Chemistry by Touch

Blind scientist fashions new models of molecules

By RICHARD LIPKIN

In the world of chemistry, nature's architecture dominates the microscopic scene. A protein may show up as hundreds of clustered spheres, while in DNA, atoms spiral up a long helix. People appreciate chemical forms mainly with their eyes.

But what if a person cannot see? Can a blind person comprehend molecular structure?

"Blind students have struggled with molecular structures for years in studying chemistry," says Lawrence Scadden, the National Science Foundation's program director for persons with disabilities. "I'm one of them. I'm blind. I got my Ph.D. many years ago, and taking chemistry was difficult. It's hard to grasp molecular structures without asking someone to build a model."

Now, chemist William J. Skawinski, a postdoctoral research associate at the New Jersey Institute of Technology in Newark, is doing just that.

Sitting at his computer workstation, he puts the finishing touches on a 150-atom molecule he has just designed. Having made the calculations for a chemical destined to bind to a receptor with lock-and-key precision, he enters information about its chemical structure and shape into his terminal. After formatting the data with his unique program, he feeds the file into a computer that controls a laser stereolithography machine.

Several hours later, a plastic model of the molecule emerges.

Photos: Brian Buckley/NJIT

Chemists Skawinski and Venanzi look over a plastic model of a molecule made by the laser stereolithography system.

Skawinski, who is himself blind, has devised a system for translating descriptions of molecules into three-dimensional plastic models. "Originally, I got interested in this project because, being blind, I thought it would help me work with molecules represented on computer screens," he says. "But then I realized that this would be a useful research tool for sighted chemists as well."

In a science rich with glitzy computerized pictures, Skawinski's system permits a chemist to design a molecule, image it on a computer screen, and create a three-dimensional representation directly from calculations. The final product accurately portrays the atoms' relations to one another.

The secret lies in laser stereolithography, a technology that forges models quickly from a light-sensitive liquid polymer (SN: 8/3/91, p.72). Most commonly used in industry for modeling new parts, stereolithography has been slow to find its way into scientific laboratories. Whereas computer-aided design systems easily meet auto and aerospace needs, they have not been adapted for use in basic science. The critical missing link has been software that can convert molecular descriptions into a form the machine can interpret.

Skawinski has supplied that link in the form of a computer procedure that creates molecular prototypes directly from quantum mechanical calculations.

Stereolithography begins with an elevated table in a 10-inch-deep vat of liquid plastic. "The table sits at the top of the tank, covered by a polymer film," Skawinski explains. "A laser traces the bottom of the molecule [to be modeled], hardening a slice. The table eases down, and the laser draws another slice." The table falls gradually through the liquid, allowing the laser to forge the model from bottom to top. "When it's done, you get one solid piece," he says. "Then we cure it in an ultraviolet oven."

It takes 8 to 12 hours to fabricate the average molecular model. The final product emerges as a translucent sculpture. Each atom has a textured surface that reveals details of the element and its bonds.

"The beauty of this system is that the models come directly from X-ray crystallography or quantum mechanical data, so they're extremely accurate," says New Jersey Tech chemistry professor Carol A. Venanzi, who worked with Skawinski to develop the system. "With these, you can represent a molecule's transition states and electrostatic forces, which can't be done with standard models."

The molecular modeling system has proved itself as a research tool, Venanzi says. It enabled her team to see how specific molecules bind to proteins, how a drug binds to a cell's receptor, and how sucrose binds to taste buds.

"We've made models of several compounds, and just having them around has made a difference," she adds. "We could look at them, fit them together, compare them with other molecules. You can see more clearly how each molecule's structure relates to its biological activity."

Even with high-quality software, she says, it's hard to grasp a molecule's three-dimensional qualities from a computer screen.

"This project could have a major impact on chemistry education, which is one of our reasons for supporting it," says Richard L. Hilderbrandt, a chemist at NSF. "I've seen these models. They can be tremendously helpful . . . in understanding chemical structures."

While many new computer aids for the blind have come along in recent years, Hilderbrandt maintains that "there have been few in chemistry. So this is an

Models of beta-cyclodextrin and amiloride molecules.

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important new tool."

"There's a great need for tactual tools in teaching chemistry to students who are blind, or disabled, or who simply learn better by holding something in their hands," adds Scadden. "Tactile models reinforce the learning process better than drawings."

Roughly 1.1 million U.S. residents are legally blind, according to the American Foundation for the Blind. Best estimates hold that several thousand working scientists are blind or visually impaired.

Yet "blind and disabled people are severely underrepresented in the scientific community," Scadden says. "With the right educational technologies, more students with disabilities could participate in science and choose it as a career."

"There's still a great barrier for blind people in mathematics and science," concurs Virginia W. Stern, director of the project on science, technology, and disability at the American Association for the Advancement of Science in Washington, D.C. "There's a tremendous need for better teaching tools at every academic level."

Skawinski expects people in many fields — biology, physics, toxicology — to benefit from his system. "We're trying to expand the system to model other three-dimensional physical phenomena, like electrical or gravitational fields around an object, or even mathematical functions."

"The limit, really," he observes, "is a person's imagination." □

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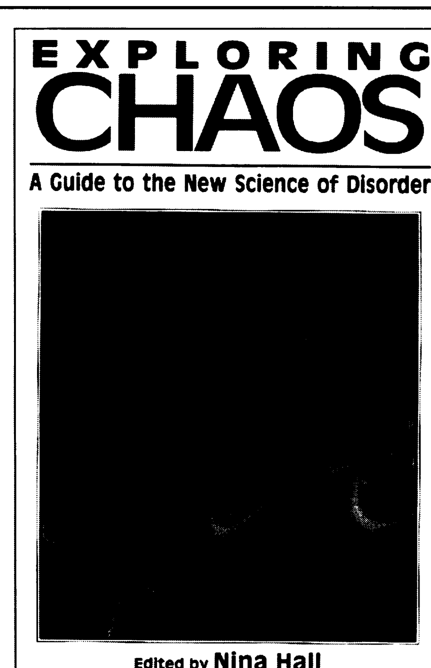

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