Classification of Topological Isomers: Knots, Links, Rotaxanes, *etc.*

Jan Cz. Dobrowolski[a,b]

[a]*National Institute of Public Health, 30–34, Chełmska Street, 00–725 Warsaw, Poland*

[b]*Industrial Chemistry Research Institute, 8, Rydygiera Street, 01–793 Warsaw, Poland*
(E-mail: janek@il.waw.pl)

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Topological isomers, *i.e.*, knots, catenanes, rotaxanes, pseudoknots, hook-and-ladder, and Möbius molecules have so far been left out from the isomer classification schemes discussed. To expand the classification schemes to include the topological molecules such as knots and links, questions about the number of components and the number of crossings are incorporated into the scheme. In the case of rotaxanes and pseudoknots, which are topologically trivial, a procedure making them not trivial is described. For the hook-and-ladder as the well as Möbius type of isomers, a procedure is given that allows their classification. All the new procedures are included into the new classification scheme in such a way that all questions about topology precede the ordinary question tree. In that way, a molecule is first classified as a topological object, and then classical questions about its structure are asked.

INTRODUCTION

The concept of isomerism was introduced by Berzelius in 1830 for compounds having an identical chemical composition and molecular mass, but different properties. Since then isomerism has been one of the most fruitful concepts in chemistry.[1] A modern definition of isomerism[2] says that isomers are individual chemical species with an identical molecular formula and display at least some differing physico-chemical properties, which are stable for periods of time that are long in comparison with those during which measurements of their properties are made. A number of classification schemes have been proposed[1] but the discovery of novel molecular structures has made repeated verifications and revisions of the schemes necessary.[3,4] The two main classes of isomers are differentiated with respect to the molecular connectivity: structural (constitutional) isomers have

different whereas stereoisomers have identical connectivities. Next, either chain, position and functional group isomerism (tautomerism included) or optical, geometrical and orientational isomerism is defined.

One recent type of stereoisomerism (first discussed,[5,6] then discovered in different forms of nucleic acids[7–20] and synthesized: knots,[21–24] hook-an-ladder and Möbius,[25,26] catenanes and rotaxanes[27–49]) is topological isomerism.[50,51] Topological isomers can be either constitutional isomers or stereoisomers; therefore, they can be both optically active and/or geometrical and/or orientational isomers. Thus, an unique definition of topological isomerism is desired. Intuitively, there is a difference between the »cycle-knot«, link(*i*)-link(*j*), »cylinder-Möbius strip« and »sphere-torus« isomerisms. The aim of the present paper is to extend the classification scheme[3,4] to include knots, links (catenanes) and some of the less frequently synthesized or observed topological isomers.

RESULTS AND DISCUSSION

Motivation for Extension of the Classification Scheme

The classification scheme of isomers[3] is presented in Table I. This scheme seems to be quite satisfactory as long as we deal with the molecules that are not topological isomers. In very detailed classiffication scheme,[4] topological isomers are included, yet only as having the same connectivity.

Let us consider the molecular cycle (unknot) and the simplest isomeric molecular trefoil knot (Figure 1). These two molecules have identical connectivity matrices, however, to say that they are configurational diastereo-
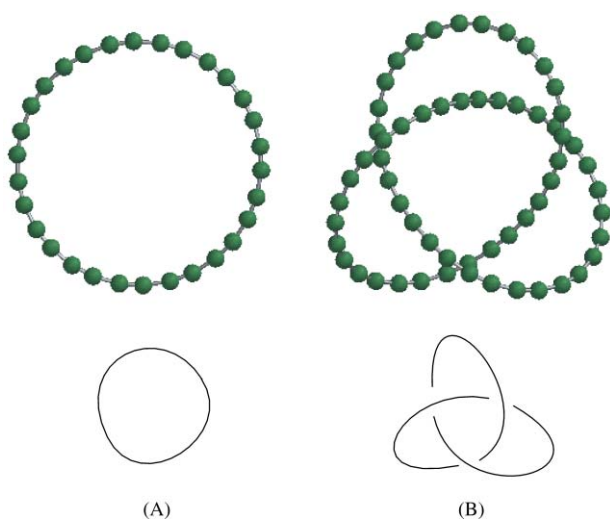
isomers (Table I) is not adequate. The same holds for any pair of molecular isomeric knots of different topological type (*cf.* Figure 2).

Let us now consider molecular links (catenanes) and separate two cyclic molecules of the same size, like those interlocked in the catenane structure (Figure 3). Again, the catenane molecule and the two separated molecules have the same connectivities. However, the mass spectrum of the former should exhibit a molecular peak corresponding to the sum of catenane components masses whereas that of the latter should not. Therefore, the connectivity matrix of the former can be written in the form of a single, two diagonal block matrix whereas that of the latter in the form of two matrices.

Let us now consider two catenane molecules of identical molecular formulas and topological type but

Figure 1. Cyclic (A) and trefoil knot 3_1 (B) carbyne C_{30} molecules have identical connectivity matrices.[58–60]
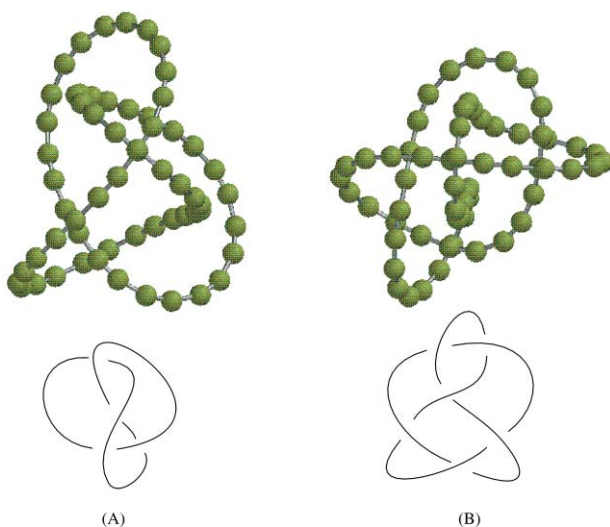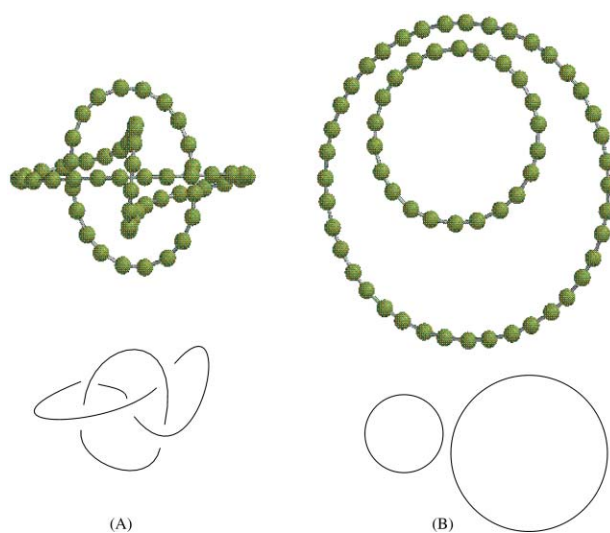

Figure 2. Connectivity is the same for any pair of isomeric knot molecules; *e.g.*, the figure-eight 4_1 knot (A) and the 6_2 (B) carbyne C_{60} knot molecules.[60]

Figure 3. The molecular 5^2_1 link (catenane) (A) and two separate cyclic carbyne molecules (B) and the have identical connectivities; however, the former is one molecule and the latter are two molecules.[61]
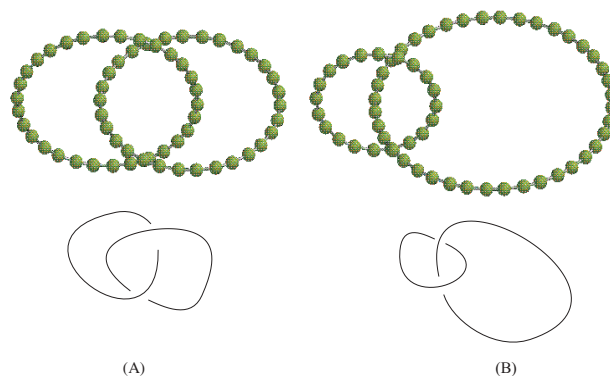

Figure 4. Two isomeric catenane molecules are of the same topological type 2^2_1 (Hopf links) but they have different connectivities: rings are of different size – it has been proposed to name them *catenamers*.[61]

TABLE I. The classification scheme for isomers of organic molecules according to Ref. 3

Two molecules have the same molecular formula				
Are they completely superimposable?				
YES: They are IDENTICAL STRUCTURES	NO: Any pair of compounds beyond this point are ISOMERS			
	PLACE TO DETERMINE THE MOLECULAR TOPOLOGY (this work)			
	Do they have identical connectivity matrices?			
	YES: They are CONSTITUTIONAL ISOMERS	NO: They are STEREOISOMERS		
		Are they non-superimposable mirror images?		
		YES: They are ENANTIOMERS		NO: They are DIASTEREOISOMERS	
		Are they identical after rotation around a single bond?		Are they identical after rotation around a single bond?	
		YES: They are CONFORMATIONAL ENANTIOMERS	NO: They are CONFIGURA-TIONAL ENANTIOMERS	YES: They are CONFORMATIO-NAL DIASTEREO-ISOMERS	NO: They are CONFIGURA-TIONAL DIASTEREO-ISOMERS

differing in the size of the components (Figure 4). These molecules have different connectivity matrices and, in that sense, they are constitutional isomers; and yet they are of the same topological type; therefore, we have named this kind of isomers *catenamers*.[60]

Now, let us consider two catenanes with identical connectivity matrices, *i.e.,* identical in the size of the components, but differing in topological type (Figure 5). Once again, in terms of the classification scheme pr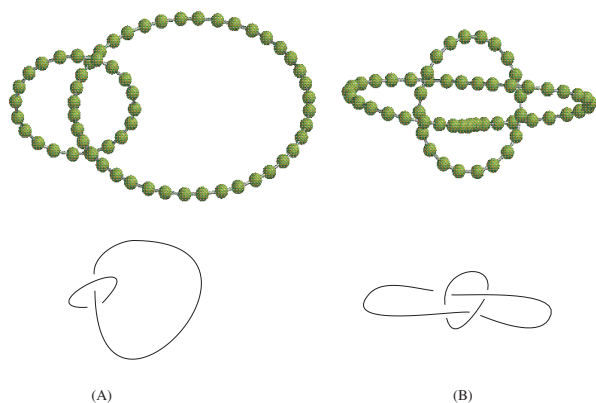esented in Table I, these molecules would be classified inadequately. They should be named configurational diastereoisomers; however, this would be an oversimplification: the number of different catenanes is large and all those with a relatively small number of crossings are to be classified analogously to the mathematical classification of links.[52–56]

The above examples show why the classification scheme[3,4] (Table I) has to be revised and extended. In the revised approach, new questions must be asked, concerning:

a) structure connectivity (catenanes, rotaxanes),

b) number of components (catenanes, rotaxanes),

c) possibility of structure decomposition without bond breaking (rotaxanes), and

d) number of crossings (knots, catenanes, rotaxanes, and pseudoknots).

The aim of any classification scheme is to sort the existing molecules, but also to show the possibility of the existence of new categories of compounds. On the other hand, extending the classification scheme towards topological molecules involves the risk of going too far, *i.e.*, of including the objects that are mathematical figures rather than potential molecules. Therefore, it is important to balance the descriptivity and the predictivity of the classification developed. This is why the modified

Figure 5. Two isomeric catenane molecules (A) 2^2_1 and (B) 4^2_1 have identical connectivities but different topological types.[61]

scheme proposed below continues to maintain some questions, which are easily to generalize, in their simple forms.

Concept of Simplified Reduced Regular Diagram

Before new elements of the question tree are introduced and discussed, the regular diagram, an elementary concept of the knot theory,[53] must be defined: A regular diagram $D \subset \mathbb{R}^2$ of a (molecular) knot, link, or rotaxane (knotted molecular structure) $S \subset \mathbb{R}^3$ (molecular graph in $\mathbb{R}^3$) is such a projection of the molecule S onto the diagram D in which:

(i) The diagram D has at most a finite number of points of intersections.

(ii) Inverse image of each intersection point has exactly two points.

(iii) A vertex (atom) can be a point of intersection but it is never mapped onto a double point.

The situations presented in (Figures 6A-6C) are not allowed in a regular diagram.
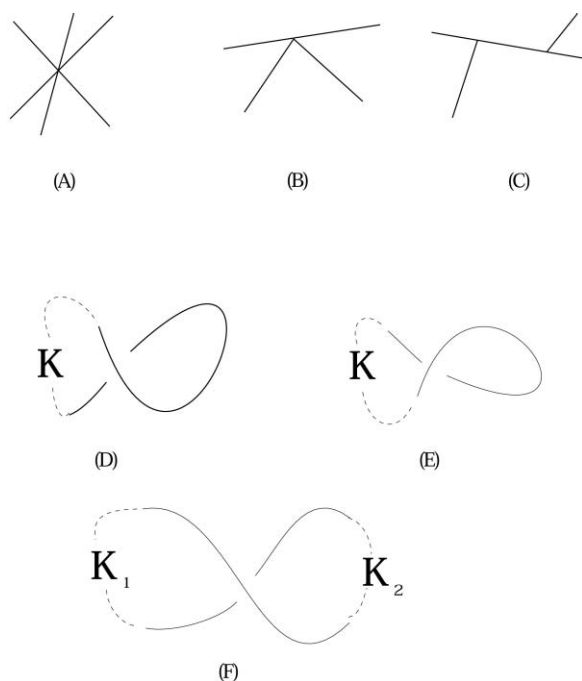

Figure 6. The cases not permissible in the regular diagram (A-C) and types of crossings that have to be reduced to obtain the reduced regular diagram (D-F). K stands for knot.

The number of regular diagrams is countless,[53] because they may have the crossing points of the type shown in Figures 6D-6F, therefore, a reduced regular diagram (RRD) does not possess any crossing point of this type.

The presence or absence of side chains or substituents does not affect the topological type of molecular structure. Moreover, all the side chain and substituent subtleties are included into the molecular connectivity

and are classified by reference to Table I. In particular, the (phenyl, naphthyl, *etc.*) rings in the main chain can be replaced by one segment. Therefore, for the analysis of the topological type of a molecular structure, the reduced regular diagram can be further simplified by cutting off the side chains and substituents and replacing small untied chains by segments. In that way, we obtain a simplified reduced regular diagram (SRRD), which can be further examined as a sheer topological object.

Concept of ρ-link

The idea of a (simplified) reduced regular diagram is very useful if we deal with non-trivial topological structures. However, a very important class of topological compounds, rotaxanes, treated in terms of RRD, reveal their trivial topological structures: reduction of a regular diagram of a rotaxane molecule leads to several untied components in a rotaxane diagram. (In general, some rotaxane components may still be tied because they may be topologically knotted or linked).

To avoid the problem of rotaxane classification, as a topologically trivial molecule, Dodziuk and Nowiński attached two (infinite) planes to two ends of the interlaced component of a rotaxane molecule.[50] Here, let us imagine that we close the rotaxane molecule in a 3-dimensional sphere (a figure homeomorphic with the sphere) that has only two common points with the rotaxane structure, which are the ends of the interlaced component. If there is more than one interlaced component, the sphere has mutual points with all the ends. On the sphere, we choose an arc or arcs (figures homeomorphic with arcs) that join all the pairs of ends of the interlaced component(s) and are mutually disjoint. As a result, we obtain here a link that can be classified in full analogy to the catenane structure (Figure 7A). The above concept is similar to the concept of an *(n, n)*-tangle;[53] in a tangle, however, all the ends of an internal segment placed at the sphere are joined by a single circle. Let us name the object that results from closing the rotaxane molecule within a sphere and joining the 2*n* ends of interlacing components the ρ-link.

Concept of ψ-knot

In the mid-1990's Mislow and Liang presented several examples of pseudoknots.[57] The pseudoknots are knotted structures which, however, are not closed and therefore are topologically trivial. In this case, the idea of closing the molecule in a sphere and then joining its ends, placed on the sphere, by an arc is very useful (Fig 7B). We shall refer to the knot resulting from a pseudoknot as the ψ-knot. In that way, the ψ-knot can be classified analogously to the ordinary knot.
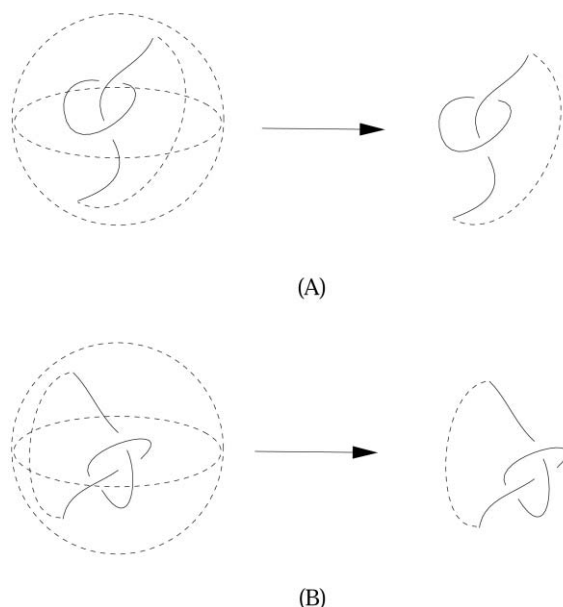
Figure 7. Illustration for ρ-link (A) and ψ-knot construction (B).

Hook-and-ladder and Möbius Strip Molecules

A connected bi-, tri-, ..., *j*-cyclic molecule can be topologically not trivial, *i.e.*, it can have *k* crossings. In general, any cycle can have crossings with itself and/or with another cycle. So far, two types of molecules belonging to this class have been known in chemistry: the hook-and-ladder and the Möbius strip[25,26] compounds. In the former type the ending two cycles are linked (Figure 8A) and in the latter the binding cycle is twisted (Figure 8B). Here, we address solely these two types of molecules. Unlike in mathematics, a chemical Möbius strip (and any other molecule) can always be classified as one-dimensional figure, because the bonds can be transformed into segments in $\mathbb{R}^3$. We propose to classify the two types of compounds analogously to the classification proposed in our recent paper on hook-and-ladder carbyne structures.[64]

The following three factors have to be considered to classify the topological type of hook-and-ladder structures:[64]

The first is the *M-H* (Möbius-Hook-and-Ladder) isomerism at the (*j*)-cycles, the idea first formulated as *cis-trans* isomerism at the cyclobutadiene ring for hook-and ladder structures.[64] Let us replace the (*j*-2)-cycles by a rectangle with the longer pair of bonds representing all the (*j*-2) binding cycles. In that way, we obtain a simplified tricyclic structure. We shall refer to such a simplification as the 3-cyclic reduction. Now, assuming that the segment ends at two neighbouring vertices of the rectangle, the structure is named the *H*-structure (Hook-and-Ladder) (Figures 8C and 8D), and if otherwise, *i.e.*, with the ends attached to the diagonal vertices, the
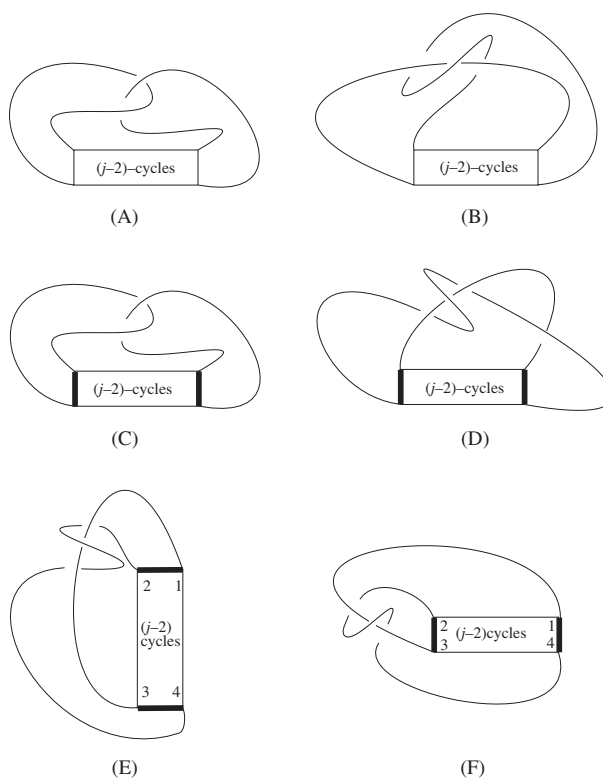

Figure 8. Scheme of hook-and-ladder (A) and Möbius (B) structures, and two possible hook-and-ladder (C, D) and Möbius (E, F) isomers.

structure is called the *M*-structure (Möbius) (Figures 8E and 8F). Notice, that the H-structures of type as in Figure 8D may be named also Belt structures.[66]

The second is the path over the structure: if we agree that the molecular path goes through the shorter bonds of the rectangle (represented in Figure 9 by broader lines), two situations are possible: (i) the path runs over the whole structure, (ii) the path runs over two separated circles. The two situations exist only for the *H*-structures.

For the *M* (Möbius) isomers, the path is always over the whole structure. However, in their case, there is also a topological invariant, which is the path orientation, *i.e.*, the order of the labels of the four vertices of the rec-
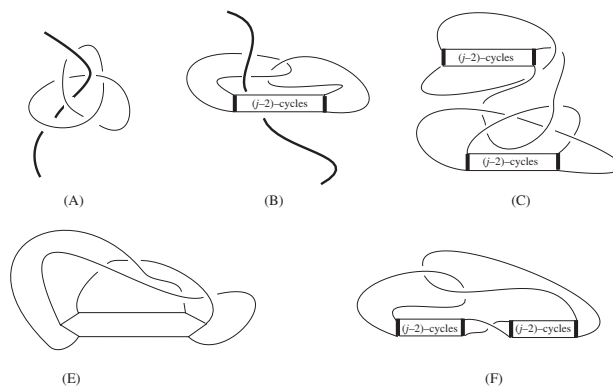

Figure 9. Scheme of different new types of topological compounds.

tangle determined by the path. Assume that the vertices are labeled counterclockwise and the path runs from the first vertex through the long segment to the diagonal third. Then, the path goes either to the second or to the fourth vertex. Abstraction classes of the sequences either (1243) ≡ (1342) or (1423) ≡ (1324) determine the type of the *M* isomers.

If the *H-M* isomerism occurs at the (*j*-2)-cycles, two kinds of *H* and two kinds of *M* isomers appear (Figures 8C–8F). Thus, let us introduce the following notation of the isomers:

$$\kappa \, k_n(\mathrm{J})$$

where *k* – number of crossings,

     n – serial number,

     J – path over the structure running either over the whole structure (J = I) or over two independent cycles (J = II) for the *H* isomers, or orientation equivalent to the rectangle vertices numbering (1243) ≡ (1342) then (J = I) or (1423) ≡ (1324), then (J = II) for the *M* isomers

     κ – *H* or *M* arrangement around the rectangle (resulting from 3-cyclic reduction) separating the two linked (*H*) or knotted (*M*) segments.

In a search for topological classification, there is no need to address the number of cycles (*j*-2): we assumed that these cycles are neither linked nor knotted and the number of cycles will be found by connectivity examination based on Table I.

Classification of Topological Molecules

The concepts of (simplified) reduced regular diagram, ρ-link, ψ-knot, and (*H-M*)-isomerism allow us to classify the known knot, link, rotaxane, pseudoknot, hook-and-ladder, and Möbius molecular structures. Assume that for the molecule to be classified, the molecular graph, the simplified reduced regular diagram, the ρ-link and the ψ-knot diagram are well known.

Than we can find the following numbers:

    1. Number of connected components *m* of the molecular graph.

    2. Number of cycles *c* in the simplified reduced regular diagram.

        2.1. If *m* – *c* = 0, then we deal with

            2.1.1. knot (*m* = 1, *c* = 1), or

            2.1.2. link (*m*>1).

        2.2. If *m* – *c* > 0, then we deal with a rotaxane molecule, and

            2.2.1. ρ-link must be formed.

            2.2.2. Number of connected ρ-link components *μ* must be checked.

        2.3. If *c* = 0, then we deal with a pseudoknot or a not knotted molecule, and

            2.3.1. ψ-knot must be formed.

        2.4. If *m* – *c* < 0, then we deal with a hook-and-ladder or Möbius strip molecule (*m* = 1, *c* >1), and

            2.4.1. A 3-cyclic reduction of *j*-cycles of the molecular graph must be applied.

            2.4.2. Hook-and-Ladder or Möbius-isomerism must be distinguished.

   3. Number of crossings of the simplified reduced regular diagram *k*.

    4.1. Classified topology of the molecule can be written using the Alexander and Briggs notation:[65] (k_n^m) in the case of links (catenanes) and knots (then *m* = 1 is omitted in the notation) where subscript *n* is the prime knots or links counting index.

    4.2. In the case of rotaxanes, we propose to use a similar notation: ($\rho k_n^{(\mu,c)}$), where *ρ* stands for the ρ-link procedure applied, and the superscript is the number pair (*μ*, *c*) where *μ* is the number of ρ-link components and *c* is the number of parent cyclic components.

    4.3. In the case of ψ-knots, we propose to use a notation similar to the knot notation: (ψk_n), where letter ψ stands for the ψ-knotting procedure applied.

    4.4. In the case of Hook-and-Ladder or Möbius isomers, we use the notation (κk_n(J)), where *κ* = *H* or *M* (optionally Hook or Moeb), and J stands for the type of two segments binding to the model rectangle (see previous section).

    4.6. If *k* = 0, symbols are omitted.
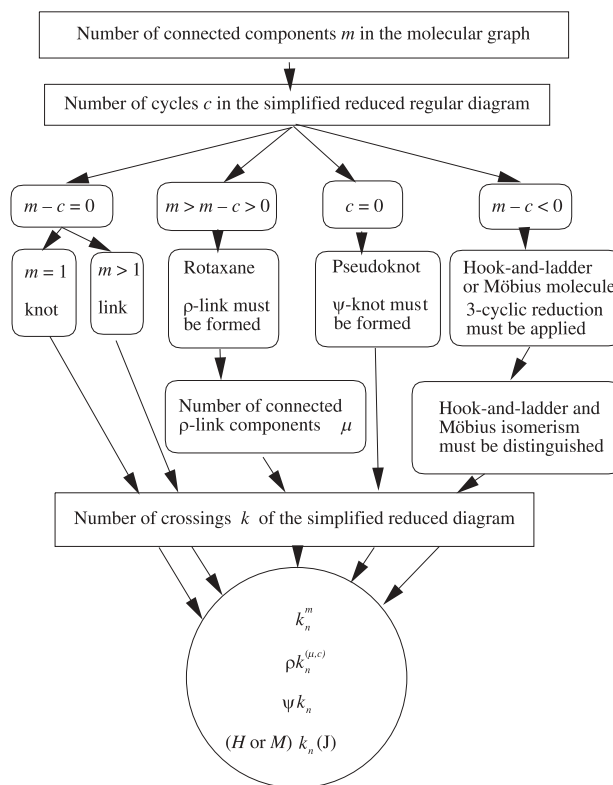
Scheme 1

The above numbers should be found (Scheme 1), and the Alexander and Briggs notation should be given to molecules, just after we state that the two molecules are isomers (see PLACE TO DETERMINE THE MOLECULAR TOPOLOGY, Table I). Once the topological notation is assigned to the classified molecules, the remaining questions in Table I can be asked.

Final Remarks

The present paper focuses on the known types of topological molecules rather than on a multitude of possible new compounds. Some new topological chemical structures may be generated by combining the known types of structures and some by generalizing their definitions:

(i) knot and chain would give a ro-knot structure (Figure 9A),

(ii) knot and Möbius strip, or cycle and hook-and- ladder may yield a new type of catenanes (Figures 9B and 9C),

(iii) if not only two ending rings are linked or knotted in the hook-and-ladder or Möbius strip structures, then a new topological type of molecules is formed (Figure 9E),

(iv) if more than two segments in the hook-and-ladder or Möbius structure can be linked and/or knotted, this would lead to another new topological compound (Figure 9F),

(v) *etc*. ...

We believe that the fascinating new kinds of topological compounds will be found in Nature and/or synthesized soon. Thus, the problem of how to extend the classification will be confronted with future needs.

CONCLUSIONS

The classification scheme for chemical compounds[3,4] has been extended to include topological molecules such as knots, catenanes, rotaxanes, pseudoknots, hook-and-ladder, and Möbius. The extension required a few additional questions to be included into the classification. They have been added so that all the questions about topology precede THE ordinary question tree. In that way, a molecule is first classified as a topological object, and then classical questions about its structure are asked.

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SAŽETAK

Klasifikacija topoloških izomera: Uzlovi, spone, rotaksani i srodne molekule

Jan Cz. Dobrowolski

Dosadašnje sheme za klasifikaciju izomera nisu razmatrale topološke izomere za npr. uzlove, katenane, rotaksane, pseudouzlove, kuke-i-ljestve i Möbiusove molekule. Stoga su prvo sheme za klasifikaciju uzlova i spona proširene time da uključuju pitanja o broju komponenti i broju križanja. Za topološki trivijalne rotaksane i pseudouzlove opisan je postupak koji ih čini netrivijalnim. Za izomere kuka-i-ljestva i Möbiusovih molekula također je dan postupak za njihovu klasifikaciju. Svi ovi navedeni postupci uključeni su u novu klasifikacijsku shemu u kojoj upiti o topologiji prethode uobičajenom redoslijedu pitanja, naime, molekule se prvo klasificiraju kao topološki objekti, a tek se onda postavljaju pitanja o njihovoj strukturi.