CHEMISTRY

Computerization of chemistry

The FBI isn't the only government agency interested in centralizing computerized data for rapid identification. The Chemical Information System, developed by researchers at the National Institutes of Health and the Environmental Protection Agency, has on file experimental fingerprints—mass spectra, carbon-13 nuclear magnetic resonance spectra or X-ray diffraction patterns—for more than 30,000 compounds and also about 70,000 literature citations for the use of research chemists.

In the Jan. 21 SCIENCE, Steven R. Heller of EPA and George W.A. Milne and Richard J. Feldmann of NIH describe the current state of this ambitious computer project. The mass-spectra search system, the oldest component, now provides about 4,000 searches a month. Researchers anywhere in the world can use a telephone-coupled terminal to contact the computer. To identify a compound, the chemist describes the spectrum he has obtained in his laboratory. The computer identifies spectra with the same peaks that are stored in its file.

Cost for use of the computer is low, usually $1 to $6 per search, but laboratories also pay a subscription fee. In the next years, the developers expect the system to grow both in number of components and in use.

Links in the hydrocarbon chain

When chemists analyze a long-chain molecule, they usually assume that the structure of the subunits is the same as in shorter, more easily analyzed, molecules. Researchers studying n-hexadecane, a 16-carbon molecule, have now discovered that bonds in that hydrocarbon chain are longer than in short-chain molecules.

Susan Fitzwater and L.S. Bartell of the University of Michigan analyzed the diffraction pattern of electrons deflected by a vapor of n-hexadecane molecules. The angles between the chemical bonds were the same as in shorter hydrocarbons, but the bond lengths between carbons were longer. The average carbon-to-carbon bond was determined to be 1.542 angstroms, which is 0.01 angstroms longer than the length reported for vapors of a seven-carbon hydrocarbon. The researchers suggest, in the Dec. 22 JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, that internal chemical bonds are longer than bonds at the ends of the chain due to repulsions between atoms not bonded to each other but forced close together within the molecule.

Under the influence of marijuana

A simple chemical test for marijuana intoxication may be just around the corner. In the January ANALYTICAL CHEMISTRY Joe Vinson, Dinu Patel and Arun Patel report success in detecting tetrahydrocannabinol (THC) in blood samples of volunteer smokers. The researchers are currently adapting this technique to saliva samples.

"My procedure can only be accomplished in the laboratory and hence is not fully comparable to the alcohol balloon test," Vinson says. "However, it can be done by relatively untrained personnel in about two hours of laboratory time."

In the test, THC in a sample reacts with the chemical 2-*p*-chlorosulfophenyl-3-phenylindone. The product is identified by thin-layer chromatography. Narcotics, tranquilizers and psychoactive drugs do not interfere with the results.

The major problem has been obtaining high enough sensitivity. Two hours after smoking marijuana, THC in blood is only one part per billion and in saliva it is even less. Vinson's technique can detect two tenths of a part per billion in blood.

This quick and inexpensive test has aroused considerable interest from police and crime labs, Vinson says.

SCIENCE & SOCIETY

Women scientists earn less

In 1973, a National Research Council survey of scientists and engineers found that women were bearing the burden of unemployment in scientific positions. Now, two new NRC surveys following up the 1973 data find that women scientists still account for most of science's unemployed and that women's salaries are considerably lower than men's.

The recent surveys profiled doctoral scientists and engineers in 1975 and compared them with the 1973 figures. Women's unemployment rate in 1973 was 3.9 percent, compared with 0.9 percent for men. In 1975, women's unemployment decreased to 3.0 percent, while the men's rate was 0.8 percent. Most of the unemployed women were recent and young graduates, while unemployed men were distributed evenly through all age groups.

Median income for women Ph.D. scientists was $19,000 compared with men's $23,500. Women Ph.D. engineers fared slightly better with a $21,000 median income but were still far behind the male engineers who reported a median income of $25,000.

The number of women in science and engineering has grown over the period, but women still remain a small minority of the scientific community. In 1973, the 18,049 women Ph.D.'s in science accounted for 7.9 percent of all scientists. In 1975, some 23,188 women made up 9.6 percent.

Many more women had secured only part-time jobs but were looking for full-time work. In 1973, the survey found 3.5 percent of all women scientists in this category, while only 0.7 percent of the men were in comparable positions. By 1975, the picture had improved a little: only 2.4 percent of women and 0.5 percent of men were part-timers seeking full-time jobs.

Employment in the sciences

While scientists may bemoan their lack of funding and loss of esteem, unemployment figures show that scientists still occupy a unique status in the United States. Two studies by the National Research Council show that unemployment rates for scientists were well below the national average in 1973 and 1975.

Unemployed Ph.D.'s in science and engineering decreased from 1.2 percent in 1973 to 1 percent in 1975, compared with an increase in the national unemployment rate from 4.9 percent to 8 percent in the same period. Physics and astronomy had the highest percentage of unemployed, 1.6 percent, while mathematics had the lowest rate, 0.5 percent. In 1973, chemistry had recorded the highest unemployment, 1.7 percent. Not surprisingly, young scientists and recent graduates were unemployed more often than their older colleagues.

Energy and the future

In July 1975, the Energy Research and Development Administration asked the National Academy of Sciences to conduct a survey of long-term energy use to help set future policies. The final Academy report will not be out until this June, but an interim report reveals two important trends:

- "Total demand for energy will grow at a lower rate in the future than the historical rate, and . . . such [slow] growth is desirable and possible without detriment to other possible [national] goals."
- The gross national product can continue to grow without having to expand energy consumption as quickly as in the past. "There may be considerable leeway, over the long-term, in the amount of end-use energy required for a given rate of growth of GNP and employment."