Knot Theory and Applications

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Abstract

Knots are used in our everyday life, such as to tie our shoes, to make a swing, dock a boat, or wrap packags. A knot is a knotted loop of string, except that we think of the string as having no thickness, its cross-section being a single point. The knot is then a closed curve in space that does not intersect itself anywhere. Knots have certain rules, such as the Reidemeister moves, links, and braids that are the main contributers to the applications of Knot Theory. Knot theory has been around for hundreds of years, but has recently begun to contribute to the fields of physics and biochemistry, and when applied to mathematics, knots lead to in depth results about topology and geometry.

Rules

Reidemeister Moves

The Reidemeister moves allow for two different projections of the same knot to be rearranged, so they can resemble the same projection.
The Type 1 Reidemeister move allows us to put in or take out a twist in the knot.
The Type 2 Reidemeister move allows us to either add two crossings or remove two crossings.
The Type 3 Reidemeister move allows us to slide a strand of the knot from one side of a crossing to the other side of the crossing.

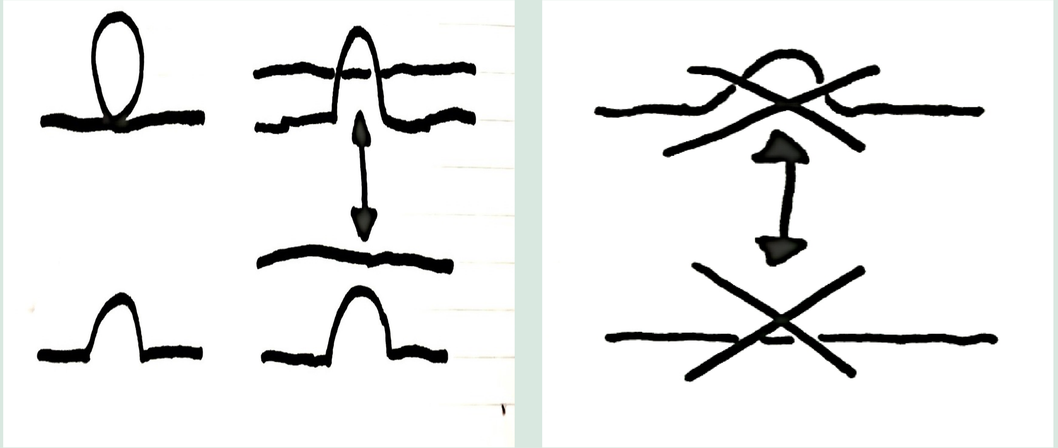


Figure 1: The pictures are in the following order: Type 1, Type 2, Type 3.

Links

A link is a set of knotted loops all tangled up together
You can have two projections of the same link as long as we can deform the one link to the other link without ever having any one of the loops intersect itself or any other loops in the process.

Braids

A braid is set of n strings that are attached to a horizontal bar at the top and bottom.
Similar to knots braids can be rearranged through Reidemeister moves to determine if two projections are the same.
Braids are important because every knot or link is a closed braid!

Topological Chirality

Chirality

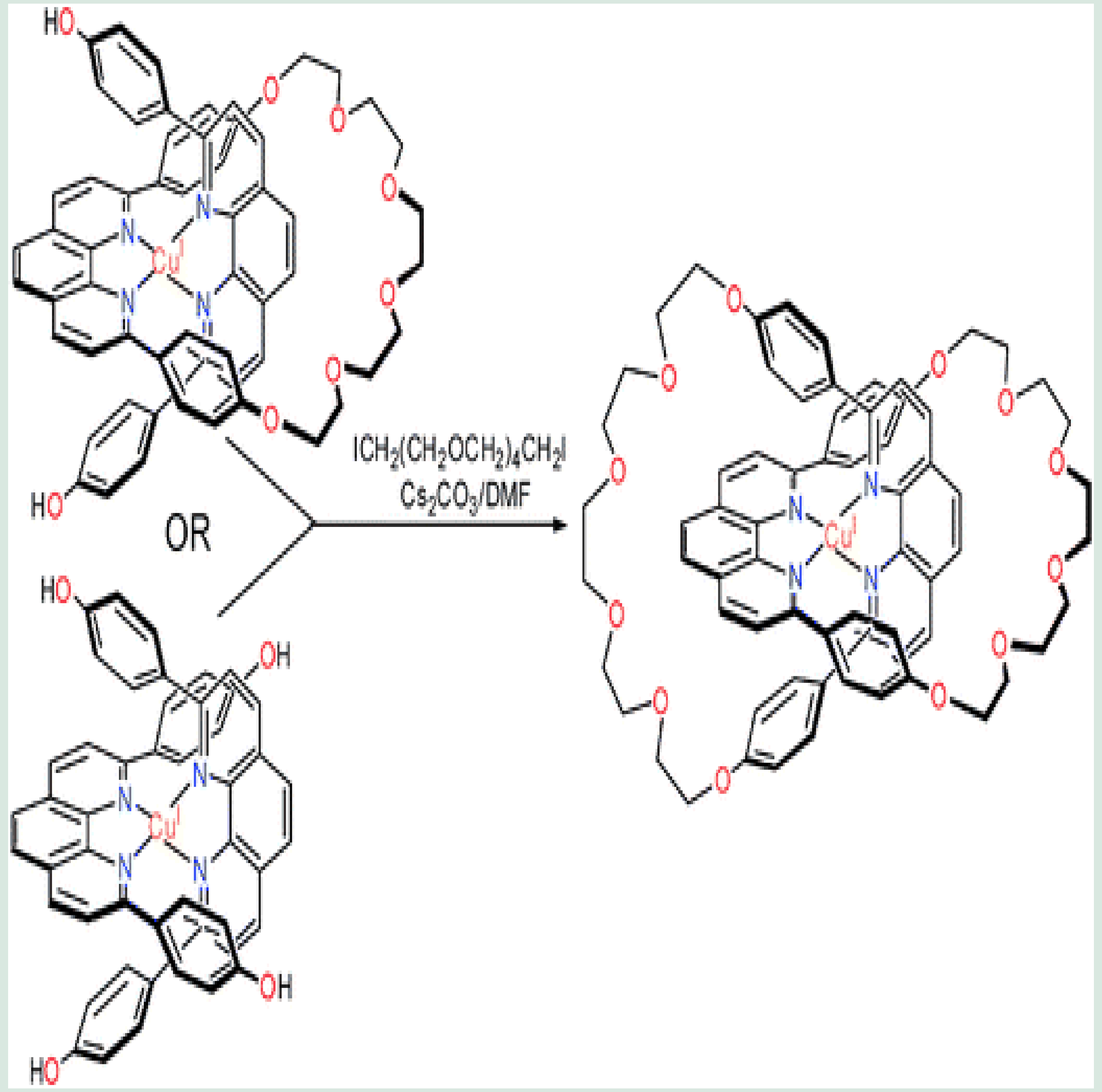
A molecule is said to be topologically achiral, assuming complete flexibilty, there is an isotopy which takes it to its mirror image. If there is no such isotopy, the molecule is said to be topologically chiral.
Why is chirality important?
1. Organisms react differently to the two forms of a chiral molecule.
2. Two mirror forms of drugs ussually have two different uses.
3. Amino acids in human body are chemically chiral.

Knots

Knots can be used to determine if a molecule if topological chiral.
Using knot polynomials of knots and links to determine if a molecule is topologically chiral has been used since 1989.
A knot polynomial is a polynomial made up by the different crossings in a knot. If the polynomial assigned to its mirror image, then we know that the molecule is topologically chiral.
Here is an example of a molecule that would topoligical chiral with its isotopy: $x + x^3 - x^4$ and $x^{-1} + x^3 - x^{-4}$
You may have noticed tthe polynomials in the example have both positive and negative exponents, but for the sake of terminology this is still considered a polynomial. Having a different signed exponent means the knot is different because the crossing would be different at that location.
This method is called the Jones polynomial and is really useful for finding if a molecule is topologically chiral, but it does not tells us if a molecule is topogically achiral.
Also, Jones polynomial cannot work on molecules that are not knotted.

Pictures of chirality!

On the left is the first synthesized knotted molecule by Dietrich-Buchecker and Sauvage. On the right is an example of Jones polynomial.



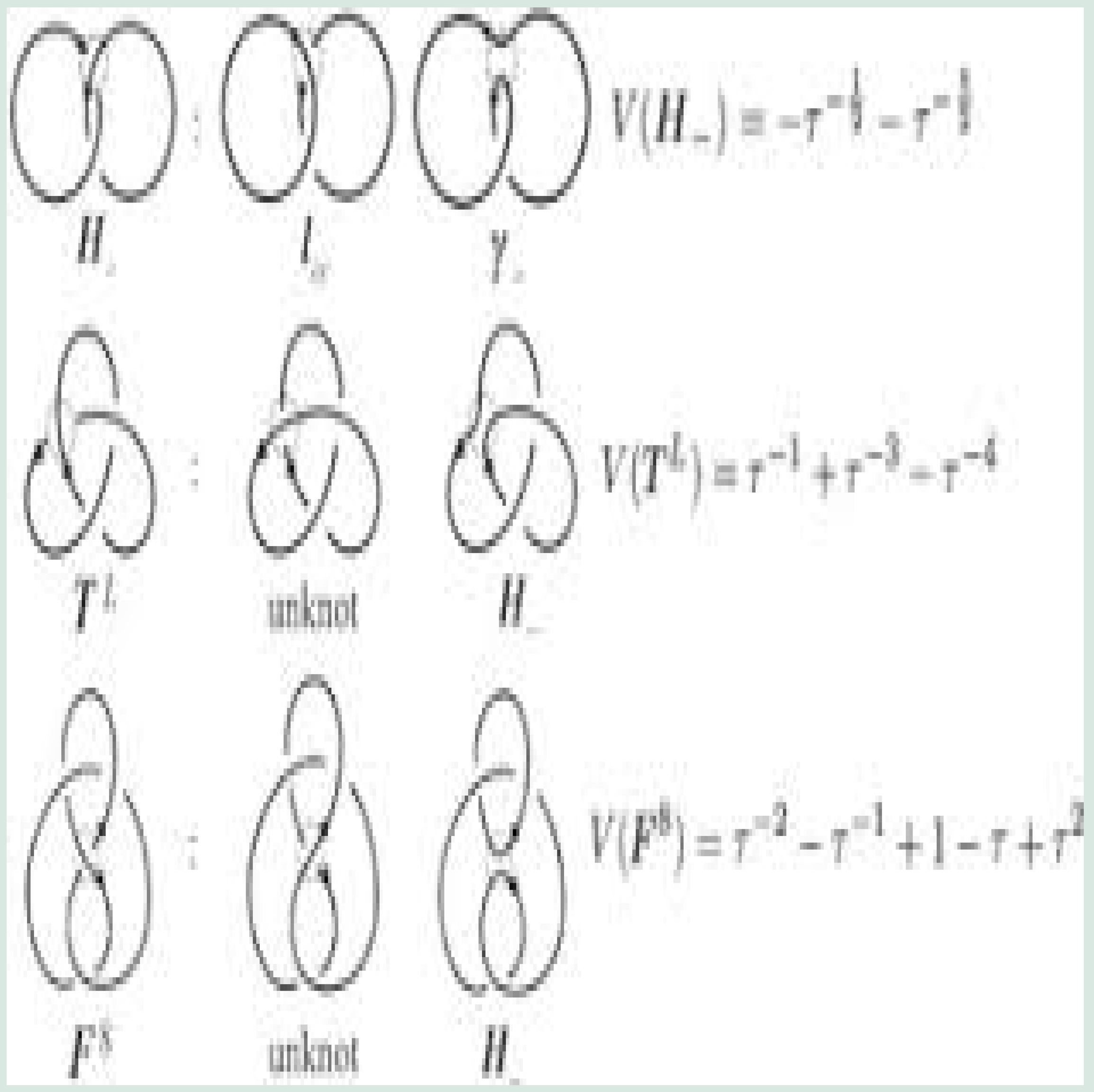


Figure 2: The pictures are in the following order:
First synthesized knot (http://pubs.rsc.org/en/Content/ArticleHtml/2013/CS/c2cs35218d)
Jones polynomial (http://iopscience.iop.org/article/10.1088/0169-5983/46/6/061412).

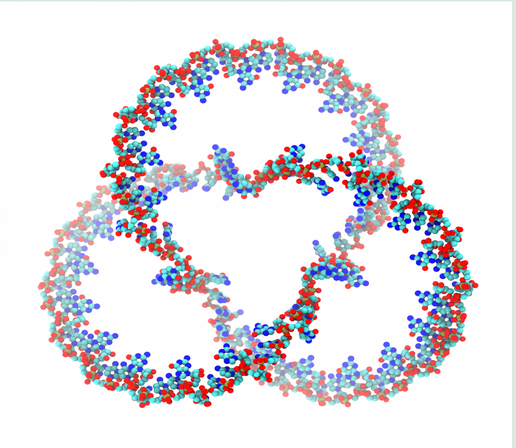
DNA

Definition

DNA is a molecule that encodes the genetic information required for the development and functioning of all living organisms and many viruses. It is not only used as a template for replication but it is also involved in RNA synthesis, which, in some cases, leads on to protein synthesis. DNA consists of two complementary polynucleotide chains that are intertwined around each other, forming a right-handed double helix, which is linear or circular.

Knots and DNA

In many cases, it is well established that DNA becomes knotted as a direct result of biological processes such as recombination, replication and transcription. In these cases, knotting is problematic. Due to this problem enzymes exist to prevent knotting.



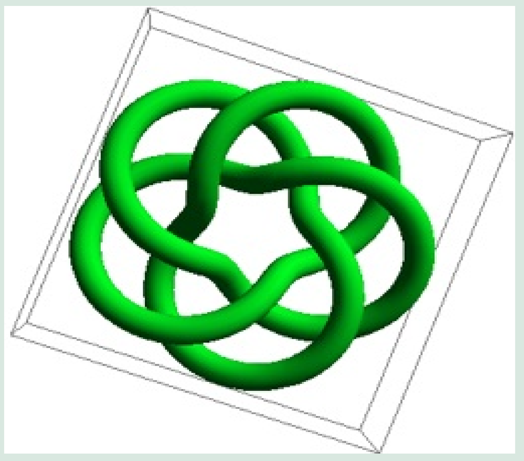


Figure 3: Trefoil Knot (https://3c1703fe8d.site.internapcdn.net/newman/gfx/news/hires/2015/rnatheunknot.png)
Torus Knot (www.tony5m17h.net/torusknot35.jpg)

Consequences

How does DNA knotting affect biological activity within cells?
As discussed above, several processes such as DNA compaction, topoisomerisation, site-specific recombination, replication and transcription can result in the formation of DNA knots in cells. The presence of knots in DNA has potentially detrimental effects in several cellular processes such as transcription and replication and, if unresolved, can lead to mutational defects in the genome or even cell death.

Topoisomerases

Topoisomerases are enzymes that unknot a DNA chain through a cut and paste mechanism in which the DNA is first cut, then moved/ rotated and subsequently religated. Effectively, this breaks the chain into small segments and rearranges them to eliminate the knot. In theory these enzymes are using knot theory to untangle DNA by cutting the DNA into braids then using some Reidemeister moves to help untangle.

References

[1] ref 1 Colin C. Adams. The knot book. W.H Freeman and Company Illustrations, 2004.
[2] ref 2 Erica Flapan. Advanced school and conference on knot theory and its applications to physics and biology. The Abdus Salam International Centre for Theoretical Physics, May 2009.
[3] ref 3 J. Ellis-Monaghan and G. Pangborn. Using dna self-assembly design strategies to motivate graph theory concepts. Math. Model. Nat. Phenom. 6(6):96-107, 2011
[4] ref 4 Nicole C H Lim and Sophie E Jackson. Molecular knots in biology and chemistry. Journal of Physics: Condenssed Matter, 2015.

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