Chemists tie a knot using only 54 atoms

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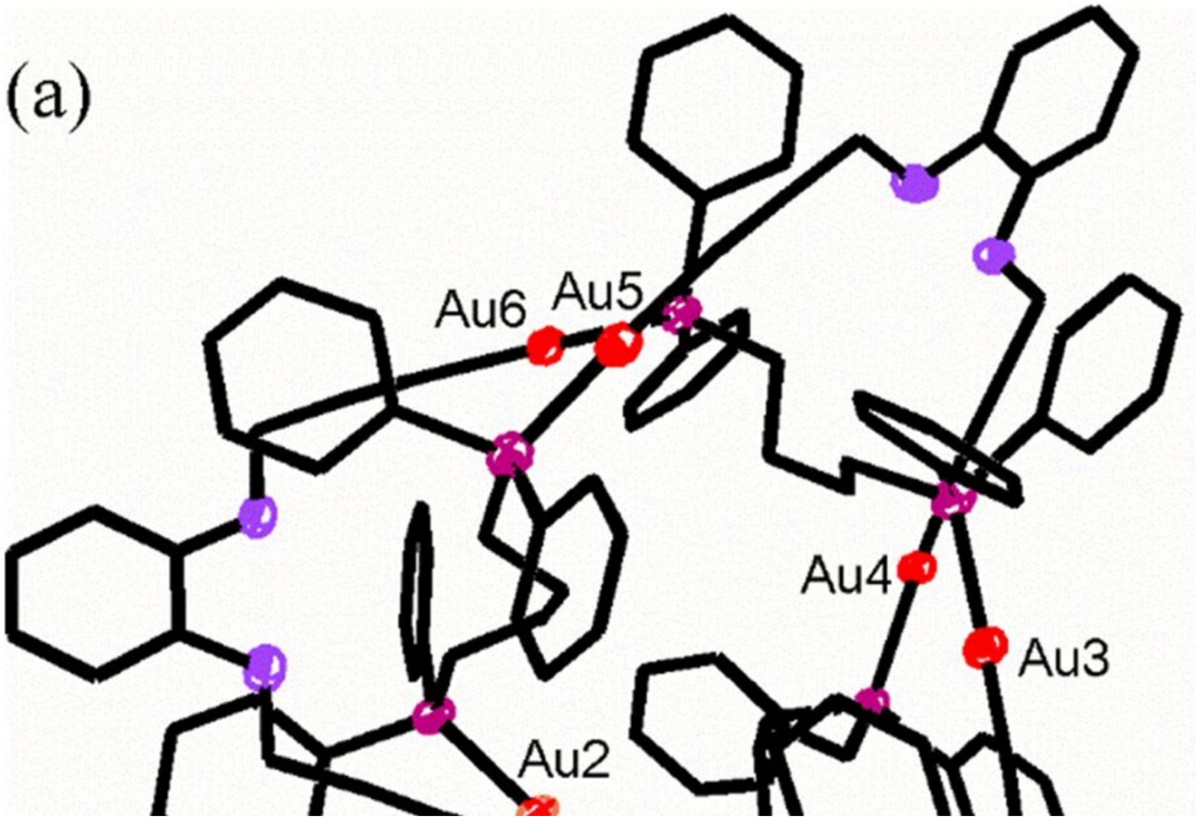

The structure of the trefoil metallaknot $[Au_6(L)_3(dppb)_3]$, Au_6. Separate sections are **a** the structure (color code: Au, red; P, purple; O, mauve); **b** the core structures of enantiomers (H atoms and dppb phenyl groups omitted for clarity); **c** the ideal left- and right-handed trefoil knots. Credit: *Nature Communications* (2024). DOI: 10.1038/s41467-023-44302-y

A trio of chemists at the Chinese Academy of Sciences' Dalian Institute of Chemical Physics, working with a colleague from the University of Western Ontario, has tied the smallest knot ever, using just 54 atoms. In their study, published in the journal *Nature Communications*, Zhiwen Li, Jingjing Zhang, Gao Li and Richard Puddephatt accidentally tied the knot while trying to create metal acetylides in their lab.

The researchers were attempting to create types of alkynes called metal acetylides as a means to conduct other types of organic reactions. More specifically, they were attempting to connect carbon structures to gold acetylides—typically, such work results in the creation of simple chains of gold known as caternames.

But, unexpectedly, the result of one reaction created a chain that knotted itself into a trefoil knot with no loose ends. Trefoil knots are used in making pretzels and play a major role in knot theory. The researchers noted that the knot had a backbone crossing ratio (BCR) of 23. Knot BCRs are a measure of the strength of the knot. Most organic knots, the team notes, have a BCR somewhere between 27 and 33.

The knot represents a record—its three-leaf clover shape beats out a previous record held by a different team in China that created a 69-atom knot back in 2020. The prior record holder was created on purpose by that team using techniques developed to entwine strands into knots. The new record holder self-assembled, and the team behind it still does not understand how it happened. It is not yet known if it is possible to make a knot any smaller.

The creation of such tiny knots, the research team points out, is not just an interesting lab trick—microscopic knots are formed in many natural settings, such as in RNA and DNA and several other proteins. By creating tiny knots, chemists are learning more about how and why they come about in nature. It also could help in the discovery of new types of polymers and/or plastics.

More information: Zhiwen Li et al, Self-assembly of the smallest and tightest molecular trefoil knot, *Nature Communications* (2024). DOI: 10.1038/s41467-023-44302-y