

# A Molecule with Half-Möbius Topology

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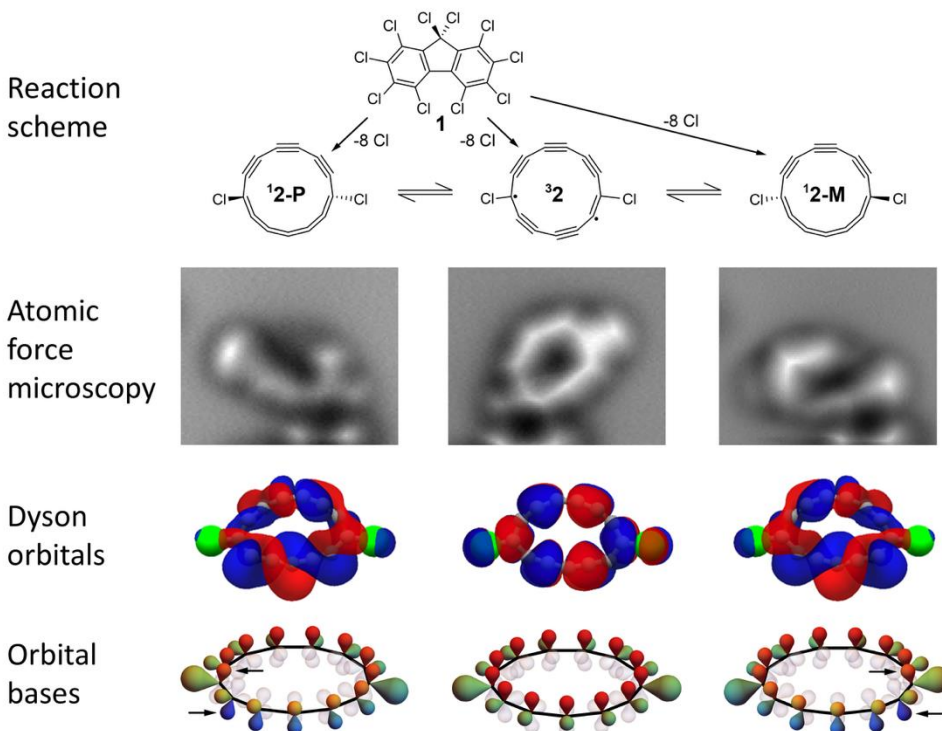
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$\pi$ -Conjugated systems are fascinating because their electrons are highly delocalised, while remaining bound by their orbital basis. In  $\pi$ -conjugated rings a key phenomenon is aromaticity, or the presence of a ring current in a magnetic field, which demonstrates that the electronic wavefunction is coherently delocalised around the whole molecular ring. Topologically trivial  $\pi$ -conjugated rings with ring currents obey Hückel's rule: they are aromatic if they have  $4N+2$   $\pi$ -electrons, and anti-aromatic if they have  $4N$   $\pi$ -electrons, where  $N$  is an integer.

In rings that resemble a Möbius strip, which is a body with a single edge, Hückel's rules are reversed [1]. This reversal is a consequence of a  $180^\circ$  twist in their orbital basis upon one circulation of the ring.

This talk will present our recent work on the characterisation of a molecule with half-Möbius topology (Fig. 1), in which the orbital basis twists by  $90^\circ$  upon one circulation of the ring [2].



**Figure 1.** A molecule with half-Möbius topology.

## References:

- [1] D. Ajami, O. Oeckler, A. Simon, R. Herges, *Nature* **426** (2003), 819–821.
- [2] I. Rončević, F. Paschke, Y. Gao, L.-A. Lieske, L. A. Gödde, S. Barison, S. Piccinelli, I. Tavernelli, J. Repp, F. Albrecht, H. L. Anderson, L. Gross, *Science* (2026), in press, DOI: 10.1126/science.aea3321.