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M. G. Wu, M. W. Deem, S. A. Elomari, R. C. Medrud, S. I. Zones, T. Maesen, C. Kibby, C. Y. Chen, I. Y. Chan, *J. Phys. Chem. B* **2002**, *106*, 264-270.

FUNDING

National Science Foundation, Petroleum Research Fund, ChevronTexaco, and Energy Research and Technology Company.

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Discovery of a New Molecular Sieve: Zeolite SSZ-55

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Scientists at the University of California in Los Angeles, and the ChevronTexaco Energy Research and Technology Company in Richmond, California, have discovered a new large-pore zeolite, which is a compound that can be used to separate molecules of various sizes and shapes, and can act as a sieve by constraining a chemical reaction medium. Due to their high thermal stability, zeolites are also used as catalysts, both in the petroleum and the chemical industries.

Zeolites, which are primarily made of silicon and oxygen, have found widespread use as catalysts, molecular sieves, and ion exchangers. High-silica zeolites are of particular interest because of their importance in refining and petrochemical applications.

In virtually all instances involving high-silica zeolites, the crystallization involves complete filling of the void regions by an organo-cation guest molecule. Then, the guest molecule is thermally decomposed, leaving the ordered void regions of the zeolite, which can later be studied for catalysis or separation applications.

Our team has found a novel zeolite: $\text{Si}_{0.97}\text{B}_{0.03}\text{O}_2$, designated as SSZ-55 by using the organo-cation guest molecule shown in Figure 1. A key feature of this molecule is that it has both structural rigidity, conformational flexibility, and a positive charge for overall system neutrality.

It is usually difficult to grow zeolite crystals for single crystal diffraction experiments, although progress is being made at synchrotron sources to collect data from micrometer-

sized single crystals. Instead, micrometer-sized crystals are easily grown and are ideal for powder diffraction. At NSLS beamline X7A, which is dedicated to powder diffraction, our team has collected high-resolution data on micrometer-sized zeolite crystals.

The unit cell was determined by indexing the experimental data with the commonly used Visser, Werner, and Louer programs. The structure was solved using ZEFSA-II, a Monte Carlo program designed specifically for solving tetrahedral

framework structures. The final structure parameters were obtained by Rietveld refinement with a widely used program called General Structure Analysis System (GSAS).

SSZ-55 is tetrahedral (has four faces) with large pores surrounded by twelve silicon atoms, also called ATS. Figure 2 shows projections of the zeolite molecule in each of the three crystallographic directions. Of particular interest is a one-dimensional channel composed of 12 tetrahedral (T) atoms. The oxygen atoms are omitted for clarity but are located halfway between each pair of silicon atoms. (Silicon-oxygen-silicon angles are usually in the range 140 – 160 degrees.)

Adsorption experiments with argon and selected hydrocarbons support the results of the structure determination. Argon adsorption shows that the pore opening is $7 \pm 1 \text{ \AA}$, which is in good agreement with the structural values of $6.5 \text{ \AA} \times 7.2 \text{ \AA}$. Hydrocarbon adsorption of molecules of various shapes and sizes reveal that the material has a pore opening of 12 to 14 rings, in agreement with our structural results.



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Though ATS framework structure has been previously found in a variety of metal-substituted aluminophosphates (compounds containing aluminum and phosphate), SSZ-55 is the first discov-

ered high-silica zeolite with an ATS structure. Also, the synthesis conditions are considerably different for the two classes of compounds. SSZ-55 is also interesting in that the structure does not contain any

five-ring silica subunits, which tend to predominate in high-silica zeolites. Instead, the structure contains only four-ring and six-ring subunits.

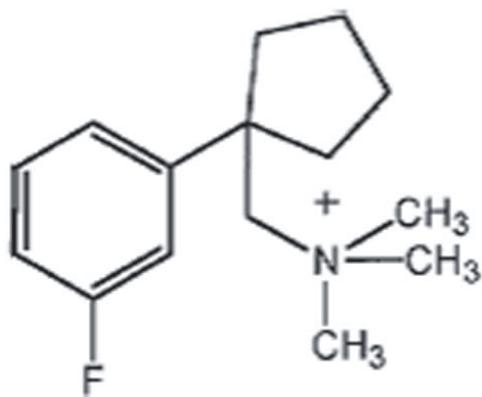


Figure 1. Molecule used in the SSZ-55 synthesis: [(1-(4-fluorophenyl)cyclopentyl)-methyl]trimethyl ammonium ion.

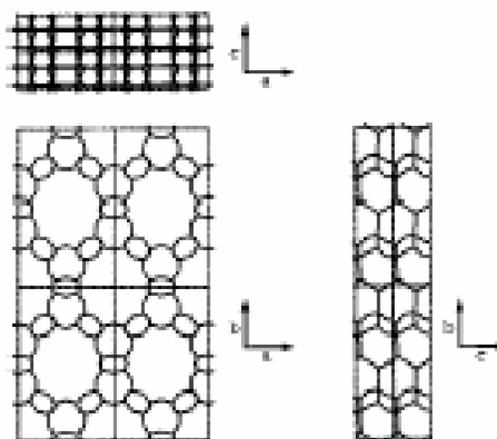


Figure 2. Three axial projections of the SSZ-55 structure obtained from Rietveld refinement. Note that only the silicon atoms are shown.