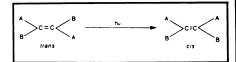
The program attempts such discrimination after studying an appropriate training set of "knowns."

Tests using those training sets indicate that ADAPT now accurately classifies only if the molecular pool is limited to one class of compound - polyaromatic hydrocarbons (PAH's) for example. Eventually, though, ADAPT may be a useful tool for setting toxicological testing priorities by screening diverse batches of suspect chemicals.

The screening potential of computer chemistry programs already is being exploited in a Battelle search for dyes that can store a sufficient amount of solar energy. The energy of light can cause the structure of those dye molecules to convert from the trans to the cis configura-



tion. Since it takes light energy to drive this transformation, the resulting cis configuration has stored energy. The Battelle researchers knew that a series of indigo dve derivatives could undergo lightdriven, trans-cis conversions. What they did not know, however, was which dye derivatives in the cis form could store at least 15 kilocalories per mole (6.023 x 10^{23} molecules), the estimated minimum for profitable storage devices. molecules of this complexity, synthesis and characterization can be very difficult," says Battelle's Wolken. "In fact, for a typical compound in this series, approximately a man-year of effort could be required to make the compound to investigate its properties thoroughly.

To save those years of synthetic effort, the researchers decided to use a computer program to screen all of the potential dye derivatives - a procedure "far more economical than a purely experimental approach." Although the computer could not calculate the precise energy storage value for each dve, it was able to calculate trends that helped identify "the best prospects for success ... among the many possible structures.

In addition to enlisting the aid of the computer in their search for chemical solar energy collectors, Battelle researchers have used computers to study chemical corrosion and to calculate the heat of different reactions - a program that eventually may be used to analyze the many chemical steps that occur among shortlived molecules involved in the combustion of fuels.

"New uses for the computer are emerging," Wolken says. "In more and more laboratories, computers are being used to predict the properties of molecules before they have been produced." And although "much work has been done," says Wolken, "much work needs to be done."

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ANNUAL REVIEW OF ANTHROPOLOGY, VOL. 9 — Bernard J. Siegel, Alan R. Beals and Stephen A. Tyler, Eds. An article by Cora Du Bois, "Some Anthropological Hindsights," introduces this volume. Annual Reviews, 1980, 646 p., illus., \$20.

ANNUAL REVIEW OF PHYSICAL CHEMISTRY, VOL. 31 — B.S. Rabinovitch, J.M. Schurr and H.L. Strauss, Eds. Activity in diverse newer branches of physical chemistry has been matched by a resurgence of interest in some of the more traditional areas. This volume reflects prog-ress across the broad spectrum of this field. Annual Reviews, 1980, 675 p., illus., \$20.

BIGFOOT: A Personal Inquiry into a Phenomenon — Kenneth Wylie. For many years controversy has raged over the existence of Bigfoot, a two-legged creature of enormous size said to be roaming the backwoods of America. The author, a historian, anthropologist and amateur naturalist, follows the many dubious and not-so-dubious physical trails of the beast, surveys the extensive literature, consults scientists and interviews leading Bigfoot hunters. This is a history of a strange phenomenon together with studies of the people who maintain the pursuit. Viking Pr, 1980, 268 p., illus., \$14.95.

THE COMPUTER: From Pascal to von Neumann — Herman H. Goldstine. A history of the computer concentrating on the ideas and the people who conceived them. This work is presented in three parts: pre-World War II; the war period, particularly at the Moore School of Electrical Engineering, University of Pennsylvania; and the postvar years at the Institute for Advanced Study in Princeton through 1957. Originally published in hardback in 1972. Princeton U Pr, 1980, 378 p., illus.,

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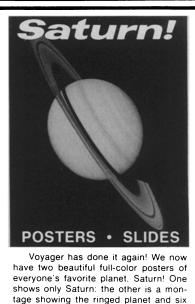
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