COMMENTS ON HARDWARE DEVELOPMENTS IN CHEMISTRY

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The subject matter placed under the broad heading of Computers in Chemical Education can be separated into two categories. The first, and probably more important to this readership, is the subject of "Teaching Chemistry Better by Using Computers", and the second is the subject of "Teaching Better Chemists About Using Computers". The former often relates to lower level students, and the latter topic is nearly always reserved for upper level or graduate students. Some observations about trends in computer use in chemistry may well be useful.

First, a few comments about the computers being used in chemical laboratories: these comments are based on the instrument show at the 1984 Pittsburgh Conference. On the floor there were many companies using personal computers as the controller for their instruments. On the other hand, there were computers being designed expressly for the laboratory/professional user.

In the former category, I was impressed by the extent to which Apple and IBM PC computers dominated: typically used in chromatography to control pumps and massage data. Other personal computers on the floor included a few S-100/CP-M machines and some more sophisticated applications using DEC machines. Unfortunately, although the term "user-friendly" was often bandied about, there was a conspicuous absence of that quality: non-descriptive menus, poor error recovery, cumbersome command sequences, and a lot of "it can't be done" explanations. Few instrumentation houses have caught up with the quality of WordStar and similar packages.

What about the newer computers? Although 16-bit personal computers have gone the 8086/8088 route, scientific computer companies, Hewlett-Packard, Perkin-Elmer, Instrumentation Laboratories, and IBM Instruments, are all using the Motorola 68000. (One small company did point out, and correctly so, that their 8086 computer with an 8087 co-processor was the most powerful micro on the floor.) Software for all of these machines is somewhat slow in developing. In any case, commitment has been made to the 68000 for scientific computers, and this should hold up as Motorola produces support chips.

The previous two paragraphs probably have little relevance for applications akin to CAI in the freshman lab. Here other factors dominate: software availability, cost, and capability for communication with an operator/student. (Note that software comes first; unless we want to study about computers or indulge in specialized activities, a useful procedure is to select the software and then purchase a computer on which to run it.) The development of networks and the "mouse" will have significant impact on lower level applications.

In the teaching environment, networks will bring back the advantages of the time-shared computer without its disadvantages. Picture a room filled with 20 inexpensive Commodore 64's (computer and color monitor for less than $500 each). A relatively simple network, with a central 64 with fast hard disk, could load programs into the sattelite computers as fast as local floppies could, but also could maintain log of computer use and store results from student sessions. At $50 per machine for interfacing and about $4000 for the hub, the total drops to well under $1000 per machine.

Operator/computer interactions found in most systems is awkward. The question should be asked, how do we make the computer more "user-friendly"? One way is to improve the method of interaction: reduce the use of the keyboard and replace it with a light-pen or, better yet, a mouse. The mouse, first developed for the Xerox Star, is getting more press in its application in the Apple Lisa and Macintosh. It is a hand-held device which is used to control a cursor position by rolling it about on a table surface. The skill develops very naturally. The result is that the operator, whether secretary or student, readily interacts directly with the information; the computer facilitates rather than complicates this process. And that means more education takes place.

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