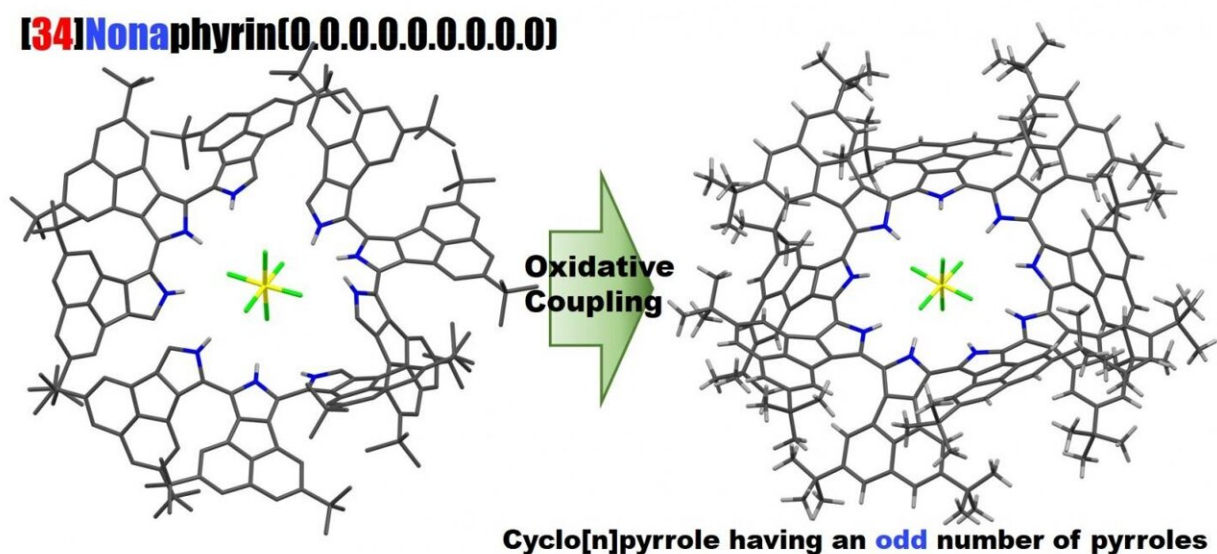


# Synthesis of a near-infrared light absorbing macrocyclic aromatic compound

June 23 2021



Selective Synthesis of Cyclo[9]pyrroles Based on an Oxidative Coupling. Credit: Tetsuo Okujima, Ehime University

Profs. Okujima and Uno at Ehime University, in collaboration with Prof. Kobayashi at Shinshu University, reported the selective synthesis, the molecular structure, optical properties and electronic structure of cyclo[9]pyrrole, a ring-expanded porphyrin consisting of directly connected pyrrole rings.

Porphyrins, which are well-known natural porphyrin molecules,

including heme and chlorophyll, are attractive for use in practical materials because of the easy optimization of their optical and [physical properties](#) by conjugation expansion and functionalization. In 2002, Sessler reported the first synthesis of cyclo[n]pyrrole (n: the number of pyrrole rings). Peripheral alkyl-substituted cyclo[8]pyrroles were obtained via an oxidative coupling of 2,2'-bipyrrole, and showed an intense L band at ca. 1,100 nm.

The team successfully synthesized a good yield of cyclo[9]pyrroles via the oxidative coupling of terpyrrole. A relatively distorted structure with a C<sub>2</sub>-like symmetry was clarified by NMR and X-ray diffraction analyses. Intense absorption was observed at ca. 1,740 nm. They analyzed the optical and electronic structures using magnetic circular dichroism spectroscopy and time-dependent density functional theory calculations. Comparison of cyclo[8], [9], and [10]pyrroles showed the electronic structures don't significantly depend on the number of pyrroles.

**More information:** Hiroki Matsumoto et al, Cyclo[9]pyrrole: Selective Synthesis of [34]Nonaphyrin(0.0.0.0.0.0.0.0.0), *Organic Letters* (2021). [DOI: 10.1021/acs.orglett.1c00899](https://doi.org/10.1021/acs.orglett.1c00899)

Provided by Ehime University

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