Making catenanes and a molecular trefoil knot out of para-connected benzene rings

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A team of researchers affiliated with several institutions in Japan has developed a way to create catenanes and a molecular trefoil knot out of para-connected benzene rings. In their paper published in the journal *Science*, the group describes their process and possible uses of their results. Jeff Van Raden, and Ramesh Jasti with the University of Oregon, have published a Perspective piece on the work done by the team in the same journal issue.

In recent years, carbon-based materials such as graphene, fullerenes and carbon nanotubes have captured the imagination of scientists—such materials have a wide range of unique physical properties that make them useful for certain applications. Graphene, for example, is a zero-gap semiconductor. Scientists have also been looking at ways in which such structures can be formed. In this new effort, the researchers have found a way to get benzene rings to form into two kinds of catenanes, and also a trefoil knot. Catenanes are a type of molecular architecture with two or more interlocking macrocycles. And a trefoil knot, as its name suggests, is a molecular structure that that resembles a knot with three crossings. By creating these structures, the researchers have added molecules that are mechanically bonded to the list of carbon nanostructures.

To create their structures, the researchers built on prior work that involved synthesizing benzene rings—but this time around, they introduced a silicon template on adjoining fragments of nanorings. After the fragments had cyclized into rings, the researchers removed the silicon, which left behind small rings interlocked with larger rings, structures called catenanes. They used a similar process to create the trefoil knot, but note that it was more difficult—only 0.3 percent of attempts worked out as planned.

The researchers also note that during testing of the nanocarbons they had created, they found something surprising—the chains in the structures moved around when exposed to magnetic resonance. They had expected all of the structures would be rigid. They suggest that the ability to control the topology of such nanocarbons could lead to the development of products that take advantage of their unique configurations.

More information: Yasutomo Segawa et al. Topological molecular nanocarbons: All-benzene catenane and trefoil knot, *Science* (2019). DOI: 10.1126/science.aav5021