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### FIRST ORGANIC-FREE SYNTHESIS OF A VERY LARGE-PORE MOLECULAR SIEVE SETS THE STAGE FOR NEW MATERIALS

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To help the U.S. dig deeper into its collective oil barrel, scientists at the Georgia Tech Research Institute (GTRI) have developed a very large-pore molecular sieve which doesn't require expensive organic substances.

*Findings will be presented during the Materials Research Society conference in Boston on Tuesday, November 27 at 11:45 a.m. in the America Center, as part of the symposium on "Synthesis and Properties of New Catalysts."*

Molecular sieves are essential to a variety of industrial processes. To generate high-octane gasoline, for example, oil companies process large hydrocarbon molecules by converting crude oil over a molecular sieve. Known as "catalytic cracking," the process selectively alters certain oil molecules, depending on the size of the molecular pores in the sieve. Larger molecules are then refined to generate high-grade fuels. To produce better quality crudes, oil companies must capture larger hydrocarbons, but the pores in existing sieves are too narrow.

#### H1(GTRI)

Dubbed H1(GTRI), the new molecular sieve is an organic-free, synthetic version of another large-pore sieve known as VPI-5, reports Dr. Rosemarie Szostak, a senior research scientist with the Georgia Tech Research Institute.

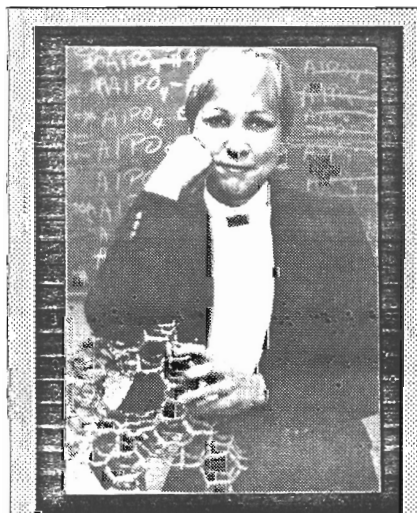
Like VPI-5, the molecular pores in H1(GTRI) "shrink" when exposed to mild heat, thus transforming to a related sieve patented by Union Carbide,  $\text{AlPO}_4\text{-8}$ . Though  $\text{AlPO}_4\text{-8}$  itself is a very large-pore sieve, the transformation is not a clean one, resulting in disorder in the crystal structure, Szostak said, and a blocking of the pores results. Since heat is an essential step in the catalysis process, H1(GTRI) probably won't be used to crack large hydrocarbon molecules anytime soon.

But Szostak is confident that the new organic-free synthesis process can soon be used to produce similar sieves with very large pores. The H1(GTRI) sieve is a first-generation product of the new technology, she noted, and subsequent materials should offer much greater stability.

By removing organic substances, meanwhile, the new synthesis process promises to dramatically reduce production costs while opening the door for significant advancements in catalytic materials.

"Organic substances are extremely expensive," Szostak noted. "For example, an aluminophosphate sieve requires aluminum and phosphoric acid, which are cheap. But when you add an organic substance, your costs could increase substantially."

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Dr. Rosemarie Szostak believes large-pore molecular sieves like  $\text{AlPO}_4\text{-8}$  (shown above) can be made without costly organics.

So why add the organics? Adding an organic amine has seemed essential for the synthesis of  $\text{AlPO}_4$ -type molecular sieves because the crystallization process generally occurs at a basic, or neutral level, she said, and organics alter the material's acidity level. The presence of an organic was also believed to promote the formation of the desired pores and channels, according to Szostak.

The Georgia Tech research challenges this conventional wisdom, however, and Szostak is convinced that effective large-pore sieves can be made at high acidity levels, without organics.

### Taking Clues from a French Scientist

Working with Kristin Sorby of the University of Oslo, Georgia Tech student Bryan Duncan, and Dr. Judith Ulan of the National Center for Electron Microscopy at the University of California, Szostak obtained clues from a 1961 paper by Ferdinand D'Yvoire. A French chemist, D'Yvoire was able to synthesize a new phase of molecular sieve, which he called H1. When another sieve (VPI-5) was recently disclosed, Szostak said, it seemed remarkably similar to D'Yvoire's H1. Unfortunately, she added, efforts to reproduce D'Yvoire's findings have been unsuccessful until now, perhaps because 1960s technology prevented him from fully characterizing H1, and materials available at the time weren't completely pure. Thus, the relationship between the two structures has remained a mystery.

When D'Yvoire was synthesizing his first sample of H1, Szostak explained, impurity levels in the aluminum used to make aluminum phosphate materials were different than the starting materials currently available. Believing that D'Yvoire's H1 may have contained hydrochloric acid as a result of impurities in the synthesis of aluminum hydroxide from aluminum foil, Szostak and her colleagues added this substance to the high-grade aluminum hydroxide currently available. Manipulating acidity levels and the ratio of aluminum-to-phosphate were the key to developing H1(GTRI), she said. (Traditionally, such sieves are made by mixing and then heating an aluminum hydroxide/water solution with phosphoric acid and an organic/water solution, she added.)

Using methods such as X-ray diffraction, NMR, adsorption and infrared spectroscopy to characterize their pure samples, researchers learned that H1(GTRI) is identical to VPI-5, Szostak reported. The most convincing evidence was the conversion of H1(GTRI) to a highly faulted  $\text{AlPO}_4$ -8, she added.

Earlier this year, Szostak, Sorby and Ulan learned that many orderly stacks of atom clusters -- the "rings" which define the large pores of VPI-5 -- tend to slip when subjected to mild heat. The result, she said, is a transformation to  $\text{AlPO}_4$ -8.

"We find H1(GTRI) interesting, but it probably isn't commercially feasible," Szostak said. "Our next step is to screen other aluminophosphate systems with inorganic additives to see if we can make some of the other sieves in this fascinating family of materials."

Useful as environmental scrubbers or for producing the basic components within plastic materials, molecular sieves also contribute to the development of consumer products. By using molecular sieves, for example, manufacturing companies can make laundry detergent without harmful or non-biodegradable chemicals. Additional applications include dual window panes, where sieves prevent condensation, and refrigeration systems, where sieves help dehydrate unnecessary moisture.

*The VPI-5 research was presented at two conferences earlier this year. A paper describing H1(GTRI) has been accepted for publication in Catalysis Letters, Szostak said, and is expected to appear in December 1990 or January 1991.*

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