Molecule with a Split Personality

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If you take a strip of paper, twist one end by 180° and then stick the two ends together to form a ring, the result is called a Möbius strip, a geometric shape with only one surface and one edge.

You can prove this by making a line along the strip with a pencil: Without lifting the pencil you get back to your starting point in the end—with the whole strip marked: at each point, both sides of the strip are marked by the line. Ring-shaped aromatic molecules can also have a topology like that of the Möbius strip, with only one side.

Polish researchers have now made a porphyrin-like ring that can do something its paper analogue can't. As the team led by Lechosław Latos-Grażyński reports in the journal *Angewandte Chemie*, the new molecule can switch back and forth between the one-sided Möbius topology and a "normal" two-sided state (Hückel topology)—without breaking the ring.

An aromatic compound is a nearly planar ring (or ring system) with bonding, yet freely mobile, electron pairs from double bonds. These so called π electrons reside in a kind of "electron cloud" with a part above and a part below the plane of the ring. This is the classic Hückel topology. Even rings that are twisted into a figure eight can have this topology.

If the ring system is twisted by 180°, the result is a Möbius topology; there is no longer a difference between the upper and lower "electron cloud". Like the pencil line on the Möbius strip made of paper, the two clouds merge together to form a single continuous surface.

The Polish researchers have now synthesized a large molecular ring, which can be classified as an expanded porphyrin analogue, which can do what the glued-together paper strip cannot: Without having to break a single bond in the figure-eight-shaped ring system, it can switch back and forth between the Hückel and Möbius topologies.

Even the figure-eight shape is retained. The trick to this molecule with a "split personality" is two aromatic six-membered rings that lie directly opposite each other in the large ring system and form the crossing point of the figure eight. These two freely spinning rings can either lie flat on top of each other, with their planes lying in parallel, or one of the rings can be twisted by 90° so that their planes lie perpendicular to each other. In the parallel arrangement, there is a clear distinction of the upper and lower parts of the π-electron cloud, in accordance with a Hückel topology—a solution of the compound in this configuration is green in color.

The perpendicular arrangement is the Möbius arrangement and is blue in color. The rotated six-membered ring provides the twist required to unite the upper and lower electron clouds. Which topology the molecule prefers depends on the type of solvent and the temperature.

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