Single molecule ties itself into famous knot

17:48 07 November 2011 by **Chelsea Whyte**

A single molecule consisting of just 160 atoms has been tied into a knot that is more complicated than any other synthetic compound.

The Moroccan flag carries a pentafoil knot *(Image: Image Broker/Rex Features)*

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The molecule constitutes the smallest version of the pentafoil knot – which has both cultural and mathematical significance – in existence. The feat could help us understand the properties of naturally occurring molecular knots, and lead to the creation of materials with exotic new properties.

The pentafoil knot, also known as the cinquefoil, or Solomon's knot, is an object of fascination to mathematicians because it is a "prime knot". Its woven star-shape contains five crossing points and cannot be built from smaller knots, similar to the way a prime number cannot be built by multiplying smaller numbers. The knot is also found on the flags of Ethiopia and Morocco (pictured).

Chemists have previously created a prime knot called a trefoil with three crossing points. David Leigh at the University of Edinburgh and colleagues set out to make the next most complicated knot.

Molecular needle

To do it they needed the molecular equivalent of needles-and-thread. In this case, the needles were positively charged iron ions which were attached to the threads – long, skinny organic molecules.

When the team added negatively charged chloride ions, the ions became hubs, each attracting exactly five needle-and-thread compounds. In the process of arranging themselves around the central hub, the metal ions fold the organic molecules over one another, braiding them into a woven star shape. Finally, chemical bonds form that connect the strands at the points of the star, turning the whole arrangement into a single molecule (pictured).

"One of the neat things about the knot-forming reaction is that it's just a single reaction," Leigh says. "You choose your building blocks so they're designed to assemble into the thing that you want, just like a bit of IKEA furniture."

Chiral control

Previously, most molecular knotting has been done with DNA. Slobodan Zumer, a physicist at the University of Ljubljana in Slovenia says creating a complex knot like this out of non-DNA material is a much bigger challenge. "DNA is like a rope that you can tie into knots on a larger scale," he says. "But here you just have pieces of chemical units which are rather small and you have to get the appropriate amounts of these units to get them to link together."

An interesting thing about the original pentafoil knot is that, rather like a left and right hand, its mirror images cannot be superimposed upon each other. Molecules with this quality are called chiral.

Leigh and his team can select which of two types of knot to create by using left or right-handed building blocks. That has impressed physicist Uroš Tkalec at the Josef Stefan Institute in Ljubljana. "They have control of chirality," he says, noting that this is the first time both left and right-handed forms of a molecular knot have been made (in the case of the trefoil, only one form was made).

Knotty chainmail

Left and right-handed versions of a molecule can have different properties. Leigh says that the way the two versions of the pentafoil knot interact with light would differ. "The material would rotate light in equal and opposite directions," he says. "It would be a different colour if you looked at them through polarised lenses."

Leigh and his team will continue to attempt more complicated knots, those with seven crossing points, for example, and not just for the sake of exploration. He would like to try to make materials that exploit the unique properties of knotted molecules.

"Perhaps we could make a chainmail type of material in which, just like a suit of armour, you've got a very strong but very flexible material," he says. Zumer and Tkalec also see potential for these molecules, including using them to trap pollutants in water or even for small-scale energy storage.

Journal reference: *Nature Chemistry*, DOI: 10.1038/NCHEM.1193