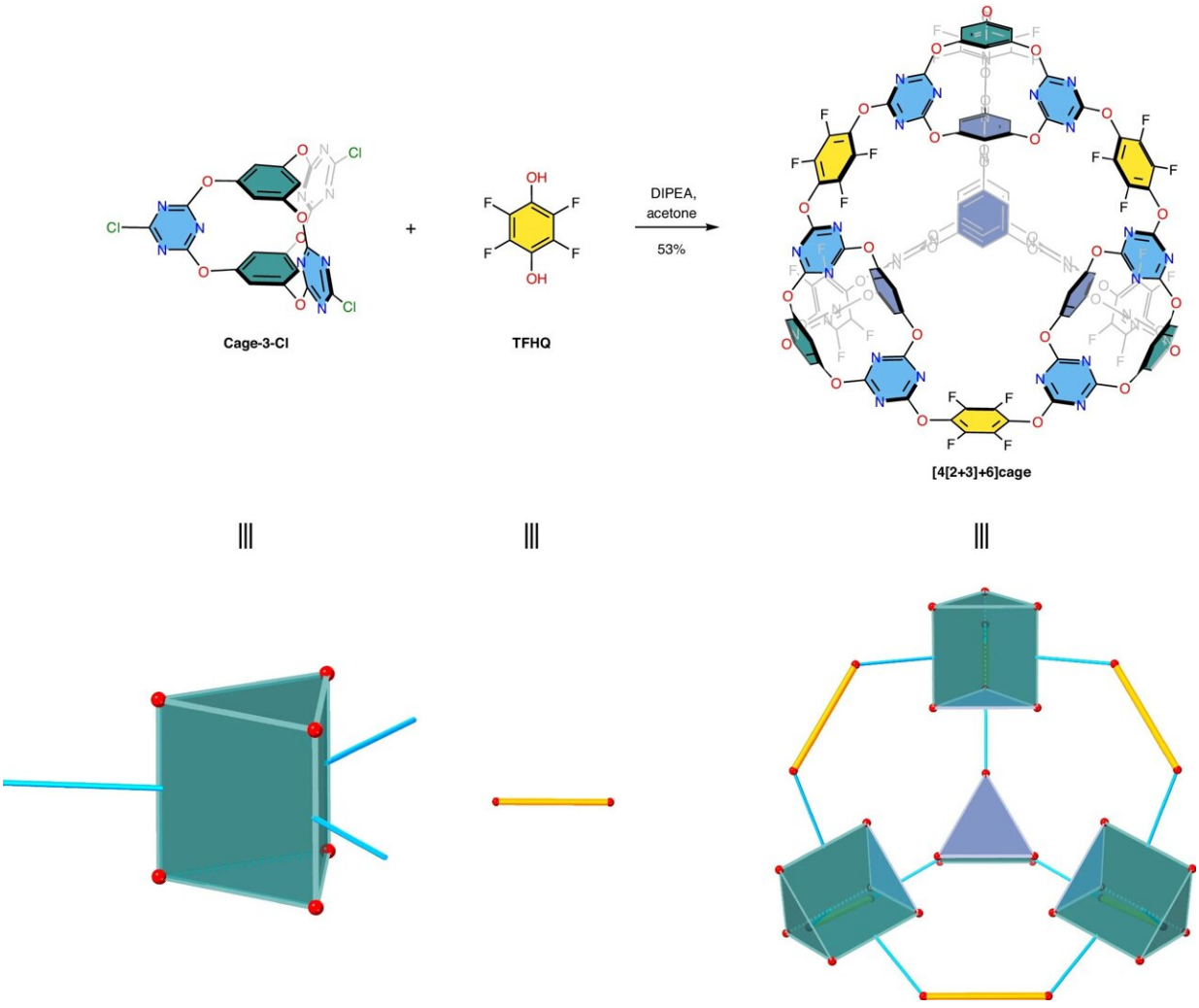
Scientists discover a new type of porous material that can store greenhouse gases

April 29 2024, by Victoria Masterson



Synthetic route for the [4[2+3]+6]cage molecule. Credit: *Nature Synthesis* (2024). DOI: 10.1038/s44160-024-00531-7

A new type of porous material that can store carbon dioxide and other greenhouse gases has been developed by a team of scientists jointly led by Heriot-Watt University in Edinburgh, Scotland.

In a collaboration with the University of Liverpool, Imperial College London, the University of Southampton, and East China University of Science and Technology in China, the team used computer modeling to accurately predict how molecules would assemble themselves into the new type of porous material.

The research, published in the journal *Nature Synthesis*, details how the scientists created hollow, cage-like molecules with high storage capacities for greenhouse gases like carbon dioxide and sulfur hexafluoride. Sulfur hexafluoride is more potent greenhouse gas than carbon dioxide and can last thousands of years in the atmosphere.

These cage molecules were assembled using other cages to create a new type of porous material that the scientists say is the first of its kind in its porous "cage of cages" structure.

Materials scientist Dr. Marc Little, an Assistant Professor at Heriot-Watt University's Institute of Chemical Sciences and an expert in porous materials, jointly led the research.

He said, "This is an exciting discovery because we need new porous materials to help solve society's biggest challenges, such as capturing and storing greenhouse gases."

Computer modeling specialists at Imperial College London and the University of Southampton created simulations to help the team understand and predict how their cage molecules would assemble into this new type of porous material.

Integral to the team were Professor Kim Jelfs from Imperial's Department of Chemistry and the Institute for Digital Molecular Design and Fabrication (DigiFAB), and Professor Andy Cooper from the University of Liverpool and Materials Innovation Factory.

Dr. Little added, "Combining computational studies like ours with new AI technologies could create an unprecedented supply of new materials to solve the most pressing societal challenges, and this study is an important step in this direction."

Dr. Little added that molecules with complex structures could also be used to remove toxic compounds known as volatile organic compounds from the air and could play an important role in medical science.

"We see this study as an important step towards unlocking such applications in the future," he said.

More information: Qiang Zhu et al, Computationally guided synthesis of a hierarchical [4[2+3]+6] porous organic 'cage of cages', *Nature Synthesis* (2024). DOI: 10.1038/s44160-024-00531-7

Provided by Heriot-Watt University