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HEAT DIMINISHES THE PROMISING CHARACTERISTICS OF A NEW MOLECULAR SIEVE, PRELIMINARY STUDIES SUGGEST

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Microstructural analysis of a new molecular sieve (VPI-5) touted for its potential as a chemical catalyst may help explain heat-induced events which can limit industrial processes such as refining gasoline from crude oil.

At two recent conferences, scientists observed that VPI-5 transforms when subjected to mild heat -- and preliminary studies suggest the end result is $AlPO_4$-8, a well-known sieve previously characterized as having smaller pores. The finding resulted from a collaboration involving the Georgia Institute of Technology, the Lawrence Berkeley Laboratory and the University of Oslo.

In its original state, VPI-5 consists of many orderly stacks of atom clusters, known as "rings," which define wide pores, making the material attractive for separating large molecules, explained Dr. Rosemarie Szostak, a senior research scientist at the Georgia Tech Research Institute.

But after being subjected to 100 degrees Celsius for 18 hours, these stacks apparently slip so that the pores -- defined by 18 rings -- are no longer aligned. The result, she said, is a smaller pore.

"Molecular sieves are adsorbers as well as catalysts," Szostak explained. "VPI-5 has 18-membered rings, giving rise to channels which are 12 angstroms wide. If you want to catalytically convert a substance that is 11 angstroms wide, it won't fit through the pores of any of the smaller sieves such as $AlPO_4$-8. This is why oil companies are interested in an 18-membered ring. Well, we're showing that $AlPO_4$-8 is actually the thermally treated form of VPI-5; a very large pore material, but with stacking faults, which limits its adsorption properties."

An aluminophosphate sieve patented by Union Carbide in 1982, $AlPO_4$-8 has generated little excitement in recent years because of its limited adsorption capacity, Szostak said. Using high-resolution electron microscopy at the Lawrence Berkeley Laboratory, however, Dr. Judith Ulan produced images showing slip planes in a sample of thermally-exposed VPI-5.

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The finding was initiated by Dr. Kristin Sorby of the University of Oslo, a visiting scientist at Georgia Tech. Sorby and Szostak had been studying VPI-5 using several different analytical techniques when they noticed unusual, thermally-dependent changes in their samples. After spotting similarities between the altered samples and $AlPO_4$-8, the scientists became even more curious about the transformation.

At that point, Szostak asked Ulan to take high-resolution micrographs using samples prepared at Georgia Tech. Unfortunately, Szostak said, the resulting images were initially even more puzzling than the X-ray diffraction patterns.

But Szostak soon recognized the features in Ulan's microscopic images. "I set that picture down in my office and it didn't seem to make any sense whatsoever," she said. "Then I was working late one night and it finally hit me that what happens is, when you heat VPI-5, the sheets slip and block the pores, although the 18-membered rings remain intact. This model explains the surprising adsorption, X-ray, and microscope data we had recorded."

Ulan then provided preliminary confirmation of Szostak's hypothesis by generating a computer model of the material showing definite VPI-5 domains in the $AlPO_4$-8 sample.

Additional research is needed to completely confirm the new model of $AlPO_4$-8, but Szostak remains optimistic that initial findings will ultimately help prevent the development of stacking faults in VPI-5, thus preserving the material's large-pore structure.

Molecular sieves are useful for a variety of industrial processes. Oil companies utilize the sieves' unique activity in the "cracking" or transformation of crude oil. Sieves may also be used as environmental scrubbers, or for the production of monomers in the plastics industry. Makers of consumer products, including detergent, frequently use sieves instead of harmful or non-biodegradable chemicals. These tiny structures can also be found in refrigeration systems, where they help dehydrate unnecessary moisture, explained Dr. Tudor Thomas, director of the molecular sieve research program at the Georgia Tech Research Institute. In weatherstripping, molecular sieves prevent condensation from accumulating on dual window panes, he added.

EDITOR'S NOTE: Preliminary results from the VPI-5 project were presented at the recent Materials Research Society Conference in San Francisco, Calif. on April 18, and during the Pittsburgh-Cleveland Catalysis Society Conference in Cleveland, Ohio on April 19. To receive photographs or copies of the presentation proceedings, members of the media are invited to contact Ginger Pinholster or John Toon at (404) 894-3444. Non-media inquiries should be directed to the scientists.

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