MOLECULAR KNOTS

By Colin Byfleet

Close relation to Guild's logo knot (4B,3L TH) makes news in the journal Science

Just over a year ago in *KM* 130 there were photographs of some knots in graphene oxide which were about 0.1mm across. In a recent issue of the magazine *Science* there is a paper[1] from Professor David Leigh's group at the University of Manchester, UK, which announces a new *molecular* knot.

In this beautiful rendition in Figure 1 (right) of the shape of the knot, you can see that it is a single pass, three-lead, four-bight Turks Head (the basis of our IGKT logo). The difference here is that the tucking is over-over, under-under, rather than the normal alternating pattern. In topological jargon, this is knot 8-19 (8crossings, no 19 in Rolfsen's list): the IGKT logo is 8-18[2]. The spheres in the image represent atoms which are removed in the final step of the synthesis.

Figure 2 (right) shows a three-pass version of the 8-19 knot, tied on a cylindrical former. It looks like a mixture of a normal 3-stand plait and two strands twisted together. Because of the o,o-u,u pattern, it is not very stable until tightened, like quite a number of non-standard Turks Head arrangements.

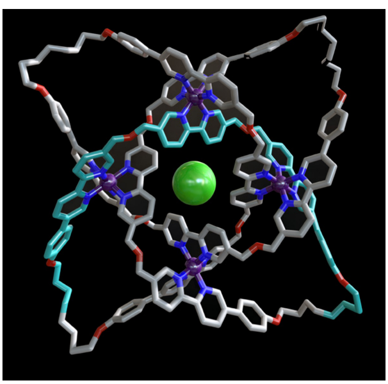


Figure 3 (left) shows the structure of the strands of atoms. In these images, atoms are at the bends of the strand, the links between them represent chemical bonds. The 8-19 molecular knot is claimed to be the tightest (in the sense of having the smallest radius loops) ever made.

The length of the 'rope' (a chain of carbon and oxygen atoms) is about 20 nanometres (one nanometre is a millionth of a millimetre) and since there are 8 crossings, each of these occurs in about 2.5nm and is made of just 24 atoms. There is a lovely animation of this molecule at:

http://www.catenane.net/media/2017_Knot_819_molecule_flyaround.mp4

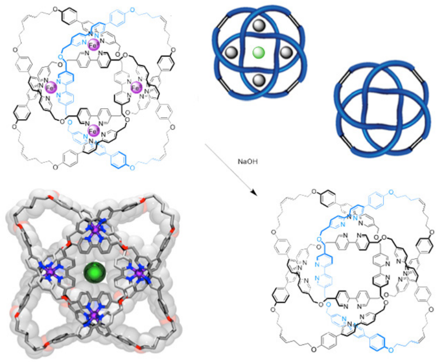
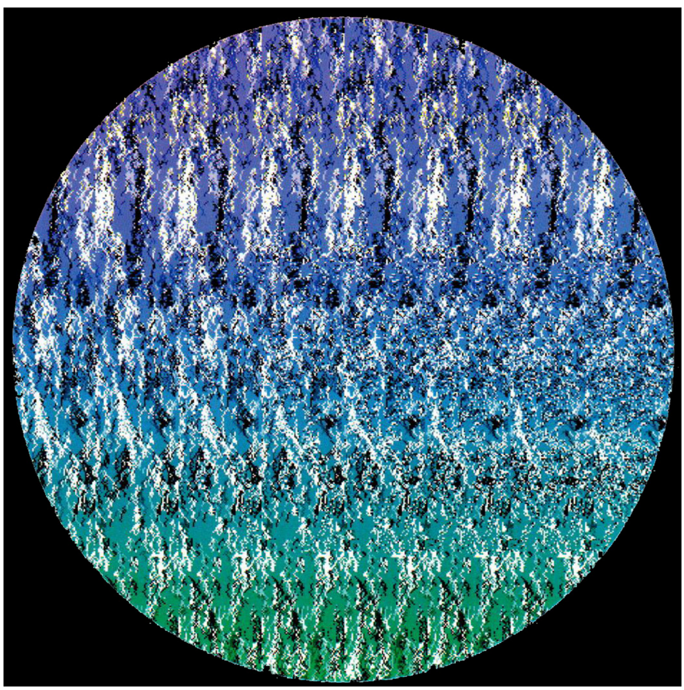


Figure 4 (left) shows diagrams of the removal of the iron and chlorine atoms to leave a completely organic knot. Because, like string, chains of atoms are flexible, removing these atoms enables the knot to flop around and so a 3D picture is not so easy to visualise. If you trace the strand around, the blue and black shading shows the ‘over-over’ part of the crossings.

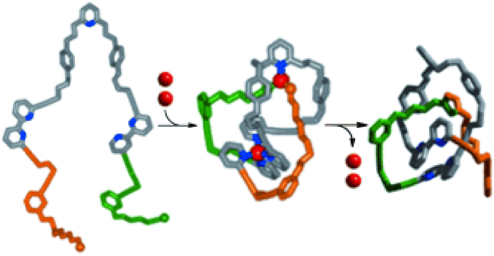
Molecular knots have been seen in DNA strands, in proteins and in polymers like nylon. It is useful to find how to create such knots both because it increases our understanding of biochemistry and because it could well lead to the production of new and useful materials.

Leigh’s co-workers have, for some years, been making a family of molecules with loops and interlocked crossings called catenanes (from the Latin *catena*, a chain, which gives rise to our catenary for supporting cables).

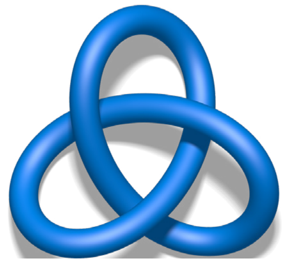
One of these chains, with just two links, was shown as a ‘magic eye’ picture on the cover of the journal *Angewandte Chemie,* Vol 34 No11 in 1995, shown in Figure 5 (right). It took me a while to see it, but there is an image of a molecule in this seemingly random pattern. To visualise the 3-D image stare at the page from about 30-40cm away and try to focus on your reflection which will be the same distance behind the page.



As with all optical illusions, it takes some time for your brain to be persuaded.

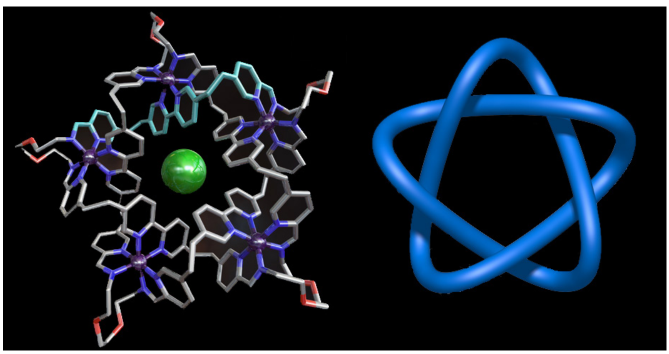


As we have seen, many of the Leigh group molecules are more complex than simple chains: they are real knots (Figure 6, left).



One of the first was a synthetic trefoil knot, made in 2011 and announced then as the 'smallest knot ever tied'. The trefoil (opposite) was followed by a more complex cinquefoil (Figure 7, below)a year later[3].

These knots are the simplest two-lead Turks Heads. Trefoil 3B, 2L, cinquefoil 5B, 2L.



Interestingly the cinquefoil, flattened, appears on both Moroccan and Ethiopian flags as a pentagram – the Seal of Solomon.

Acknowledgements: *KM* is grateful to the following for permission to use the illustrations.
Figures 1 & 3 Stuart Jantzen www.biocinematics.com
Figure 7 Robert W McGregor www.mcgregorfineart.com
Figures 4,5,6 Professor David Leigh, University of Manchester

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[1] 'Braiding a molecular knot with eight crossings' Jonathan J. Danon et al, Science, 355, 159-162 (2017).

[2] See, for example http://katlas.org/wiki/8_19

[3] 'Active-Metal Template Synthesis of a Molecular Trefoil Knot' Perdita E. Barran et al, Angew. Chem. Int. Ed., 50, 12280-12284 (2011).

Colin Byfleet

Growing up in Harrow, north-west London, I enjoyed an excellently-run Scout group where knots and lashings were enthusiastically taught and used. We even had a precious copy of Ashley, although I little realised its importance at that time.

Distractions followed (girls and exams) and knotting took a back seat. Learning to sail on a gravel-pit lake at St Ives in Cambridge and a bit of dinghy sailing brought them back to the fore for a while.

Thirty busy years of work, family etc followed and knotting again disappeared into the background until involvement with the now sadly-defunct Exeter Maritime Museum, via my wife, Jackie, began in the mid-1990s. A visit to the maritime festival Brest 2000 brought us into contact with Ken Yalden and the Solent branch, and we joined the Guild very soon thereafter.

I foolishly replied to a request in *Knotting Matters* for a new Supplies Secretary - and was given the job because of the lack of competition. At the 2010 meeting in Weston-super-Mare, I was cajoled into joining the Council and discovered the inner workings of the Guild. The following year, at the meeting in Coventry, I was asked to be President, an honour for which I was ill-prepared, especially since our long-standing Treasurer and Secretary both finished their time in office at the same meeting.

I am pleased that the re-organisation into Council of Trustees and Executive Committee, forced upon us by our status as a Registered Charity, now seems to be running smoothly.

Following the Autumn meeting in Sweden in 2010, I became interested in circular mats and their mathematical analysis. Whilst rather immobile recovering from knee surgery, I was able to sit and make many of the mats.

After a career as a chemical physicist, my time with the Guild has taken Jackie and me to many really interesting meeting places and, more importantly, put us in contact with many splendid colleagues. The Guild is quite the friendliest organisation I know and I am delighted to have been a small part of it.