Chemists devise a way to create a five point knotted molecule

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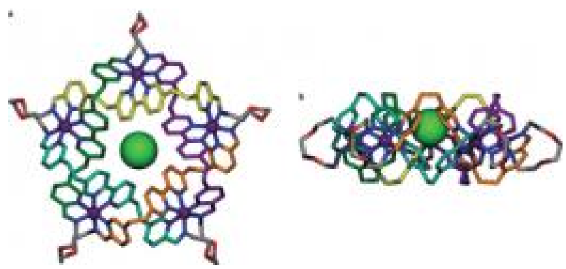

X-ray crystal structure of molecular pentafoil knot [6]Cl(PF6)9. Image: Nature, doi:10.1038/nchem.1193

(PhysOrg.com) -- Chemists have for a long time been interested in a type of molecule that is literally tied up into a knot. This is where atoms are bonded together to form strands, which are then twisted around one another in a way that looks very much like a length of rope tied into an everyday knot. Such molecules when used to make whole structures can provide both strength and elasticity. Unfortunately, forcing atoms to bind together in ways that result in knotted molecules has proven to be an especially difficult task; so much so, that until now, no one has been able to make a molecule that has more than three points. Now, researchers at the University of Edinburgh, have figured out a way to create one with five points, as they describe in their paper published in *Nature Chemistry*, essentially creating what looks like a flat five point star.

Called a pentafoil, the five point knot is the most complex kind of molecule synthesized from other building blocks, other than those found in DNA, and having a means for building them could lead to all sorts of new materials that could be both strong and flexible.

To build the molecule, the team started with a negatively charged chloride ion, to serve as a pulling force, or anchor. They then added other parts, such as iron ions with a positive charge, and chains of carbon atoms. They then chemically "programmed" the whole works to assemble itself into the pentafoil, with five chains looped over and under one another and connected to form one single knotted strand, with a single chloride ion sitting squarely in the center holding the whole knot together. The finished product is made up of just 160 atoms and very much resembles a traditional two-dimensional five pointed star.

As an interesting side note, the researchers found that if they removed the single chloride ion after the knot was completed, they were left with a molecule that was hungry for that missing ion, which could mean they've found a new type of chlorine sensor.

In devising a means to create a pentafoil, the researchers have created not just a new type of man-made molecule, but a blueprint for creating other types of knotted molecules which could lead to all sorts of new and exotic materials.

More information: A synthetic molecular pentafoil knot, *Nature Chemistry* 4, 15–20 (2012) doi:10.1038/nchem.1193

Abstract
Knots are being discovered with increasing frequency in both biological and synthetic macromolecules and have been fundamental topological targets for chemical synthesis for the past two decades. Here, we report on the synthesis of the most complex non-DNA molecular knot prepared

to date: the self-assembly of five bis-aldehyde and five bis-amine building blocks about five metal cations and one chloride anion to form a 160-atom-loop molecular pentafoil knot (five crossing points). The structure and topology of the knot is established by NMR spectroscopy, mass spectrometry and X-ray crystallography, revealing a symmetrical closed-loop double helicate with the chloride anion held at the centre of the pentafoil knot by ten CH···Cl– hydrogen bonds. The one-pot self-assembly reaction features an exceptional number of different design elements—some well precedented and others less well known within the context of directing the formation of (supra)molecular species. We anticipate that the strategies and tactics used here can be applied to the rational synthesis of other higher-order interlocked molecular architectures.

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