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The Role of Chemistry in Computers

Chemists are relying more and more on computers to solve problems which tax human patience and human capability. But another fact about chemistry and computers is less generally known: Computer manufacturers are relying increasingly on chemists for solutions to certain problems related to computer development. These problems involve not so much a set of requirements determined by present computer needs as a series of open questions raised by future computer possibilities. Research in chemistry could conceivably improve computers, and might revolutionize them; but the search itself serves a more general purpose as it uncovers new information and encourages awareness of scientific interdependence.

To those of us in research, this interdependence is obvious and urgent now; more general recognition of this fact will eventually help industry as much as it helps science. Progress in science and technology depends on common efforts by chemists, physicists, and other scientists in laying claim to the "no man's land" where the different sciences overlap and where any one science alone is inadequate. Common efforts among scientists are under way, as evidenced by news of interdisciplinary conferences and cross-disciplinary publications. Such efforts may be seen in current computer research.

Computers in Chemical Research

Consider first, by way of introduction, the more familiar side of the subject—the role of computers in chemistry. Computers help the chemist in two distinct ways: They save his time in solving relatively straightforward but tedious problems; and they enable him to attack new problems too complex for solution by other means. A look at some typical problems of each kind will suggest some reasons for the chemist's appreciation of computers.

Fitting a line to a number of points by the least squares method—a relatively trivial yet common kind of problem—involves calculations which are highly repetitive but almost exorbitantly time-consuming without mechanical assistance. Even with a desk calculator, hours of work are necessary. But with a computer, the answer is available almost immediately.

Another example: Computers have made numerical analysis a practical way of handling the integration of differential equations. In physical chemical problems, one can often write a differential equation describing, for instance, the successive rates of reaction of a polymerization mixture; but the integration of the equation rapidly becomes unmanageable, and one must make approximations to reach a solution. Attempted manually, these approximations involve a lengthy process; but numerical analysis, performed mechanically, can find the shape of the curve with relative speed and ease. To accomplish this, the computer requires only the boundary conditions for the problem and the incremental step, ΔX, to be evaluated numerically. The ΔX chosen may be so small that even a fast computer cannot quickly solve the problem to the degree of precision desired; but in principle, numerical analysis is always possible.

Computers also make possible the solution of new kinds of problems, as in X-ray crystallography, where the application of computers to chemistry has been most successful. X-rays of known wavelength, sent through a crystal, are diffracted by the ordered atoms which act as a three-dimensional diffraction grating. When the rays reach a photographic plate or film positioned behind the crystal, a diffraction pattern of the crystal is visible in the form of spots of varying intensity. Any experimental technique used to detect the X-ray diffraction pattern from a crystal determines the intensity of a diffracted spot. The intensity observed at each spot is related to the sum of the diffracted waves from various atoms in the crystal, reaching that spot with various positive and negative amplitudes (i.e., phases). Since the intensity of a wave is the square of the resultant wave amplitude, the sign of the wave (negative or positive) is lost in the experimental determination of intensity. Without this information it is not possible to deduce the structure of the crystal from the diffraction pattern.

The ability of the X-ray crystallographer is taxed to the utmost at this point. He must now assume, by induction, a "reasonable" atomic structure for the crystal. With the computer, he then simulates the X-ray diffraction pattern that would be produced by the assumed crystal structure and compares the simulated diffraction pattern with the actual pattern. By a series of such successive approximations, discarding erroneous assumptions, the actual crystal structure is obtained.

To help him make these "reasonable" approximations, the X-ray crystallographer incorporates a

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"heavy" atom in the crystal structure whenever possible, since it scatters the X-rays much more effectively than the other atoms can and thus produces easily identifiable spots in the diffraction pattern. These spots are all assigned the same phase relationship; and then it is materially simpler to determine a probable structure and to make reasonable approximations. With this technique, it has become possible to determine a structure as complex as that of vitamin B_{12} with more than sixty carbon atoms and one (heavy) cobalt atom.

More recently, however, the X-ray crystallographer has begun to enlist the computer even in the work of making the necessary reasonable approximations. That is, the computer can be used to make a statistical analysis of spot intensities and to correlate the intensities with the respective atoms of differing atomic number assumed to be present, and possibly with their wave phase.

With these computer techniques, it may be possible in the future to determine the structure and configuration of almost any polymer or protein. Biophysicists are becoming increasingly aware that the spatial configuration and the chemical structure of a particular protein are equally important in biological processes. Since X-ray crystallography determines both structure and configuration, it is a powerful tool for the biological sciences.

As these examples suggest, many chemists who have no direct contact with computers are nevertheless aided in their work by data obtained through various applications of computers to chemistry problems. It is obvious that computers relieve the chemist of drudgery and enable him to learn more than he once thought he could know. And appropriately enough, some of the very facts the chemist is learning with the aid of computers may be applied directly to the improvement of these machines.

Chemical Research for Computers

Historically, computer development has not depended heavily on chemistry. Mechanical, electrical, and electronic engineers have successively taken the lead in designing increasingly complex business machines, with no more than marginal help from chemists. As the machine technology advanced from the manual key punch to the digital computer, and as the business market broadened to include general purpose data processing equipment, certain trends became apparent in the kind of improvements required by the customer and produced by the manufacturer. The changes generally increased the speed of machine operation to handle vast computations within reasonable times, without raising power consumption or lowering mechanical reliability. In recent years, the emergence of electronics provided the principal basis for these improvements in speed and capacity.

The single event most responsible for drawing chemistry into participation in computer research was the introduction of the transistor, which marked a major change in computer development and in technical progress generally. Faster, more compact, and requiring less power than the vacuum tube it replaced, the transistor recommended itself strongly to computer manufacturers. This solid state device made it theoretically possible to increase the speed and complexity of computer operation while decreasing the size of the machines.

This possibility led to intensive study of the semiconductor materials from which transistors are made. Computer research staffs were enlarged to include new specialists: Physicists and chemists analyzed semiconductors to determine their potential advantages and to furnish facts necessary for the actual manufacture of transistors for computers.

To describe semiconductors theoretically, the solid-state physicist explained that the electron gains energy from heat or light, and jumps "quantum-mechanically" into a conduction band, leaving a "positive hole." But in addition to the theoretical description, experimental preparation of semiconductors was required; and this demanded a different and complementary approach: the chemist's view of the chemical constituents, and their arrangement, in semiconductors. The physicist had to learn chemistry and the chemist had to learn physics, so that they could specify and prepare materials with the required number of excess "holes" or electrons. Figure 1 shows such a configuration, demonstrating the meaning of a "hole."

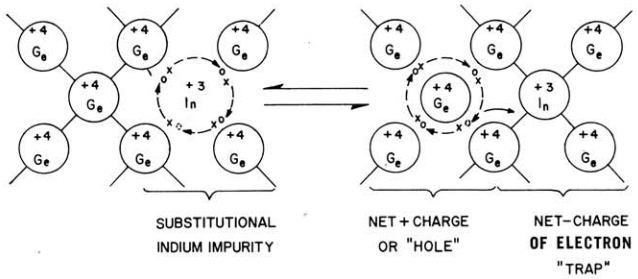

Figure 1. Chemical configuration of a hole in germanium. When indium is substituted as an impurity into a germanium lattice site, only three covalent bonds are formed to the adjacent germanium atoms. The fourth germanium valence electron has no indium electron (indicated by dotted open circle) with which to pair, because indium has only three valence electrons (shown by open circles). The resulting electron lack "resonates" (as shown by dashed arrows) among all the germanium-indium bonds. When an electron migrates from an adjacent pure germanium site, all four germanium atoms are fully bonded to the indium atom, producing a net negative charge on the indium site and a net positive charge (hole) in the germanium lattice.

As transistors have proved their value in computers, the increased study of semiconductors which resulted has firmly established the importance of chemistry, along with physics and quantum mechanics, in computer research. Physical chemists and X-ray crystallographers have been enlisted to study diffusion processes of micro-quantities of impurities in host semiconductor materials, and to grow and characterize crystals with such impurities to test the theoretical assumptions about them.

Transistors may have dramatized the emergence of chemistry as an active force in computer development, but semiconductor analysis is by no means the only assignment for chemistry in computer research. The current knowledge and methods of chemistry are also being applied to other materials and processes important to computer manufacturers. For example, photographic methods of handling data in computers are being considered and explored: Chemists are studying various photosensitive materials which might be incorporated successfully in data processing equipment for the entry, storage, and retrieval of information.

Data processing equipment could handle more information more rapidly if the computer memory units, where the information is stored, could be made more compact and more efficient. It has been known for some time that a photo-optical memory unit is theoretically possible, and that such a memory could surpass a magnetic unit in storage capacity. But present photo-optical memories are limited in that they are not reversible; tnat is, information cannot be changed once it is placed on the photosensitive medium.

Reversibility is not necessary in some applications, or is even undesirable; in such cases a non-reversible photosensitive material is acceptable and might be preferable. The translating machine developed at IBM, for example, stores an entire Russian dictionary, including idioms, in coded form on a 10-in. disk coated with a silver halide emulsion. In this application, where the information to be "remembered" by the unit is a long list, relatively permanent in content and arrangement, high-density storage is desirable for machine economy; non-erasability ensures the desired degree of permanence; and delayed processing is no particular disadvantage, since the list is seldom changed.

In other applications for a photosensitive memory unit, however, delayed processing may be a disadvantage. In connection with the problem of processing new entries to a memory unit during computer operation, we at IBM have recently studied the photoionization of a triphenylmethyl leuconitrile. This photochemical reaction has possible relevance because it produces color on irradiation alone, and thus might be a suitable medium for data storage in a computer. Our detailed study of the mechanism of this photochemical activity located certain controlling factors, and found some variations in the reaction: Under certain conditions, for example, fluorescence rather than photoionization takes place.

In the search for reversible photosensitive materials, another direction is being followed by the National Cash Register Company, whose chemists have developed the photosensitive spiropyrans shown in Figure 2—organic compounds which are bistable under irradiation by two different wavelengths of light. The usefulness of these compounds is limited by the fact that degradation products from the photochemical side reactions eventually interfere with reversibility; but in applications where only a few reversals are required, these compounds may be ideal.

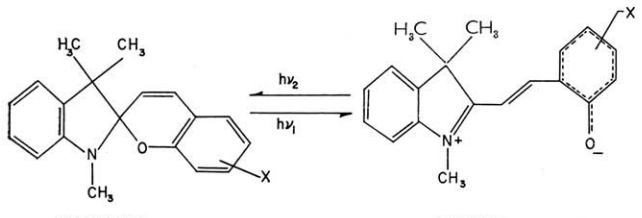

Figure 2. Spiropyrans.

Experiments reported at General Electric suggest that thermoplastic tape, which works on the simple principle of electrostatic attraction, might provide a reversible medium for data storage in computers. Their chemists prepared tape from a thermoplastic polymer such as polystyrene, charged selected areas of the tape with electrons from an electron beam, and then heated the tape. They found that electrostatic forces cause the material to deform under surface tension forces, leaving an erasable record of the electron beam.

These examples of current activity may seem to suggest that the chemist's present goal is to produce materials which could replace magnetic materials. If this were the only goal, the effort would be wasted. Rather we are examining broadly the several ways in which electromagnetic radiation affects materials. Magnetic fields interacting with ferromagnetic materials represent only one possible type of interaction. The study of the interaction of light with matter has already been mentioned to show that potentially useful processes may develop from this kind of basic investigation. It is true that the photosensitive materials developed so far cannot match all the capabilities of magnetic materials. They cannot be reversed as often or as rapidly; but they have other properties that magnetic materials do not possess. For example, photosensitive materials can store not only digital information but also photographic information; and there are numerous applications in which this ability would be useful.

Each material has its own unique advantages and disadvantages; it is necessary for the chemist to investigate these interactions to uncover all the significant variations. This area is one where physics and chemistry overlap strongly, and this fact again points up the need for inter-science cooperation.

Chemical research is attacking other problems: If we want to make smaller holes in accounting cards, we must understand the problems of dimensional stability of paper under varying conditions of humidity. If we want to specify a good magnetic ink, we must understand colloidal suspensions. If we want to make thinner and more uniform magnetic coatings on drums and disks, we must understand the mechanism of electroplating and the interaction of a pigment with its binder. If we want computers which are more sophisticated and more compact, we must—as we have seen—understand and exploit the processes of matter at the molecular level, which is also the province of chemistry.

Here again, as in our earlier examples, the chemist must work closely with other scientists. This interdependence is by no means unique to chemistry or to computer technology. Wherever the fundamental nature and processes of matter are being studied (and in this atomic age they are being studied everywhere), the old distinctions of separate sciences and separate science buildings on college campuses are now unrealistic. It is to be hoped that before long the traditional departmental division between physics and chemistry, for instance, will be abandoned in our universities. I believe this change should be recommended now on the graduate level. The terms "physical chemistry" and "chemical physics" are not semantic innovations; they are designations necessitated by the emerging facts. The facts, and the interdependence they reveal, are not new: The new element is our recognition of how important they are to our future.

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