Low-symmetry coordination cages enable sensitive recognition and selective enrichment of higher fullerene isomers

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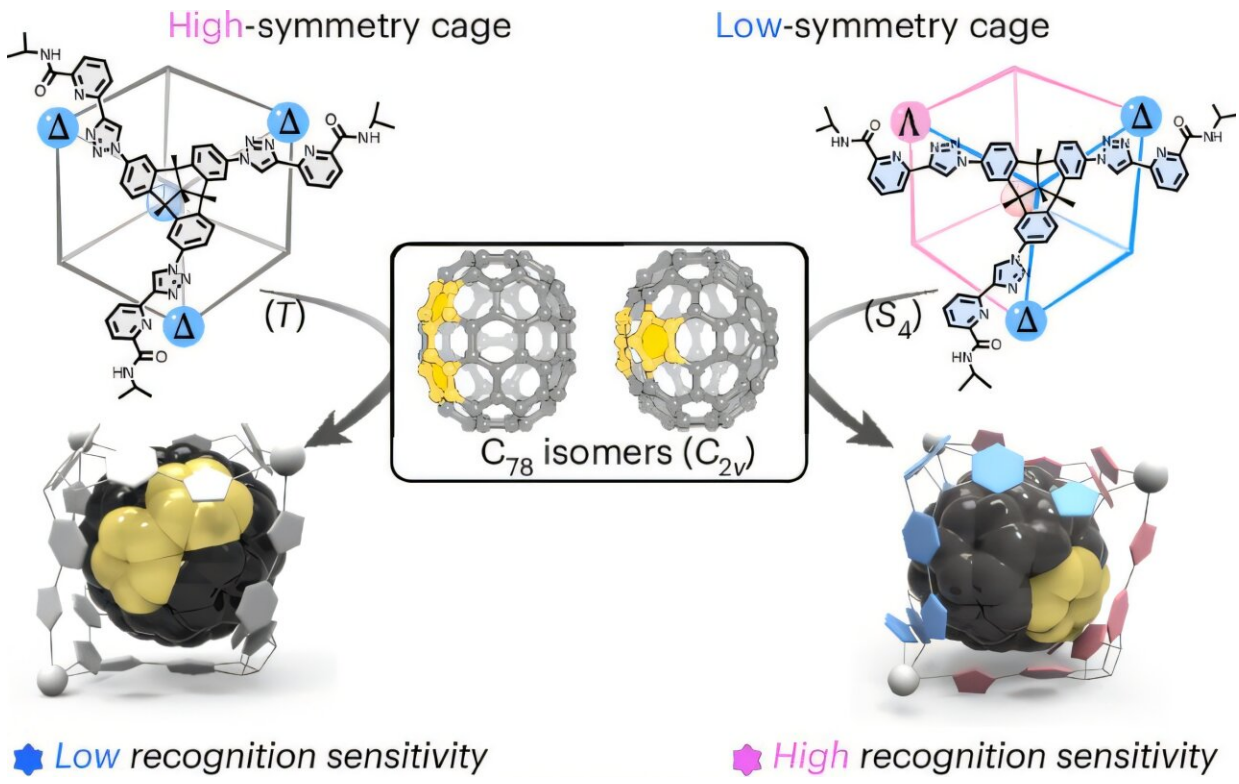

Comparison of the recognition sensitivity for a pair of closely related C_{2v}-symmetric C_{78} isomers using pseudo-cubic cages with T and S_4 symmetries. Credit: *Nature Synthesis* (2025). DOI: 10.1038/s44160-024-00697-0

Molecular recognition and binding are fundamental to biological

systems, which is exemplified by the specificity between enzymes and substrates. Drawing inspiration from these complex natural mechanisms, researchers have developed artificial systems that emulate biological recognition.

The discovery of buckminsterfullerene (C_{60}) marks a milestone in the study of three-dimensional carbon materials. However, as the number of isomers increases exponentially in higher fullerenes (C_n, n>7), achieving their selective enrichment through molecular recognition remains a challenge.

In a study published in *Nature Synthesis*, Prof. Sun Qingfu's team from the Fujian Institute of Research on the Structure of Matter of the Chinese Academy of Sciences, collaborating with Prof. Lu Xing's team from Huazhong University of Science and Technology, introduced two pseudo-cubic metal-organic cages (MOCs) with distinct symmetries, T and S_4. These cages, featuring unique cavity microenvironments, demonstrated exceptional recognition specificity toward higher fullerene isomers.

Taking advantage of asymmetric ligands to inherently generate MOCs with reduced symmetry, researchers synthesized two pseudo-cubic cages based on tribenzotriquinacenes (TBTQs), possessing T and S_4 symmetries, dictated by the C_3- and C_1-symmetric bowl-shaped ligands.

A symmetry breaking from S_4 to C_2 was observed upon encapsulating the low-symmetry, ellipsoidal D_2-C_{76} guest within the S_4-4 cage, indicating that a precise shape matching curtails the random rotation of guest. As a control, no symmetry reduction was detected for the high-symmetry T-3 cage.

Encouraged by these findings, researchers then studied selectively recognized pair of highly similar C_{2v}-symmetric C_{78} isomers, namely

$C_{2v}(2)$-$C_{78}$and $C_{2v}(3)$-C_{78}, which can be interconverted through a one-step Stone-Wale transformation (SWT).

Researchers found that compared to high-symmetry T-3 cage, the rotation restriction of C_{78} isomers within the low-symmetry S_4-4 cage more sensitively reflects the constitutional difference through changes in the host's chemical shift, and that the sophisticated void and proper shape complementarity, brought about by reduced symmetry, are responsible for the high recognition sensitivity of S_4-4 toward C_{2v}-symmetric C_{78} isomers.

Furthermore, they revealed that the discernible variances in binding affinity, stemming from heightened recognition sensitivity, positions S_4-4 as a promising candidate for isolating the inextricable C_{2v}-symmetric C_{78} isomers. These findings underscored the power of symmetry reduction in enhancing molecular recognition.

This study represents the exploration of MOCs recognizing higher fullerene isomers by employing the symmetry reduction strategy, positioning the MOCs family as promising candidates for future identification and separation of a wider range of fullerene isomers.

By mimicking the specificity observed in biological systems, these low-symmetry coordination cages can offer new insights into molecular recognition and pave the way for their future applications in material science and molecular separation.

More information: Xiao-Qing Guo et al, Low-symmetry coordination cages enable recognition specificity and selective enrichment of higher fullerene isomers, *Nature Synthesis* (2025). DOI: 10.1038/s44160-024-00697-0

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