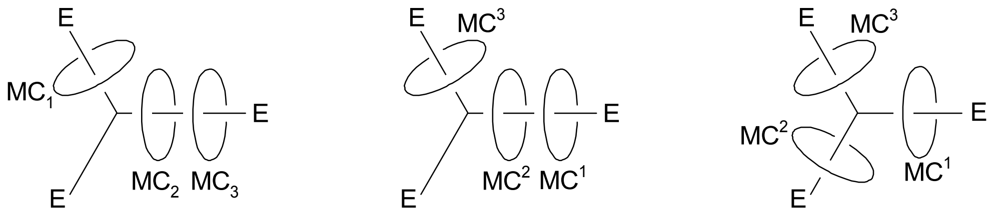
MC^1,MC^1,MC^2 MC^1,MC^2,MC^1

Figure 5.5.1.1. Isomeric [4]rotaxanes of Type 1 and the corresponding prefixes.

The prefix part of the rotaxane name cites the designations of components in the order in which they are positioned on the threading component providing the earlier citation of the components that are cited first in the name of a rotaxane.

For rotaxanes of Types 5 to 8, composed of threading components with several linear sections and different macrocyclic components, each possible isomer is specified by the prefix that cites the specific macrocyclic component designations MC^n instead of numbers for each linear section. The linear sections for specific rotaxane types are listed in the order defined in the section ROT-5.3. If there is a choice, the most populated sections are cited first, then earlier cited macrocyclic components. For rotaxanes of Type 5 the macrocyclic components are cited sequentially, beginning with the outermost one. For rotaxanes of Types 6 to 8, the components are cited from the outermost one for each linear section. Examples of rotaxanes of Types 5 and 6 and their corresponding prefixes are shown in Figure 5.5.1.2.

$MC^2,MC^1:0$ $MC^1,MC^2:MC^1,MC^2$



MC³,MC²: MC¹:0 *MC¹,MC²: MC³:0* *1:1:1*

Figure 5.5.1.2. Rotaxanes of Types 5 and 6 with different macrocyclic components and their corresponding prefixes.

Note that for the last example of [4]rotaxanes of Type 6 no isomers are possible when one macrocyclic component is threaded onto each threading section and components are symmetrical. Thus the simplified prefix described in the section ROT-5.3 unambiguously describes the structure of the rotaxane. If no isomers are possible or if the exact position of each component is unknown, simplified prefixes can be used for other types of rotaxanes with nonequivalent components.

ROT-5.5.2. Specification of positions of nonequivalent threading components

The positions of different threading components for isomeric rotaxanes with macrocyclic components with several threadable rings are specified by modification of the prefixes described in section ROT-5.2. Instead of numbers that define the number of threading components in each threadable ring, the italicized designations TC^n are used, where *TC* is an abbreviation for "threading component" and *n* is the position of the threading component name within the complete name of a rotaxane.

Figure 5.5.2.1 shows two isomeric [4]rotaxanes of Type 3 and their corresponding prefixes. The designations TC^1 and TC^2 indicate different threading components. TC^1 designates a component cited earlier in the complete name.

TC¹,TC¹:TC² *TC¹,TC²:TC¹*

Figure 5.5.2.1. Isomeric [4]rotaxanes of Type 3 and their corresponding prefixes.

If the threadable rings in a complex macrocyclic component are equivalent, the designations of threading components are cited starting from the more populated threadable ring, which results in citation of lower-numbered threading components as early as possible.

ROT-5.5.3. Specification of rotaxanes that function as molecular shuttles

The recommended method for indicating the association of a macrocyclic component with a specific recognition site is to add a prefix comprising italicized indications rs^n-*MC*, where *rs* is an abbreviation for "recognition site", *n* is a number assigned to the recognition site by consecutive numbering from one end of the threading component, and *MC* is an abbreviation of "macrocyclic component". Figure 5.6.1 shows several examples of molecular shuttles and their corresponding prefixes.

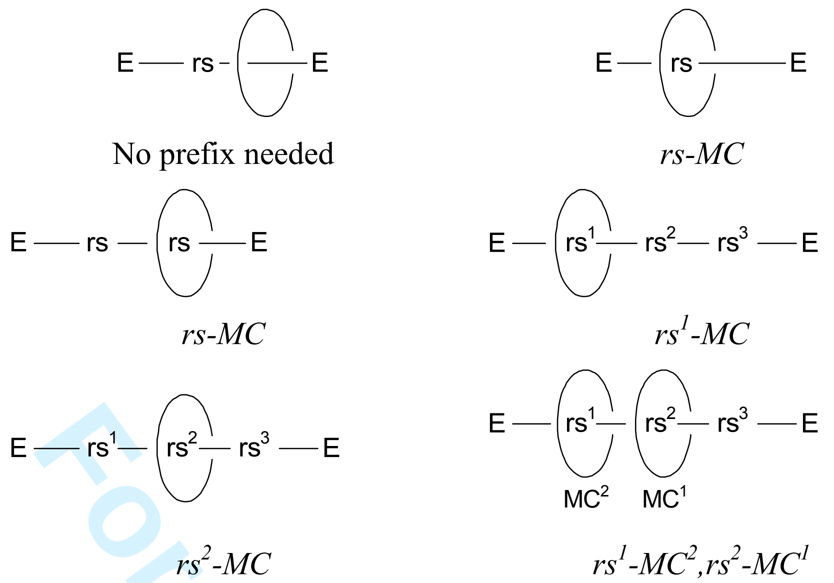


Figure 5.6.1. [2]Rotaxanes that function as molecular shuttles and their corresponding prefixes.

For rotaxanes with a single recognition site or two identical recognition sites, the designation is unnecessary. However, if it is important to distinguish between associated and non-associated forms of a rotaxane, the prefix *rs-MC* is added to indicate that a macrocyclic component resides at a recognition site (see ROT-1.6).

Different macrocyclic components are indicated by the addition of MC^n designations that are assigned as described in section ROT-5.5.1 (see the last structure on Figure 5.6.1)

If the threading component is unsymmetrical and thus recognition sites are nonequivalent, the numbering of recognition sites is established as described in section ROT-6.2.1.3.

ROT-6. ROTAXANES WITH UNSYMMETRICAL COMPONENTS

ROT-6.1. Asymmetry of rotaxane components

ROT-6.1.1. Asymmetry of threading components and linear sections

For a linear section of a threading component to have a different orientation in relation to an asymmetric macrocyclic component or another linear section, it must not have a plane perpendicular to it capable of dividing it into two identical halves. In other words, it must not have a C_2 axis of symmetry that is perpendicular to a linear section.

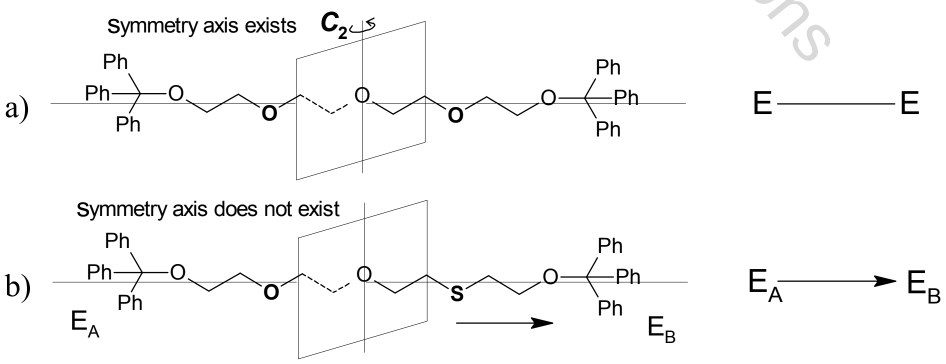


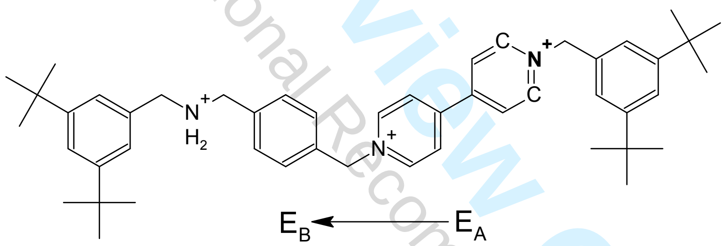
Figure 6.1.1.1. Examples of symmetric (a) and asymmetric (b) threading components and their schematic designations.

When two parts of a linear section are nonequivalent, it is possible to define seniority rules to select the senior end of the linear section. It is recommended that the senior end shall be arbitrarily designated E_A and the other end shall be designated E_B. The senior end is the one that satisfies the following criteria, applied in descending order until a decision is reached.

The direction of the linear section, and hence the seniority of ends, is defined by application of Cahn-Ingold-Prelog (CIP) seniority rules, as used for assignment of stereodescriptors [24, 25]. A decision is made by application of the following steps in descending order:

1. According to CIP seniority of elements, select the most senior atom.
2. If several atoms of the same seniority are present, compare the ligands of each atom according to CIP priority until the first point of difference is found.
3. Compare the ligands of the most senior atom(s) according to CIP priority rules until the first difference between two directions within a threading component is found. If the most senior ligand does not allow choice of direction the next most senior ligand is considered.
4. If a single senior atom defining the direction within a threading component can be identified, or a greater number of senior atoms with equal seniority lead to the same direction, the threading component is considered to have a direction. Otherwise the component is symmetrical.
5. The direction of a threading component from E_A to E_B is defined as going from the most senior atom to its most senior ligand or to the branch of the most senior ligand that allows choice of direction.

The following example illustrates an application of these principles:



1. Nitrogen atoms are senior in the threading component according to CIP rules for seniority of elements. There are three nitrogen atoms.
2. Two nitrogen atoms in pyridine rings have four carbons in the first sphere and are senior to the acyclic nitrogen having two carbon neighbors. The seniority of the nitrogen atom shown in bold over the other cyclic nitrogen is decided in the fifth sphere.
3. The two ligands of the senior nitrogen atom shown as explicit carbon atoms, “C”, have equal seniority and are senior to the ligand that starts with the CH_2 group. Both senior ligands lead to the same direction within the threading component.
4. The threading component is thus unsymmetrical.
5. The direction is from right to left in the drawn structure; the right end is designated as E_A and the left end is therefore E_B.

Note that the position of the senior atom within the threading component is not itself used to define the seniority of ends, because for asymmetric threading components it is often difficult to define the center of the linear section. Use of the direction from the senior atom to its senior ligand in some cases may lead to situations where the senior atom is closer to the less senior end. For example, for the structure b) in Figure 6.1.1.1 the senior atom is closer to E_B.

Linear sections of complex threading components are topologically asymmetric. For unbranched threading components with several linear sections the principles stated above are applied to define the seniority of terminal ends of the whole threading component. In the case of branched threading components, the terminal group of each linear section is arbitrarily defined as senior to the branching point. Figure 6.1.1.2 shows the examples of complex threading components and the corresponding seniority of the ends of linear sections.

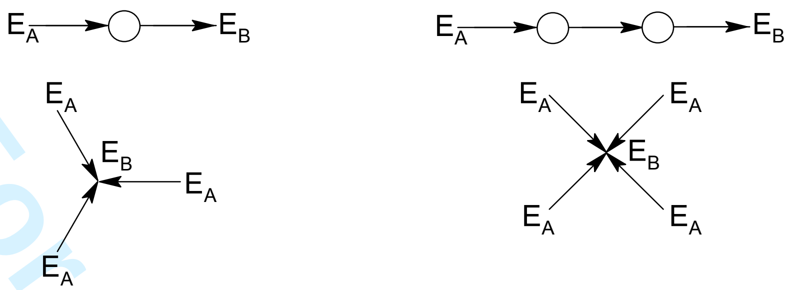


Figure 6.1.1.2. Directions of linear sections in threading components of Types 5–7.

These types of threading components are discussed in the sections ROT-6.2.2 and ROT-6.2.3.

ROT-6.1.2. Asymmetry of macrocyclic components

For a macrocyclic component to have different orientations in relation to an asymmetric linear section or another asymmetric macrocyclic component, it must not have a proper symmetry axis C_2 that lies in a nominal plane of a macrocyclic ring.

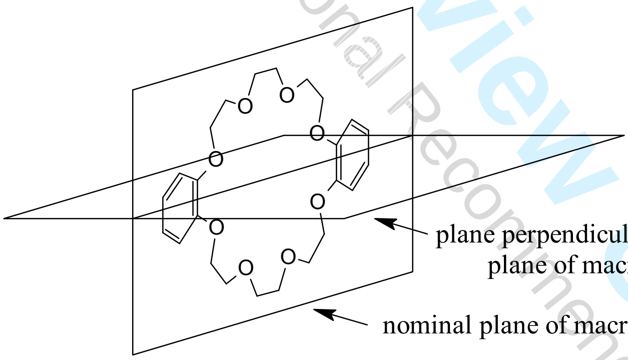


Figure 6.1.2.1. Nominal plane of a macrocyclic molecule.

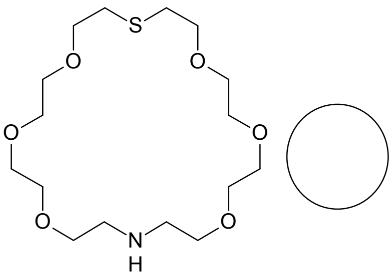
Three different situations are possible:

a) has no C_2 symmetry axis but has a symmetry plane that lies in a nominal plane of the macrocyclic ring (ring with direction or directed ring),

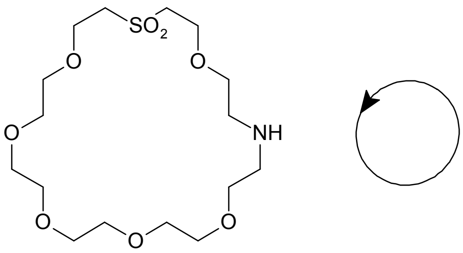
b) has no C_2 symmetry axis that lies in a nominal plane but has a symmetry plane that is perpendicular to a nominal plane of macrocyclic ring (ring with nonequivalent sides),

c) if both symmetry planes are absent, the asymmetric macrocyclic component possesses both a ring direction and different sides at the same time.

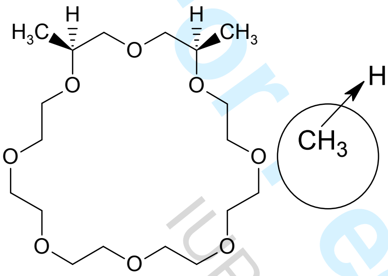
Examples of symmetrical and unsymmetrical macrocyclic molecules are given in Figure 6.1.2.2.



symmetrical ring

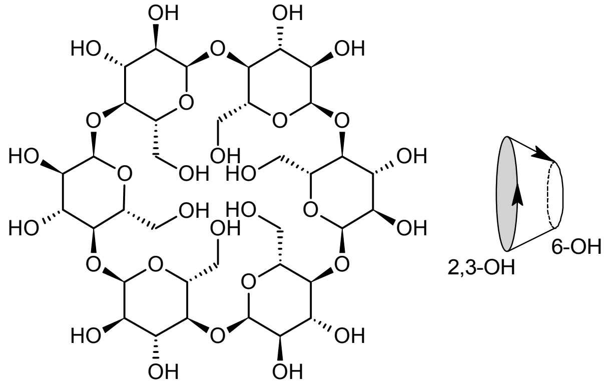


unsymmetrical with ring direction



unsymmetrical with different sides

α-cyclodextrin



unsymmetrical with different sides and ring direction[a]

Figure 6.1.2.2. Examples of symmetrical and unsymmetrical macrocyclic molecules.

[a] The spatial structure of cyclodextrins, determination of ring direction, and seniority of sides are discussed in the section ROT-6.1.2.3.

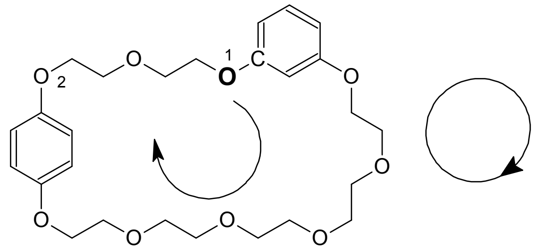
ROT-6.1.2.1. Determination of ring direction

A ring direction is described by the order in which the constitutional units responsible for the asymmetry of the macrocyclic component are encountered when going from more senior units to less senior. To define seniority within a macrocyclic component, CIP priority rules are used [24, 25].

Selection of ring direction is determined by application of the following steps in descending order:

1. According to CIP seniority of elements, select the most senior atom in the macrocyclic ring.
2. If several atoms of the same seniority are present, compare the ligands of each atom according to CIP priority until the first point of difference is found.
3. Compare the ligands of the most senior atoms according to CIP priority rules until the first point of difference between two directions within a macrocyclic ring is found. If the most senior ligand does not allow choice of direction less senior ligand is considered.
4. If a single senior atom that allows differentiation of the direction within a ring is found, or a greater number of senior atoms of equal seniority leads to the same ring direction, the ring is considered to have a direction.
5. The ring direction is defined as that from the senior reference atom to its most senior ligand or to the branch of the most senior ligand that allows choice of a direction.

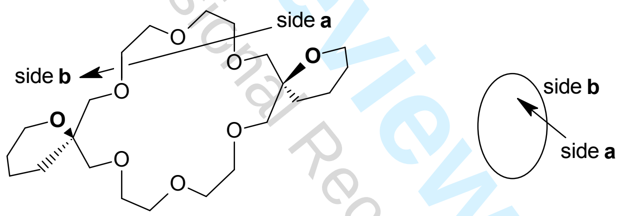
For example, in the structure below, the most senior oxygen atom number 1 is senior to oxygen atom number 2 due to the seniority of O^1-C-C-C-O-C sequence over the sequence O^2-C-C-C-C-O-. The senior ligand attached to the senior oxygen atom is the benzene ring with the explicitly shown carbon atom. Thus, the direction within the macrocycle is assigned and is clockwise when viewed from the side closer to a viewer.



ROT-6.1.2.2. Determination of seniority of sides

To select the seniority of ring sides, all rings are considered to be flat and specific conformations are not taken into account. To make a decision the following steps are applied in descending order:

1. Select the most senior atom according to CIP rules for seniority of elements.
2. If several atoms of the same seniority are present, compare the ligands of each atom according to CIP priority rules until the first point of difference is found.
3. If the most senior atom, or greater number of senior atoms, is rigidly positioned on one side of the macrocyclic ring, this ring side is considered to be senior.
4. If a decision cannot be made from application of steps 1 – 3, compare the ligands of the most senior atom(s) according to CIP priority rules until the first point of difference between two sides of a macrocyclic ring is found.
5. The side of the ring in which the senior atom or greater number of senior atoms or their senior ligands are located is defined as the senior side and designated as the **a**-side of a macrocyclic component; the other side is designated as the **b**-side.

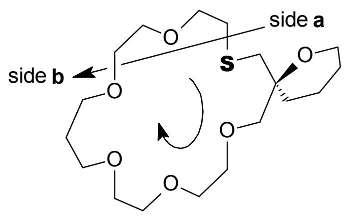


In the structure shown, both senior oxygen atoms shown in bold are rigidly positioned on the same side of the ring system, and this defines the senior side of this tricyclic system that is closer to the viewer for the drawing above.

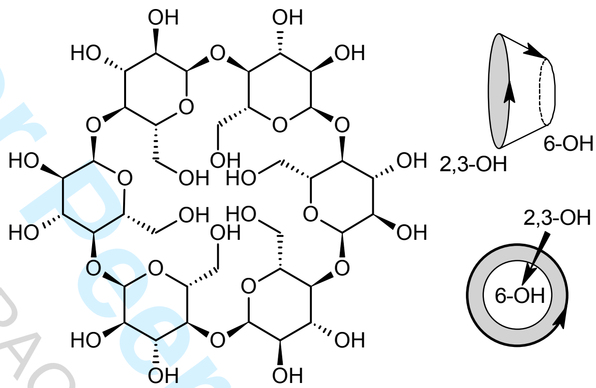
ROT-6.1.2.3. Determination of asymmetry for macrocyclic components with ring direction and nonequivalent sides

When the macrocyclic component possesses both ring direction and different sides, the specification of ring direction unambiguously describes the orientation of the macrocyclic component. All such systems can be treated as a special case of macrocyclic components with ring direction.

According to the procedures specified in section ROT-6.1.2.1 the ring direction for the structure given below is defined as clockwise when viewed from the side closer to the viewer.



Cyclodextrins represent another example of macrocyclic components with both ring direction and nonequivalent sides. The structures of α-, β- and γ-cyclodextrins are such that the secondary hydroxy groups in the 2- and 3- positions of each glucopyranose unit form a wider rim (or 2,3-rim), whereas the primary hydroxy groups in the 6-positions form a narrower rim (or 6-rim) of these macrocyclic molecules [26].The asymmetry of cyclodextrin components can be specified by ring direction according to above-specified procedures and is determined by the senior oxygen atom of the large ring and its senior ligand that is the adjacent anomeric carbon atom. Thus, viewing from the narrow 6-rim leads to clockwise direction, whereas viewing from the wide 2,3-rim leads to anticlockwise direction. At the same time, the 6-rim can be designated as the **a**-side and 2,3-rim as the **b**-side.

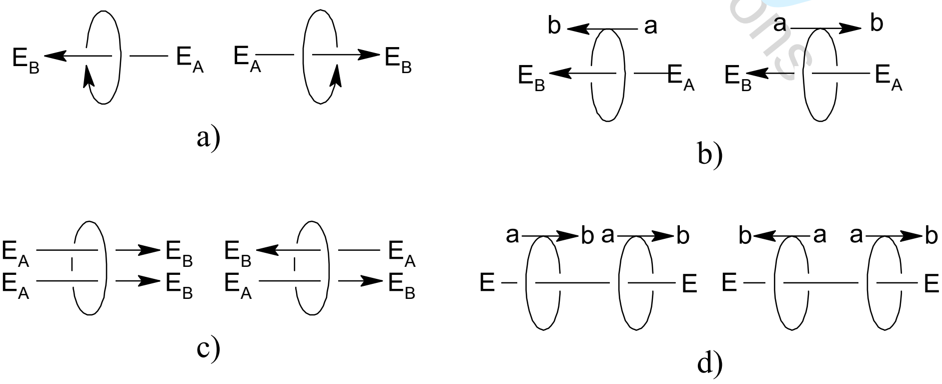


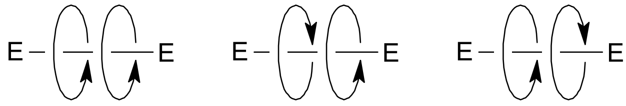
ROT-6.2. Stereoisomers of rotaxanes

The above-specified two main types of asymmetric macrocyclic components and a single type of asymmetric threading component can be classified according to the following five basic types of rotaxane stereoisomers that differ in mutual orientation of:

a) an asymmetric threading component and a macrocyclic component with a ring direction;
b) an asymmetric threading component and a macrocyclic component with different ring sides;
c) asymmetric threading components in relation to each other;
d) asymmetric macrocyclic components with different sides; and
e) asymmetric macrocyclic components with ring directions.

Five basic types of rotaxane stereoisomers are shown in Figure 6.2.1.





e)

Figure 6.2.1. Types of rotaxane stereoisomerism.

The examples shown in Figure 6.2.1 represent the simplest cases; more complex situations can exist if a greater number of asymmetric components or more complex components are present in a rotaxane.

These types of rotaxane isomerism are specified by additional descriptors introduced into the prefix of a rotaxane name as described in sections ROT-6.2.1 to ROT-6.2.7.

ROT-6.2.1. Specification of isomers of unsymmetrical rotaxanes of Type 1

ROT-6.2.1.1. [2]Rotaxanes of Type 1.1 with unsymmetrical components

[2]Rotaxanes of Type 1.1 composed of an asymmetric threading component and a macrocyclic component with ring direction can form two isomers that are enantiomeric and differ in orientation of the macrocyclic component in relation to the threading component. This type of stereoisomerism, called "cyclochirality" [27, 28], really represents a case of an axis of chirality in which a threading component defines an axis and its direction and an asymmetric macrocyclic component defines a direction around the axis.

To specify the structure of a rotaxane, the ring direction of a macrocyclic component in relation to an asymmetric threading component is designated by addition of an italicized prefix *A*- or *C*- that defines anticlockwise or clockwise direction respectively, as shown in Figure 6.2.1.1.1.

Figure 6.2.1.1.1. Enantiomeric [2]rotaxanes with asymmetric macrocyclic component with ring direction and the corresponding prefixes.
The macrocyclic component is assumed to be in the plane of the paper, the A end is in front of the plane and the B end is behind it.

Two rotaxanes shown in Figure 6.2.1.1.1 form an enantiomeric pair. In the case of rotaxanes with asymmetric macrocyclic components possessing both ring direction and different sides unambiguously described by *A* and *C* prefixes, the two corresponding isomers are diastereomeric. Examples are the rotaxanes composed of asymmetric threading components and cyclodextrins.

The descriptors *A*- or *C*- are determined by the following steps:
(1) Define the direction of the threading component as described in Section ROT-6.1.1
(2) Orient the rotaxane so that is viewed "end on" along the axis of the threading component from E_A.
(3) Define the ring direction of the macrocyclic component, as described in Section ROT-6.1.2.1.

(4) If the ring direction is anticlockwise when the rotaxane is viewed from E_A, the prefix is *A*-. Otherwise the prefix is *C*- (for clockwise direction).

For example, the generic name for a [2]rotaxane with clockwise orientation of macrocyclic components in relation to an unsymmetrical threading component is:

***C*-[2][(name for threading component)-*rotaxa*-(name for macrocyclic component)]**

[2]Rotaxanes composed of an asymmetric threading component and a macrocyclic component with different ring sides can form two diastereomers and are specified by the addition of an italicized prefix *ab*- or *ba*- that defines the orientation of nonequivalent sides in relation to the senior end E_A of the threading component. The prefixes *ab* and *ba* are assigned, in a manner analogous to assignment of *A*- and *C*-, as shown in Figure 6.2.1.1.2 in which, for example, the prefix *ab*- indicates that the senior a-side is closer to E_A of the threading component.

Figure 6.2.1.1.2. Diastereomeric [2]rotaxanes with unsymmetric macrocyclic component with different sides and the corresponding prefixes.

For example, the generic name for the left rotaxane shown on Figure 6.2.1.1.2 is:

***ab*-[2][(name for threading component)-*rotaxa*-(name for macrocyclic component)]**

ROT-6.2.1.2. [3]Rotaxanes of Type 1.2 with unsymmetric components

For [3]rotaxanes of Type 1.2 composed of a symmetric threading component and two asymmetric macrocyclic components with ring direction, three isomers are possible. The isomers are specified by the addition of a prefix that indicates the orientation of each macrocyclic component when the rotaxane is viewed from one end of the threading component. The three possible isomers and their corresponding prefixes are shown in Figure 6.2.1.2.1.

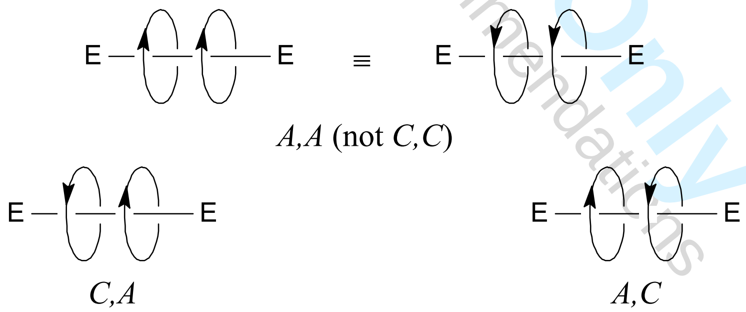


Figure 6.2.1.2.1. Isomeric [3]rotaxanes with symmetrical threading component and two macrocyclic components with ring direction, and their corresponding prefixes.

For the *A,A* isomer shown first in Figure 6.2.1.2.1, viewing from one end results in a “clockwise” designation for both cyclic components, but viewing from the other end results in an “anticlockwise”designation. The prefix *A,A* is chosen because it is first alphabetically. The other two isomers form an enantiomeric pair, and the result is the same, regardless of from which end the [3]rotaxane is viewed.

For [3]rotaxanes of type 1.2 composed of an unsymmetric threading component and two unsymmetric macrocyclic components with ring direction, four isomers are possible. The isomers are specified by addition of a prefix composed of E_A to indicate from which end the rotaxane is viewed and designations of ring direction for each component. The four possible isomers and their prefixes are shown in Figure 6.2.1.2.2.

E_A-A,A *E_A-C,C*

E_A-C,A *E_A-A,C*

Figure 6.2.1.2.2. Isomeric [3]rotaxanes with unsymmetrical threading component and two macrocyclic components with ring direction and their corresponding prefixes.

The two isomers in the upper row, and the other two isomers in the lower row, each represent enantiomeric pairs.

The same principles are used to specify isomeric [3]rotaxanes of Type 1.2 having asymmetrical macrocyclic components with different ring sides. The prefixes are generated according to the same procedure, but instead of *A* and *C* the designations *ab* and *ba* are used, as shown for the two examples in Figure 6.2.1.2.3.

ba,ab *E_A-ba,ba*

Figure 6.2.1.2.3. [3]rotaxanes with two macrocyclic components with different sides and their corresponding prefixes.

Figure 6.2.1.2.4 gives several examples of [3]rotaxanes of type 1.2 with different macrocyclic components. If the rotaxane is composed of an asymmetric threading component and two different symmetric macrocyclic components possible isomers are specified by inclusion of MC^1 and MC^2 designations in the prefix part of the name. The prefixes MC^1 and MC^2 are assigned to the macrocycles cited earlier and later, respectively, as described in section ROT-5.5.1. If a [3]rotaxane of Type 1.2 contains an asymmetric threading component, the macrocyclic components are cited starting from the component that is closer to E_A. For [3]rotaxanes with a symmetrical threading component the different macrocyclic components are cited starting from the component that is cited earlier in the rotaxane name.

E_A-MC^2,MC^1 *E_A-MC^2-A,MC^1-C*

MC¹-A,MC²-C   *MC¹,MC²-A*

Figure 6.2.1.2.4. Examples of [3]rotaxanes with different combinations of macrocyclic components and their corresponding prefixes.

The nomenclature principles described above are readily adaptable to accommodate other possibilities and more complex rotaxanes.

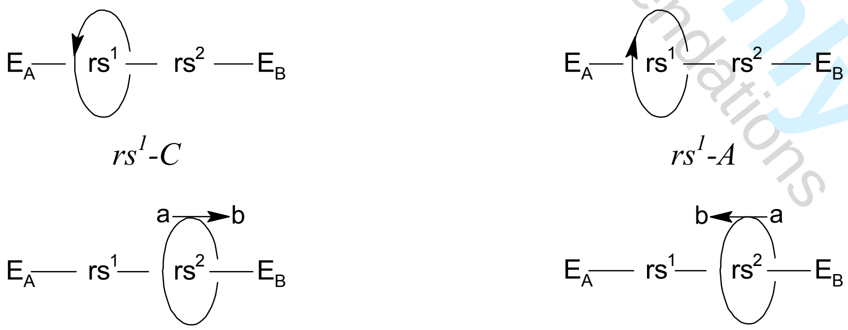
ROT-6.2.1.3. Indication of position and orientation of macrocyclic components on unsymmetric threading components with several recognition sites

The position of a macrocyclic component is indicated as described in section ROT-5.6 for molecular shuttles with symmetrical components. The only difference is that for unsymmetric threading components the recognition cites are sequentially numbered, starting from a site closer to the senior end E_A of the threading section, and are designated as rs^1, rs^2, etc.

rs^1-*MC* rs^2-*MC*

Figure 6.2.1.3.1. [2]Rotaxanes containing two recognition sites in an unsymmetrical threading component, and their corresponding prefixes.

For molecular shuttles with an unsymmetrical macrocyclic components, the recommended method for indicating the orientation and position of a component is an italicized prefix composed of a designation for the recognition site rs^n, designation *A* or *C* for each macrocyclic component with ring direction, and *ab* or *ba* for components with different sides that indicate which side is closer to the senior end E_A of a threading component. Figure 6.2.1.3.2 shows several examples of molecular shuttles with unsymmetric components and their recommended prefixes.



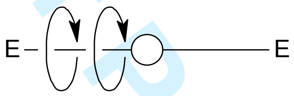
rs^2-*ab* rs^2-*ba*

Figure 6.2.1.3.2. [2]Rotaxanes containing two recognition sites in an unsymmetric threading component, and their corresponding prefixes.

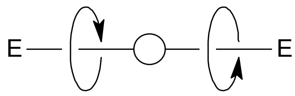
The described procedures are readily adaptable to more complex rotaxanes of different types.

ROT-6.2.2. Type 5 Rotaxanes with unsymmetric components

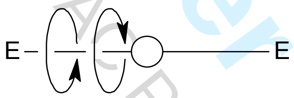
This section discusses Type 5 rotaxanes in which the linear sections of the threading component are structurally unsymmetric. For rotaxanes that include unsymmetric macrocyclic components, their orientation must be specified in order to describe the complete rotaxane structure unambiguously. For symmetrical, unbranched threading components, the prefix part of the rotaxane name cites the orientations of the components in the order in which they are positioned on the threading component when the rotaxane is viewed from one of the terminal ends. The prefix cites the most populated sections first, and then whether the threaded components have clockwise or anticlockwise orientation. For unsymmetric threading components, the orientations of components are cited when the rotaxane is viewed from the senior end E_A. Figure 6.2.2.1 shows examples of isomeric [3]rotaxanes with unsymmetric macrocyclic components and their recommended prefixes.



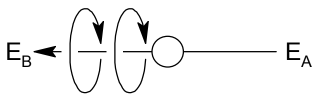
2-A,A:0 (not *0:2-C,C*)



1-A:1-C



2-C,A:0 (not *0:2-C,A*)



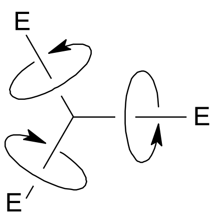
E_A-*0:2-C,C* (not E_B-*2-A,A:0*)

Figure 6.2.2.1. Isomeric Type 5 [3]rotaxanes of with unsymmetric macrocyclic components and their corresponding prefixes.

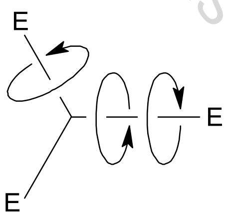
ROT-6.2.3. Rotaxanes of Types 6 to 8 with unsymmetrical components

For rotaxanes of Types 6–8 having branched threading components, clockwise and anticlockwise orientations are always defined when the rotaxane is viewed looking from the terminal end of a linear section towards the central junction point. The prefix cites linear sections for specific rotaxane types in the order defined in section ROT-5.3. If there is a choice, the most populated sections are cited first, then earlier cited macrocyclic components, and finally the macrocyclic components with anticlockwise orientation.

Examples of Type 6 rotaxanes containing three and four different macrocyclic components and their corresponding prefixes are shown on Figure 6.2.3.1.



1-A:1-A:1-A



2-C,A:1-A:0

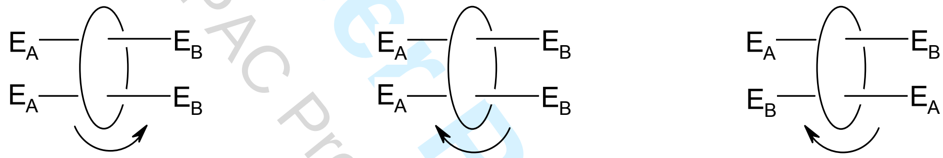
Figure 6.2.3.1. Type 6 rotaxanes of and their corresponding prefixes.

The principles specified above can be adapted for rotaxanes that have more complex threading components, for example, those having more macrocyclic components or star-shaped threading components with more than four arms.

ROT-6.2.4. Type 2 rotaxanes of with unsymmetrical components

For Type 2.1 [3]rotaxanes containing two unsymmetric threading components and one macrocyclic component, isomers differing in mutual orientation of threading components are possible. The orientation is defined by the prefix E_A,E_A or E_A,E_B, which depends upon whether the senior ends are on the same side or opposite sides of the macrocyclic component. If the macrocyclic component is also unsymmetric, the descriptor is modified to include an indication of the orientation of the macrocyclic component when the rotaxane is viewed from the end E_A of a threading component. Figure 6.2.4.1 shows examples of unsymmetrical Type 2.1 [3]rotaxanes and their corresponding prefixes.

E_A,E_B E_A,E_A



E_A,E_A-C E_A,E_A-A E_A,E_B

Figure 6.2.4.1. Unsymmetrical Type 2.1 [3]rotaxanes and their corresponding prefixes.

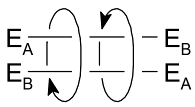
Note that the two first structures in the second row form an enantiomeric pair. The third structure is symmetrical but to highlight that the macrocycle is unsymmetrical the prefix E_A,E_B-A may be used in this case.

If Type 2.1 [3]rotaxanes shown in the second row on Figure 6.2.4.1 have asymmetric macrocyclic component with different sides, the prefixes will be E_A,E_A-ab, E_A,E_A-ba, and E_A,E_B (or E_A,E_B-ab) correspondingly.

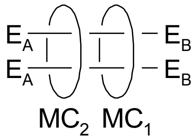
The prefixes for the Type 2.2 rotaxanes with unsymmetric components are generated according to the same principles recommended for rotaxanes of Types 1.2 and 2.1. Figure 6.2.4.2 shows several examples for Type 2.2 [4]rotaxanes and their corresponding recommended prefixes.

E_A,E_A E_A,E_A-C,C

E_A,E_A-C,A E_A,E_A-A,A



E_A,E_B-*CA*



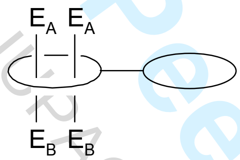
E_A,E_A-*MC*$_2$,*MC*$_1$

Figure 6.2.4.2. [4]Rotaxanes of Type 2.2 and the corresponding prefixes.

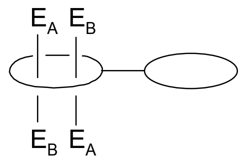
The same principles can be applied for other Type 2.2 [4]rotaxanes and other Type 2 rotaxanes .

ROT-6.2.5. Orientation of Threading Components for Rotaxanes of Type 3

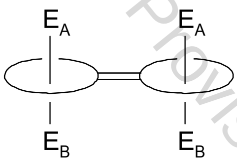
Type 3 rotaxanes with two or more asymmetrical threading components can form isomers that differ in mutual orientation of threading components. The isomers are specified by addition of E_A and E_B indications before the prefix to indicate the number of components in each threadable ring. Figure 6.2.5.1 shows several examples and their recommended prefixes.



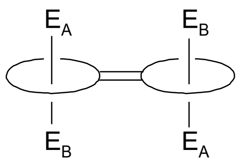
E_A,E_A-2:0



E_A,E_B-2:0



E_A-1:E_A-1



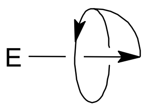
E_A-1:E_B-1

Figure 6.2.5.1. Type 3 [4]rotaxanes of and their corresponding prefixes. A double line drawn between two rings indicates that rotation of one ring with respect to the other is not possible.

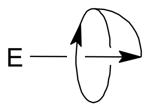
The same principles are used to define the structure of Type 4 rotaxanes with unsymmetric components.

ROT-6.2.6. Unsymmetrical Type 9 [1]rotaxanes

The linear section of a Type 9 [1]rotaxane is structurally unsymmetric and the free end that is not linked to the macrocyclic section can be arbitrarily designated as the senior end. If the macrocyclic part is unsymmetric, stereoisomers are possible and are specified by the addition of a prefix, *A*- or *C*-, in front of the complete name. The prefix is assigned according to the orientation when the rotaxane is viewed from E_A. The two possible isomers and their corresponding prefixes are shown in Figure 6.2.6.1.



C



A

Figure 6.2.6.1. Type 9 [1]rotaxane

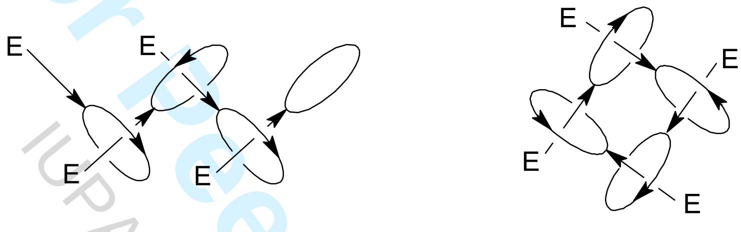
For example, the name for a [1]rotaxane in which the macrocyclic moiety has clockwise orientation is:

C-[1][*rotaxa*-(name of complete chemical substance)]

ROT-6.2.7. Unsymmetrical Type 10 [n]rotaxanes

For Type 10 rotaxanes with an unsymmetric macrocyclic component, stereoisomers are possible. Mutual orientation of components is described by addition of a prefix that cites the corresponding *A* and *C* or *ab* and *ba* descriptors generated in accordance with general procedure described in section ROT-6.1.

For acyclic Type 10 rotaxanes the prefixes are cited starting from the end with the free linear section, and the number of descriptors equals the number of components minus one. For cyclic Type 10 rotaxanes the descriptors are cited one by one along the "daisy-chain," and the number of prefixes equals the number of components. Figure 6.4.1 shows two examples of Type 10 [4]rotaxanes and their recommended descriptors.



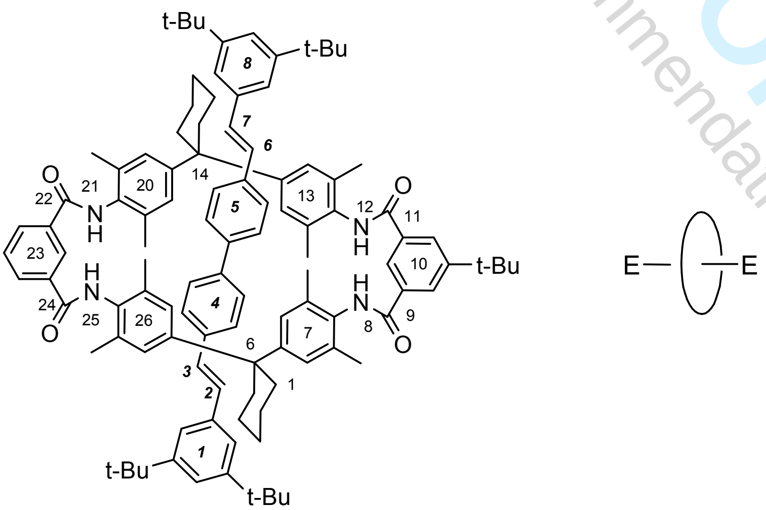
C,C,C *A,C,A,C*

Figure 6.2.7.1. Acyclic and cyclic Type 10 [4]rotaxanes and their corresponding prefixes.

ROT-7. EXAMPLES OF ROTAXANES AND THEIR SYSTEMATIC NAMES

This section illustrates the above-stated principles of rotaxane nomenclature for several examples of rotaxanes reported in the literature. Names are created according to the IUPAC recommendations for the nomenclature of organic compounds [22]. Because the rotaxane components very often contain several cyclic fragments, many compounds are named using phane nomenclature principles [29,30].

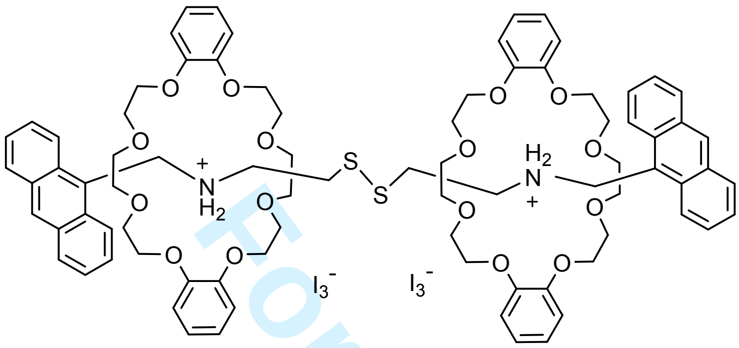
Example 1.

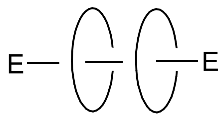


A Type 1.1 [2]rotaxane composed of symmetrical components. Isomers are not possible.

[2]([1^{3},1^{5},8^{3},8^{5}tetra-*tert*-butyl-1,8(1),4,5(1,4)-tetrabenzenaoctaphane-2,6-diene]-*rotaxa*-{10^{5}-*tert*-butyl-7^{3},7^{5},13^{2},13^{6},20^{3},20^{5},26^{3},26^{5}-octamethyl-8,12,21,25-tetraaza-7,13,20,26(1,4),10,23(1,3)-hexabenzenadispiro[5.7.5.7]hexacosaphane-9,11,22,24-tetrone})

Example 2



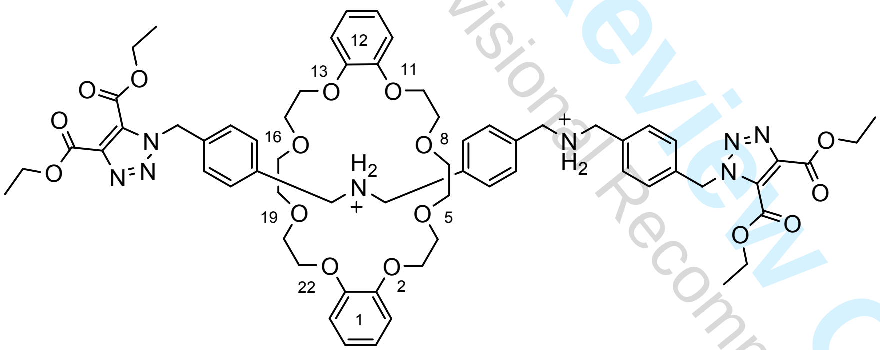


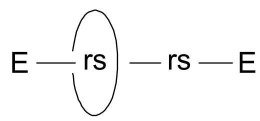
A Type 1.2 [3]rotaxane with symmetrical components. Isomers are not possible.

[3]({2,2'-disulfanediylbis[*N*-(anthracen-9-ylmethyl)ethanaminium]}-*rotaxa*-[2][2,5,8,11,13,16,19,22-octaoxa-1,12(1,2)-dibenzenacyclodocosaphane]) bis(triiodide)

Note: To highlight that macrocyclic components are associated with charged nitrogen atoms this compound can be considered as a molecular shuttle and the prefix *rs*^{1}-*MC*,*rs*^{2}-*MC* can be added in front of the name.

Example 3.



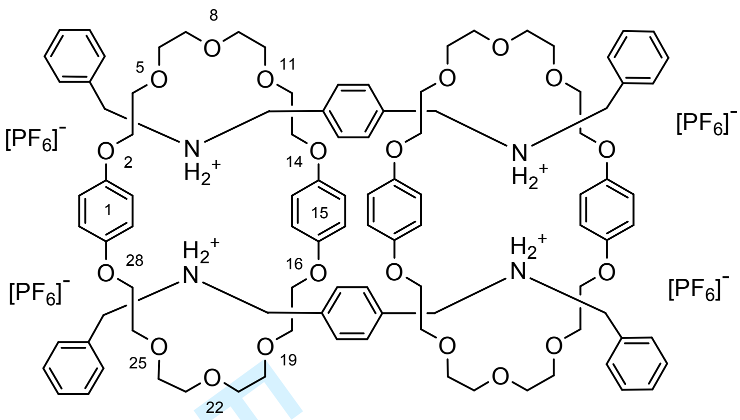


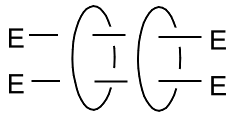
A Type 1.1 [2]rotaxane of that can function as a molecular shuttle composed of symmetrical components. Recognition sites are equivalent. Isomers are not possible.

[2]({*N*,*N*'-[1,4-phenylenebis(methylene)]bis[(4-{[4,5-bis(ethoxycarbonyl)-1*H*-1,2,3-triazol-1-yl]methyl}phenyl)methanaminium]}-*rotaxa*-[2,5,8,11,13,16,19,22-octaoxa-1,12(1,2)-dibenzenacyclodocosaphane])

Note: To highlight that the macrocyclic component is associated with one of two equivalent recognition sites the prefix *rs*-*MC* may be added.

Example 4

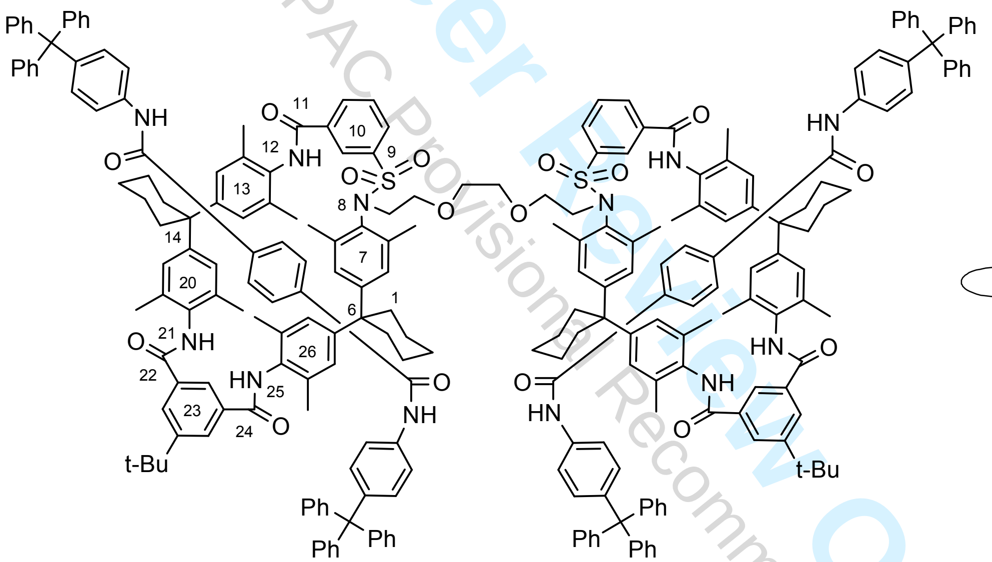


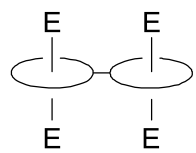


A Type 2.2 [4]rotaxane with symmetrical components. Isomers are not possible.

[4]{[2][*N*,*N'*-(1,4-phenylene)bis(*N*-benzylmethanaminium)]-*rotaxa*-[2][2,5,8,11,14,16,19,22,25,28-decaoxa-1,15(1,4)dibenzenacyclooctacosaphane]} tetrakis(hexafluorophosphate)

Example 5

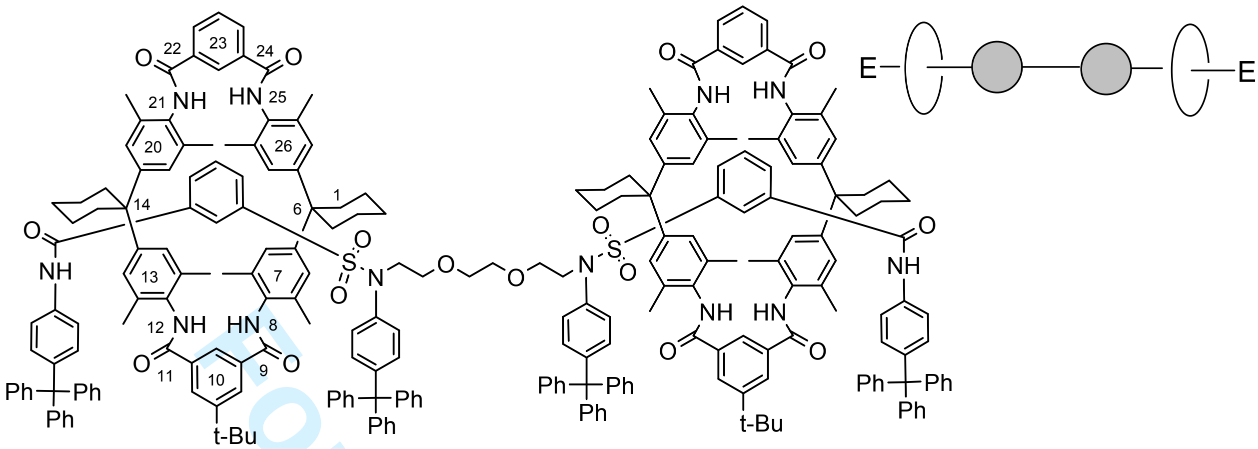




A Type 3 [3]rotaxane with symmetrical components. Isomers with different positions of threading components are possible. The prefix *1:1* is needed to specify the isomer.

1:1-[3]{[2][*N*,*N'*-bis(4-tritylphenyl)-1,4-benzenedicarboxamide]-*rotaxa*-{8,8'-[ethane-1,2-diylbis(oxyethane-2,1-diyl)]bis{23^5-*tert*-butyl-7^3,7^5,13^2,13^6,20^3,20^5,26^3,26^5-octamethyl-9λ^6-thia-8,12,21,25-tetraaza-7,13,20,26(1,4),10,23(1,3)-hexabenzenadispiro[5.7.5.7]hexacosaphane-9,9,11,22,24-pentone}}}

Example 6

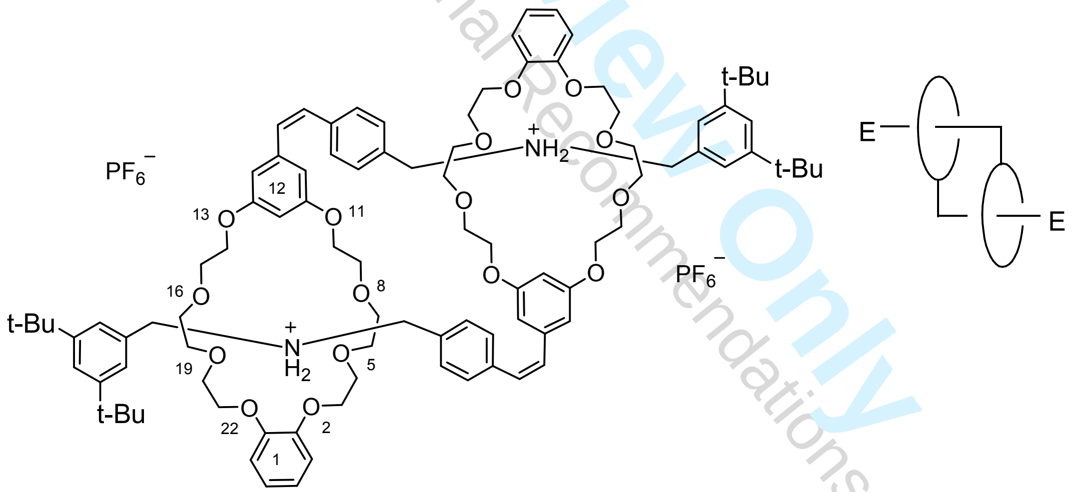


A Type 5 [3]rotaxane composed of two symmetric macrocyclic components and threading component with three linear sections. Isomers are possible. The number of macrocyclic components at each linear section must be specified.

1:0:1-[3]{[3,3'-(ethane-1,2-diylbis{oxyethane-2,1-diyl[(4-tritylphenyl)imino]sulfonyl})bis[*N*-(4-tritylphenyl)benzamide]]-*rotaxa*-[2][10^5-*tert*-butyl-7^3,7^5,13^2,13^6,20^3,20^5,26^3,26^5-octamethyl-8,12,21,25-tetraaza-7,13,20,26(1,4),10,23(1,3)-hexabenzenadispiro[5.7.5.7]hexacosaphane-9,11,22,24-tetrone]}

Note: If the threading component in this case is treated as having only two linear sections where macrocyclic component can reside, the prefix will be *1:1*.

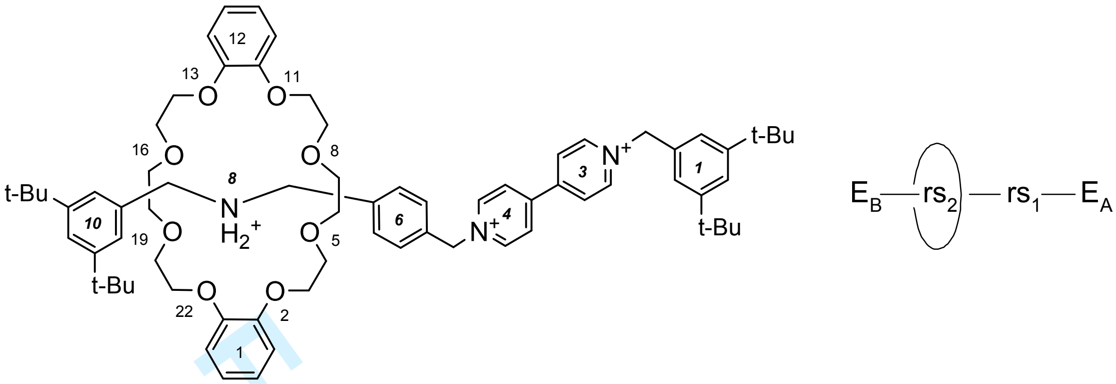
Example 7



A Type 10 cyclic daisy-chain [2]rotaxane composed of two symmetrical components. Isomers are not possible.

[*cyclo*-2]{*rotaxa*-[(3,5-di-*tert*-butylphenyl)-*N*-(4-{(*Z*)-2-[2,5,8,11,13,16,19,22-octaoxa-1(1,2),12(1,3)-dibenzenacyclodocosaphan-12^5-yl]vinyl}benzyl)methanaminium]}

Example 8

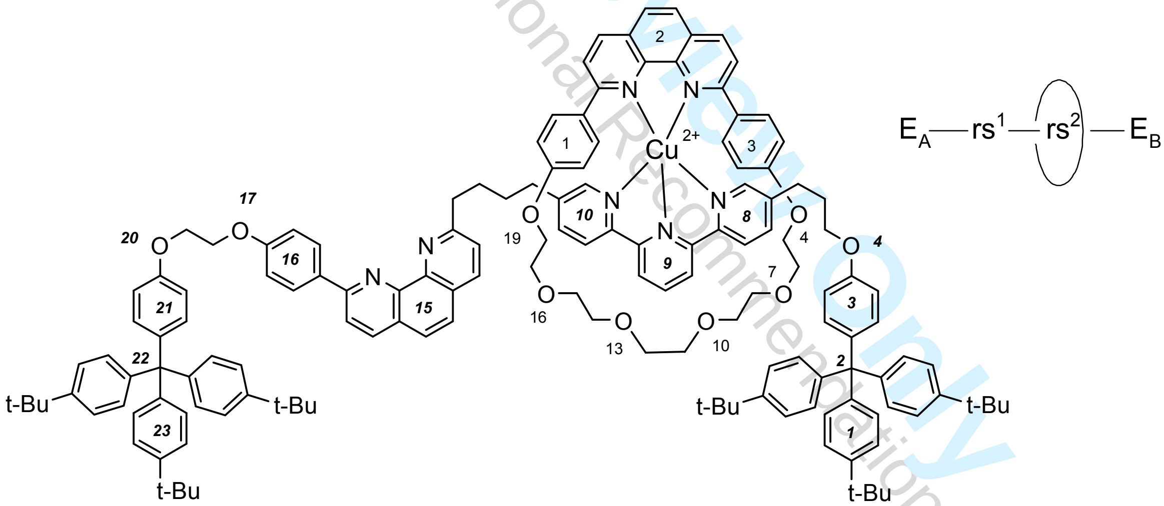


A Type 1.1 [2]rotaxane that functions as a molecular shuttle. The threading component is unsymmetrical and has two nonequivalent recognition sites. The macrocyclic component is symmetrical.

Isomers are possible. The designation of recognition sites is needed to specify the position of the macrocyclic component. The direction of the threading component is defined as described in section ROT-6.1.1. Thus the acyclic charged nitrogen is rs^2 and the resulting name for the drawn isomer is

rs^2-*MC*-[2]{[1^3,1^5,10^3,10^5-tetra-*tert*-butyl-8-aza-$3^1\lambda^5$,$4^1\lambda^5$-3(1,4),4(4,1)-dipyridina-1,10(1),6(1,4)-tribenzenadecaphan-8-ium-3^1,4^1-bis(ylium)]-*rotaxa*-[2,5,8,11,13,16,19,22-octaoxa-1,12(1,4)-dibenzenacyclodocosaphane]}

Example 9



A Type 1.1 [2]rotaxane that can function as molecular shuttle. Threading component is unsymmetrical and thus recognition sites are nonequivalent. Due to the coordination with copper atom the structure can function as a molecular shuttle depending on copper oxidation state [31]. The prefix is needed to specify an association with specific recognition site.

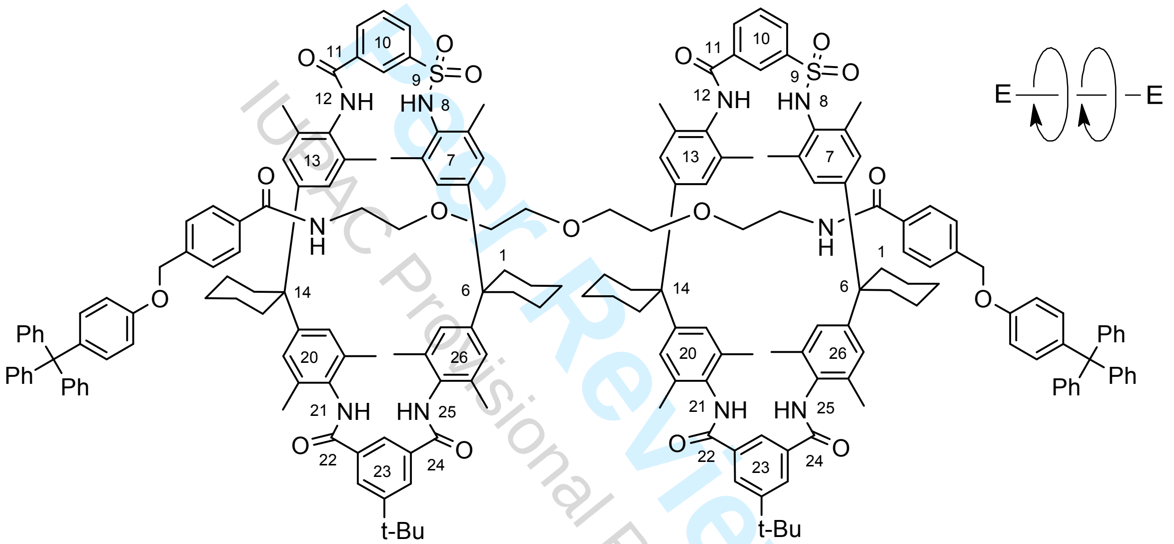
According to the procedure specified in the section ROT-6.1.1 the direction is defined by the senior oxygen atom with number 17 and benzene ring number 16 as its senior ligand. So phenanthroline site is designated as rs^1 and terpyridine fragment as rs^2 correspondingly. The resulting name for the drawn structure is

(rs^2-*MC*-[2]{[1,23-di-*tert*-butyl-2,2,22,22-tetrakis(4-*tert*-butylphenyl)-4,17,20-trioxa-15(2,9)-[1,10]phenanthrolina-8(5,2),9(2,6),10(2,5)-tris(pyridina-κ*N*)-1,23(1),3,16,21(1,4)-pentabenzenatricosaphane]-*rotaxa*-[4,7,10,13,16,19-hexaoxa-2(2,9)-phenanthrolina-1,3(1,4)-dibenzenacyclononadecaphane-κ*N*,κ*N*′]})copper(2+)

The reduced copper(1+) form of this complex has copper atom coordinated with phenanthroline fragment of the threading component and the name will be:

(rs^1-*MC*-[2]{[1,23-di-*tert*-butyl-2,2,22,22-tetrakis(4-*tert*-butylphenyl)-4,17,20-trioxa-15(2,9)-[1,10]phenanthrolina-κ*N*,κ*N*′-8(5,2),9(2,6),10(2,5)-tripyridina-1,23(1),3,16,21(1,4)-pentabenzenatricosaphane]-*rotaxa*-[4,7,10,13,16,19-hexaoxa-2(2,9)-phenanthrolina-1,3(1,4)-dibenzenacyclononadecaphane-κ*N*,κ*N*′]})copper(1+)

Example 10

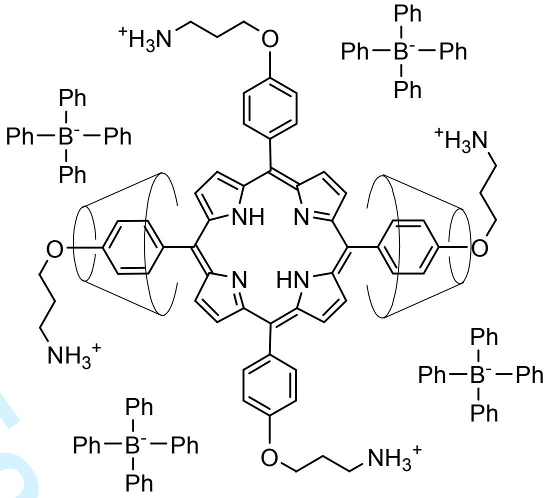


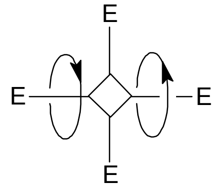
A Type 1.2 [3]rotaxane with symmetrical threading component and two equivalent unsymmetrical macrocyclic components. Isomers are possible.

The ring direction is defined by senior atom S and its senior ligand starting with the N-atom. A view from the left end of the threading component leads to the prefix *CC*- and a view from the right end to the prefix *AA*- that is chosen as alphabetically senior. The resulting name for the drawn isomer is

AA-[3]({*N*,*N*′-[oxybis(ethane-2,1-diyloxyethane-2,1-diyl)]bis{4-[(4-tritylphenoxy)methyl]benzamide}}-*rotaxa*-[2](23^5-*tert*-butyl-7^3,7^5,13^2,13^6,20^3,20^5,26^3,26^5-octamethyl-$9\lambda^6$-thia-8,12,21,25-tetraaza-7,13,20,26(1,4),10,23(1,3)-hexabenzenadispiro[5.7.5.7]hexacosaphane-9,9,11,22,24-pentone)}

Example 11

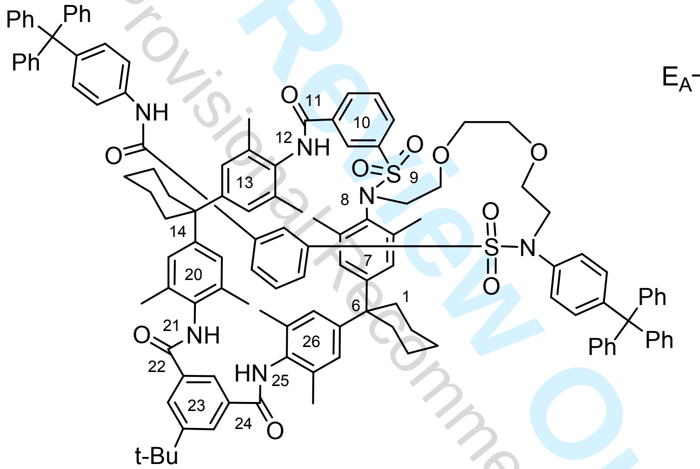


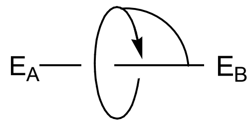


A Type 7 [3]rotaxane composed of two asymmetrical macrocyclic components and an X-shaped threading component with four linear sections with square-planar topology. Isomers are possible. The number and an orientation of the macrocyclic component in relation to the asymmetrical linear sections must be specified.

1-C:0:1-C:0-[3][{3,3',3'',3'''-[porphyrin-5,10,15,20-tetrayltetrakis(4,1-phenyleneoxy)]tetra(1-propanaminium)}-*rotaxa*-[2](β-cyclodextrin)] tetrakis(tetraphenylborate)

Example 12

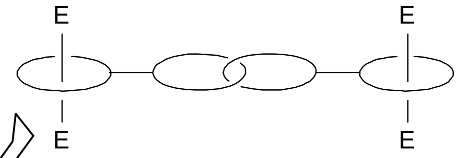


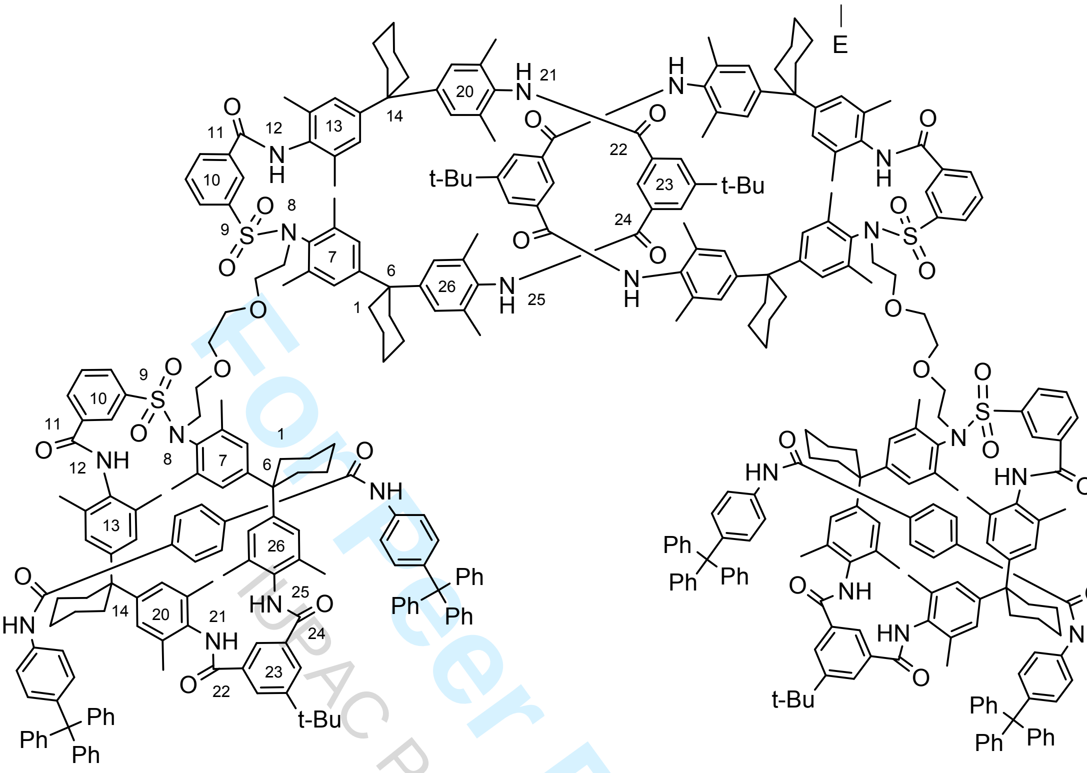


A Type 9 [1]rotaxane . Macrocyclic and threading parts are unsymmetrical. Isomers are possible. The orientation of the macrocyclic component in relation to the linear section must be specified.

A-rotaxa-[1][3-({[2-(2-{2-[23^{5}-*tert*-butyl-7^{3},7^{5},13^{2},13^{6},20^{3},20^{5},26^{3},26^{5}-octamethyl-9,9,11,22,24-pentaoxo-$9\lambda^{6}$-thia-8,12,21,25-tetraaza-7,13,20,26(1,4),10,23(1,3)-hexabenzenadispiro[5.7.5.7]hexacosaphan-8-yl]ethoxy}ethoxy)ethyl](4-tritylphenyl)amino}sulfonyl)-*N*-(4-tritylphenyl)benzamide]

Example 13





A Type 11 [3]rotaxane composed of two symmetrical threading components and a two-component catenane macrocyclic component. The catenane component has four macrocyclic sections. Isomers are possible. An indication of the number of threading components in each macrocyclic section is needed.

1:0:0:1-[3]([2]{*N*,*N'*-bis[4-(triphenylmethyl)phenyl]-1,4-benzenedicarboxamide}-*rotaxa*-{(*1-1*)-[2][*catena*-(8,8'-[ethane-1,2-diylbis(oxyethane-2,1-diyl)]bis{23^5-*tert*-butyl-7^3,7^5,13^2,13^6,20^3,20^5,26^3,26^5-octamethyl-9λ^6-thia-8,12,21,25-tetraaza-7,13,20,26(1,4),10,23(1,3)-hexabenzenadispiro[5.7.5.7]hexacosaphane-9,9,11,22,24-pentone})]}

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