Excited molecules join reaction rules

Clothed in a bulky winter coat and gloves, Peter Chen recently met with success in a laboratory cooled to four degrees below zero. There, conditions were right for the undergraduate student and his associates to finish synthesizing the first dimers, or two-part molecules, composed of the benzene ring (C_6H_6) and the three-ringed anthracene ($C_6H_4[CH]_2C_6H_4$). These new, exceptionally energetic compounds, report the students and their adviser Nien-chu C. Yang of the University of Chicago in the Jan. 27 JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, can be used to broaden an already important set of rules on the chemistry books.

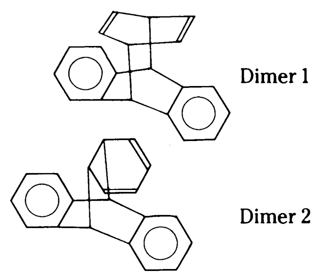
Those rules are the Woodward-Hoffmann rules. Formulated in the 1960s by 1981 Nobel Prize winner Roald Hoffmann of Cornell University and the late Robert B. Woodward, the theory-laden laws are predictive tools for researchers whose work depends on chemical reactions, or the conversion of one compound or a group of compounds into another. Such reactions play a key role in a variety of endeavors, ranging from combatting disease to preparing food and drink. In all cases, effective use of the chemical reactions depends on a solid theoretical foundation. Woodward and Hoffmann helped to provide this with their theories on the course of chemical reactions.

The theories apply to a specific subset of organic reactions called pericyclic — reactions that involve a concerted making and breaking of bonds. Under the pericyclic heading falls another way of classifying reactions — according to the energy level of the electrons in the molecules involved. In this categorization, there are three types of pericyclic reactions: those involving ground-state molecules (molecules whose electrons have a normal energy level) that convert to other ground-state molecules; those involving excited-state molecules (molecules whose electrons have a higher than normal energy level) that convert to ground-state molecules; and those involving excited-state molecules that convert to other excited-state molecules.

At its simplest level, the Woodward-Hoffmann theories predict which reactions are most likely to occur in each of those categories on the basis of the number of bonds that would be simultaneously broken and formed, Yang explains. For example, according to the rules, the ground-state-to-ground-state reactions that are most likely to occur are the ones that make and break an odd number of bonds. By contrast, the "preferred" excited-state-to-ground-state reactions are those that make and break an *even* number of bonds. But what of the excited-state-to-excited-state reactions? Yang says because so few of these have existed, the Woodward-Hoffmann rules could not be applied to them.

Enter the new benzene-anthracene dimers. Both decompose to a benzene and an excited form of anthracene in the rare excited-state-to-excited-state type of reaction. Because the dimers are structurally different, they decompose in different ways: When dimer 1 (refer to diagram) decomposes, the reaction makes and breaks an even number of bonds; when dimer 2 decomposes, the reactions involve an odd number of bond changes. Because the dimer 1 reaction proceeds in a more "efficient and facile" manner, Yang and colleagues propose, in an extension of the Woodward-Hoffmann rules, that preferred excited-state-to-excited-state reactions involve an even number of broken and formed bonds.

Hoffmann—who was out of the country at the time of this printing—could not be reached for comment. —*L. Garmon*



Mirroring a three-dimensional world

Combine an oscillating mirror with a special cathode ray tube, while relying on the same optical illusion that allows someone to watch movies or television, and the result is a glowing, three-dimensional image that shows parallax and depth. This new space-filling display may have a variety of applications, including air traffic control, seismic data analysis and computer-aided design.

The inventor, Lawrence D. Sher of Bolt Beranek and Newman Inc. in Cambridge, Mass., demonstrated his patented Space-Graph display at a recent symposium on perceptual research and military systems applications of three-dimensional displays, held in Washington, D.C.

Several people can view the display at the same time, without wearing special glasses, and see the object as it would appear from their particular viewpoints. The display also faithfully reproduces parallax effects so viewers can look over, under and around the image simply by moving their heads.

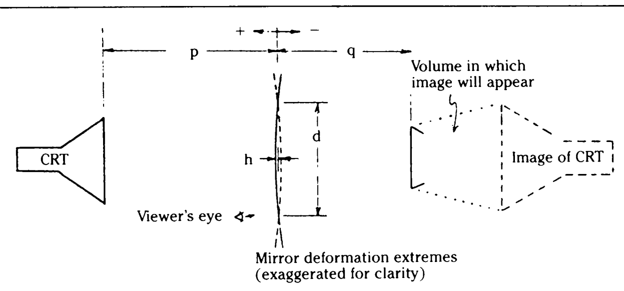
The display uses a computer-driven cathode ray tube, similar to a television picture tube but coated with a special phosphor that glows only when electrons strike, to present pictures of successively deeper layers of the desired image. A circular, aluminized acrylic mirror, facing the screen and driven by a 15-centimeter woofer at 30 hertz, oscillates from concave to convex and back again. Thus, when the mirror is synchronized with the cathode ray tube, each image layer appears farther away from the viewer than the one preceding. This occurs rapidly enough so that the eye is able to fuse the entire series into a single, flicker-free, three-dimensional image that occupies a volume equivalent to two basketballs.

One advantage of space-filling displays over conventional flat ones is in recognizing patterns and regularities in data, such as those involving earthquake zones. "Patterns may lurk in these space-filling data plots, but finding them can be difficult to impossible when their display is confined to a surface," says Sher. "From experience to date, a major value of these images is in the exploitation of eye and brain to find these patterns." Even the brightness of the individual dots that make up a display image can be adjusted to add a further dimension to data display.

A space-filling display can also show the vertical separation of airplanes in a holding pattern over an airport. At present, air traffic controllers see a stack of aircraft as a superimposed set of vectors and labels, while the height of each airplane is not displayed directly.

"The technology is already capable of doing a lot of things that people now struggle with," says Sher. He expects his display system will be useful for the analysis of all kinds of natural and man-made structures, like molecules and bridges or buildings. "We're looking now at the first instance of this technology, and it will certainly have lots of development in the next few years as it becomes more and more capable of handling certain specific applications," Sher says. —*I. Peterson*

A true three-dimensional display can be achieved by using a deforming mirror and a special cathode ray tube in the arrangement shown.



Bolt Beranek and Newman Inc.