Frustration-Induced Many-Body Degeneracy in Spin -1/2 Molecular Quantum Rings

Donglin Li,^{1‡} Nan Cao,^{2‡} Marvin Metzelaars,^{3‡} Orlando J. Silveira,^{2,4} Joakim Jestilä,² Adolfo Fumega,² Tomohiko Nishiuchi,³ Jose Lado,² Adam S. Foster,^{2,5*} Takashi Kubo,^{3*} and Shigeki Kawai^{1,6*}

¹Center for Basic Research on Materials, National Institute for Materials Science, 1-2-1 Segen, Tsukuba, Ibaraki 305-0047, Japan.

Presenting author's e-mail: LI.Donglin@nims.go.jp

Frustrated spin systems, where competing interactions prevent conventional magnetic ordering, provide a platform for uncovering emergent quantum phases and exotic many-body phenomena. Particularly, low-dimensional and symmetric geometries without boundary conditions allow us to study the unconventional spin states. Here, we present S = 1/2 antiferromagnetic Heisenberg cyclic pentamer and hexamer via homocoupling of air-stable phenalenyl derivatives on Au(111). With a combination of scanning tunnelling microscopy/scanning tunnelling spectroscopy at 4.3 K and comprehensive theoretical simulations, we found that while large magnetic exchange interactions exist in both rings, the pentamer features an increased geometric frustration of the system. This frustration induces rotational symmetry in the spin wavefunction, leading to a four-fold degenerate ground states of the pentamer. The interplay between molecular geometry and magnetic interactions creates the unique quantum spin environment. Our findings offer a powerful approach for constructing spin-frustrated molecular architectures, allowing precise control over quantum magnetic interactions.

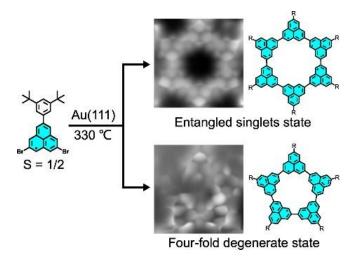


Figure 1. On-surface synthesis of cyclic [2]triangulene hexamer and pentamer. (ncAFM is on the way!)

Reference

[1] L. J. D. Jongh, et al. Adv. Phys. 50, 947, (2001).

[1] D. Li, et al. J. Am. Chem. Soc. **ASAP**, (2025).

²Department of Applied Physics, Aalto University, Espoo, Finland.

³Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka 560-0043, Japan.

⁴Department of Physics, Nanoscience Center, University of Jyväskylä, FI-40014, Finland.

⁵Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan.

⁶Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Japan.