COMBINATORIAL CRYSTALS

MATERIALS CHEMISTRY: Novel metal-organic framework compounds store, selectively trap CO_2

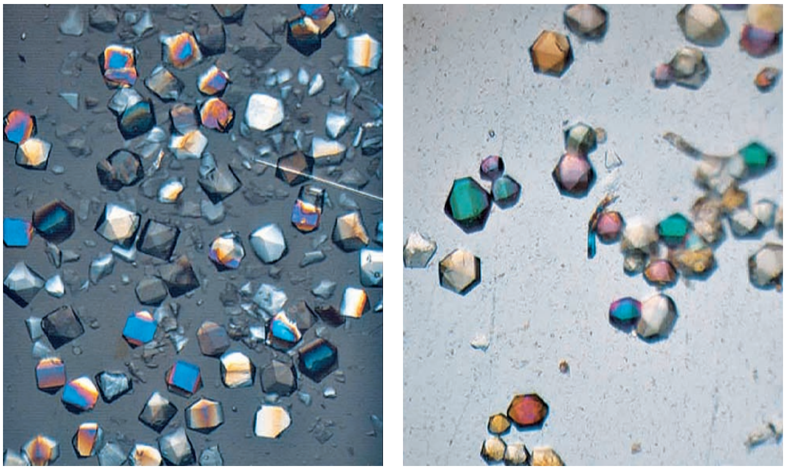
BY USING HIGH-THROUGHPUT synthesis, researchers have unexpectedly prepared a large number of novel porous metal-organic framework compounds, some with unusually large capacity for CO_2 storage and a knack for selectively trapping that gas (*Science* **2008,** *319,* 939). Those properties may help advance technologies to capture and sequester the ubiquitous greenhouse gas.

"High-throughput synthesis methods are used routinely in some areas of chemistry, but inorganic chemists have traditionally shied away from that type of synthesis," says UCLA chemistry professor Omar M. Yaghi, who led the study. The conventional thinking is that using combinatorial methods to try to make crystalline solid-state materials would probably yield only the most stable compounds, which are the ones that have already been prepared via standard bench-chemistry methods, he explains.

At least in the case of this family of framework materials, the conventional wisdom isn't quite right. The materials are composed of metal atoms linked by organic groups and are known as zeolitic imidazolate framework compounds (ZIFs). It turns out that the number of possible ZIF structures is very broad, Yaghi says. "It's just a question of examining the range of experimental conditions thoroughly," he says.

To probe a broad range of those conditions expediently, Yaghi, Rahul Banerjee, Anh Phan, Bo Wang, and coworkers used high-throughput techniques to react zinc nitrate or cobalt nitrate with one or two types of imidazolate compounds out of a group of nine imidazolates. In total, the team carried out 9,600 microreactions and generated 25 types of crystals, of which 16 exhibit compositions and structures that had not been reported previously. Several of the materials are stable at high temperatures and in reactive chemical environments.

The team also examined the crystals' propensity for CO_2 uptake. They report that one of the materials, ZIF-69, can reversibly store a record-breaking 83 L of CO_2 per liter of the crystal at 0 °C and at atmospheric pressure. In addition, they find that another material, ZIF-70, is nearly five times more selective in trapping CO_2 than standard commercial carbon-based CO_2 sorbents.



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High-throughput methods generate numerous types of millimeter-size porous crystals.

Describing the work as a "tour de force," Northwestern University chemistry professor Chad A. Mirkin notes that it demonstrates that high-throughput methods provide a convenient way to control the porosity of the materials over a wide size range by varying the organic ligands. Mirkin adds that the commercial availability of the majority of the imidazolates used in the study makes the materials potentially viable from a commercial standpoint.—MITCH JACOBY

GOVERNMENT NIH and EPA collaborate on chemical testing program

NIH and EPA last week unveiled a collaboration to rapidly test tens of thousands of chemicals for toxic effects. The work is expected to generate data specific to human health effects of exposure to a panoply of chemicals.

Ultimately, NIH Director Elias A. Zerhouni says, this information will help improve people's health.

The effort represents a major step toward moving the field of toxicology from traditional studies on laboratory animals—which are expensive and take years to complete—to rapid, automated testing using cultured human cells.

The collaboration brings together two NIH programs and an EPA research effort. One of the NIH programs, the Chemical Genomics Center, has industrial-scale equipment that can test thousands of chemicals using cells in a matter of hours. The other NIH program, the National Toxicology Program, is housed in the National Institute of Environmental Health Sciences and has tested some 2,500 chemicals through traditional animal studies during the past three decades.

EPA's National Center for Computational Toxicology will use its computer resources to compare traditional, animal-derived toxicology data with the results from the new, automated methods. Robert Kavlock, director of the EPA center, says the results from the collaboration could eventually help scientists determine health effects from mixtures of substances. The work could also identify populations of people who, due to their genetic makeup, are particularly susceptible to toxic effects of particular chemicals, he adds.—CHERYL HOGUE