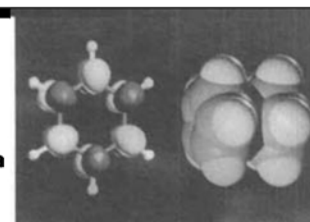


# COMPUTATIONAL CHEMISTRY COLUMN

Column Editors:  
Prof. Dr. J. Weber, University of Geneva  
PD Dr. H. Huber, University of Basel  
Dr. H. P. Weber, Sandoz AG, Basel



Chimia 45 (1991) 165-167  
© Schweiz. Chemiker-Verband; ISSN 0009-4293

## Computers in Chemistry Teaching

Computers have been used in chemistry teaching for about two decades now. Though this might seem to be a rather long period of time, we are of the opinion that the computer is still a new tool in chemistry teaching and we would like to explain why we make this contradictory statement.

In the early seventies, the only computer hardware available were mainframes and there were no personal computers (PCs). Therefore, the first computational exercises for students were at the university level where they were introduced to programming and given access to mainframes. A limited number of students took advantage of this opportunity and the situation was well away from a general use of computers in chemistry teaching. In the late seventies, the first desk computers became available, but the prices were such that at best one computer was available for a class, making it only possible to give demonstrations or to let some students work with it in a laboratory course or in their spare time. The possibility of video reproduction of computer images for demonstrations in a lecture was still very expensive and has become available in most places only in the last few years. The same is true for full classroom facilities which enable all the students in a class to do exercises on the computer. However, we are aware that these facilities are still not available in many schools and it will take a few years to reach this level. There is still a last step which is partly missing in the development of computing in teaching due to hardware availability: the possibility to integrate the computer in all kinds of exercises with the assumption that the student has his own computer at home. We think that this is a necessary step because computer exercises can often only be solved in an efficient way when the student is really familiar with the basics of computing. This is only possible if he or she has the opportunity to 'play' with it at any time. In summary, over the past twenty years the hardware used in computer-assisted chemistry teaching has evolved from

a very limited access, if any, to mainframes, to the availability of a PC (with practically the same computer power) to virtually every student.

A similar development took place in software. Whereas two decades ago everything had to be done from scratch, *i.e.* the only software available were the operating system and a compiler, complete packages of applications became available together with the desk computer. However, only in recent years have these packages become abundant and specific enough that suitable applications for chemistry teaching can be found. A major step towards a user-friendly machine was the introduction of graphical interfaces on most personal computers. Nevertheless, the compatibility of different products is a goal which still seems to be out of reach.

What is the present situation in the use of the computer in chemistry teaching in Swit-

zerland? Many teachers at all levels are using the computer in school, but we cannot speak yet of a 'computer-culture' growing out of all these efforts. Innovative teachers are lonely wolves rather than howling with the pack. In contrast to the situation for purchase of hardware (at least in some cantons), there is hardly any money available for projects in software production, evaluation, purchase and coordination. Some of the few commercial publishers are already leaving the business, as it is not profitable. Teachers who use their own software are hardly willing to make it available to others in an adequate form (debugged programs, manuals *etc.*), as this would often mean substantial additional work for which they would obtain little credit. Nevertheless, we know of some efforts in this direction. For trade and technical schools there is a federal center for information and documentation set up by the SFIB/CTIE/CTII [1]. At the universi-

### The CAT-Group of the Swiss Committee of Chemistry

For about three years, there has existed a subgroup of the *Kommission für Unterrichtsfragen/Commission pour l'Enseignement* of the Swiss Committee of Chemistry for computer assisted teaching (CAT). The first goal of this group was to create contacts among the staff of different universities and Federal Institutes of Technology who use the computer in teaching. For that purpose, we met about twice a year for the exchange of information and programs. A further activity was to establish a catalogue of software (mainly freeware produced by our members). A first draft is available (contact Dr. E. Forte, LEAO, Département d'Informatique, EPFL-Ecublens (CO), 1015 Lausanne, Tel. 021/693 47 55), but improvements are necessary.

Two years ago, we organised a small workshop at the fall meeting of the *Swiss Chemical Society* in Berne, presenting programs (similar to a poster session) on personal computers. Our next activity will be another such workshop at the fall meeting this year. We would be glad to welcome further people who would like to be active in this subject, including people from technical schools or high schools. Our next meeting will be held on June 12th in Berne. If you are interested contact us through: H. Huber, Institut für Physikalische Chemie, Klingelbergstr. 80, 4056 Basel, Telefon 267 38 30, EM: huber@urz.unibas.ch.

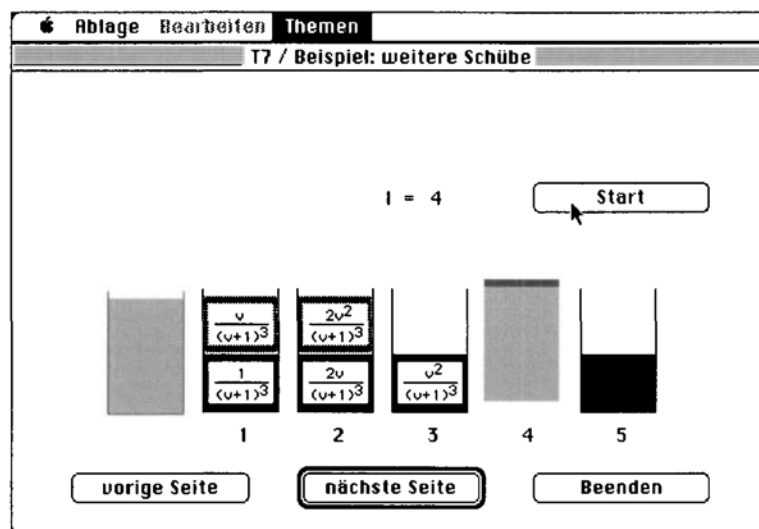


Fig. 1

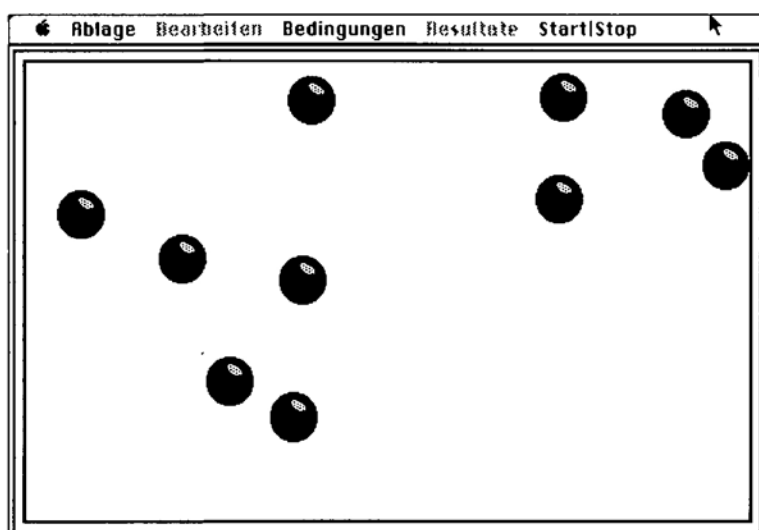


Fig. 2

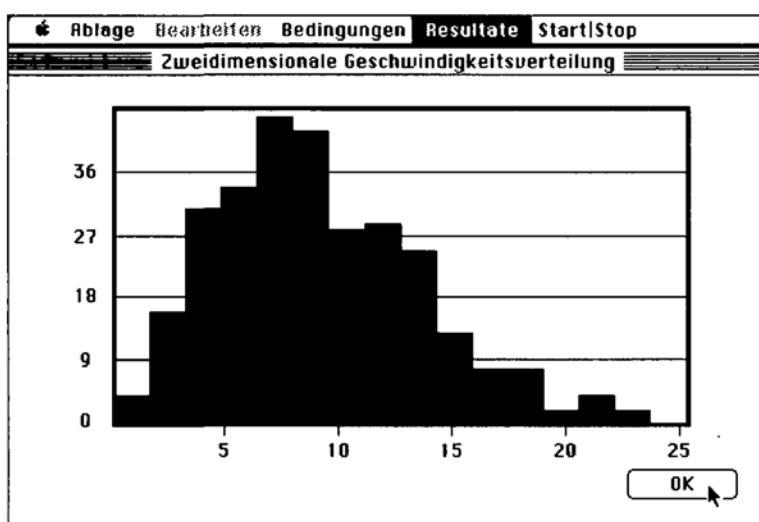


Fig. 3

teaching. The programs we used (on *Macintosh* computers; for a sample disk, see box) can be put into three different categories:

### Tutorials

We used several tutorials in fields which were treated very briefly in the lectures. The students were supposed to work through the tutorials to gain additional information, to repeat the subject at their own speed and to do some exercises to check their understanding of the subject. The programs have a simple structure which is similar to a book (mainly following the guidelines given by [3]). In addition to the standard menus used in most *Macintosh* programs, there is a menu containing the chapters of the book. Selecting a chapter results in the first page of that chapter being displayed on the screen. Each page has (at least) three buttons, which allow the user to go back to the previous page, to go to the next page or to quit the chapter (see Fig. 1 for an example from a program about the counter-current distribution). Some pages contain text only or text and graphics, others may contain animations, simulations or questions with answer buttons.

Our impression of these programs is that they are of limited value (although we did not make a scientific investigation of their use). It is usually not easy to read and assimilate a text from a computer screen, in a noisy room with many other students. This situation might change to some extent if all the students have their own computer at home. Even so, it is probably better to teach the theory in the traditional way and to restrict programs to animations and simulations which help in gaining understanding of concepts that cannot be given on paper.

### Simulations

In our opinion, computers are much better suited for simulations. We use several simulations of molecular dynamics as well as *Monte Carlo* type. Fig. 2 shows a screen produced by a program which simulates the ideal gas. Without going into the details of the program, it is possible to explain to the students the physics on which it is based, e.g. what the program has to do if a ball hits a wall. With many simulations using different conditions (e.g. varying the volume, the energy etc.) one can show that this gas behaves according to the ideal gas law. For such exercises, we usually arrange the students in large groups where each student has to do one simulation. In addition, one can learn about the *Maxwell-Boltzmann* distribution from a histogram produced by the simulation (Fig. 3). Parallel to these exercises we derive the ideal gas law in the 'classical' way by integration as in most text-books. An interesting observation is that many students are not willing to accept the results of the

ty level, some effort was made by the Federal Institutes of Technology. The IDA [2] (Informatik dient allen) project at the ETH Zürich and related initiatives produced several brochures and programs which are also very helpful for chemistry teaching. The CAT-group of the Swiss Committee of Chemistry is trying to improve the situation

by giving a platform to interested people (see box). Other activities, which we have not heard about, are probably under way. We would be glad to obtain information about such activities from our readers and to report them in a later column.

We would now like to present some of our experiences in using the computer in

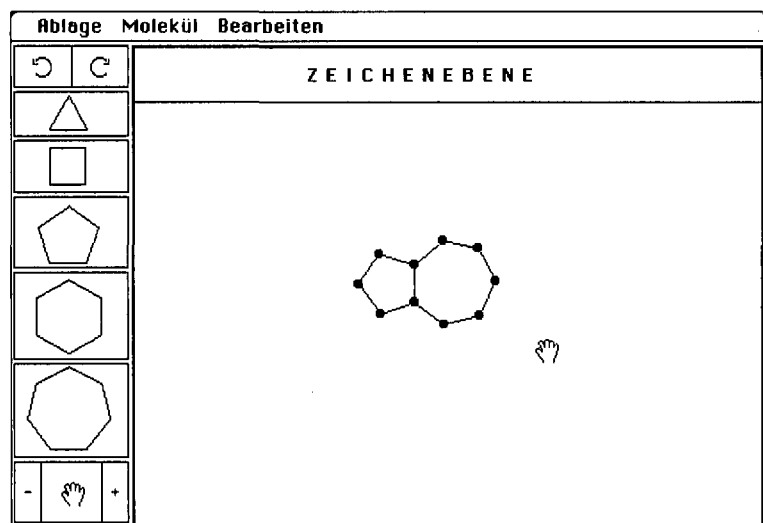


Fig. 4

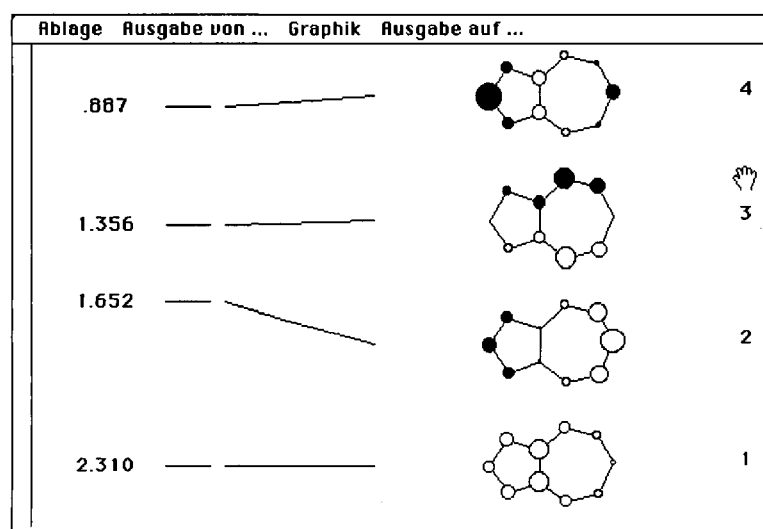


Fig. 5

simulations as a proof of equal validity as the classical method. This gives a good opportunity to stress the assumptions in both cases (which results in the surprising conclusion that usually in the classical model, one more assumption is made, namely the step from particles, *i.e.* discontinuity, to the continuum, which allows replacement of the summations by integration).

Although it is difficult to give a final rating on simulations in the classroom, we think that they are very useful in several aspects. They may help the student to visualize processes which otherwise remain abstract equations on the blackboard. This is especially valid for many microscopic processes which are usually the basis of macroscopic chemical properties. Furthermore, they are very valuable for showing the students different models or theories and to provoke discussions about the way sciences work. Last but not least, we are convinced that the era of classical theories yielding simple algebraic equations is coming to an end and that we now have to accept simulations as an equally valid description of nature. In research they are usually performed on mainframes or supercomputers without graphical representation, whereas in the classroom

visualization is an important additional feature.

### Research Tools

The last aspect of the previous paragraph brings us to a third group of programs. Today computers are used in several fields of chemical research. Therefore, the students in schools (which prepare for a profession in chemistry (technical schools like Gewerbeschulen, HTL's, universities) have to learn how to manipulate 'these machines' just as they have to be able to work on spectrometers, for example. Various tools are associated with the computer *e.g.* data banks, molecular mechanics and modelling, synthesis planning, chemometrics, quantum chemical calculations. We use several programs for molecular mechanics and quantum chemistry, one of the oldest, the *Hückel Molecular Orbital* program (Fig. 4), has already been in use for about 5 years. A good graphical interface is much appreciated by the students and usually helps to reduce to a minimum the time needed to introduce the program. The HMO-program allows a graphical input (Fig. 4) as well as a graphic repre-

### A Sample Diskette

A sample diskette for *Macintosh*-Computers is available containing the following programs (in German):

- Tutorials
  - Statistik I (answers basic questions like what is a population, sample, mean, standard deviation, distribution (binomial-, normal-), histogram)
  - Potentialkurven (gives an introduction into potential curves; the parameters of the curves (*e.g.* Morse-, Lennard Jones-, Torsion-Potentials) can be changed interactively, which replaces a mathematical discussion of the curves)
  - Verteilung (gives an introduction to the counter-current distribution, derives the equation and allows a simulation with different distribution coefficients for a two compound mixture)
- Simulation
  - Gas (molecular dynamic simulation of a hard sphere gas)
- Tools
  - HMO (a *Hückel Molecular Orbital* program with a fully graphical user interface)

The programs may be freely distributed, however, we ask for a handling fee of Fr.20.- if you want to obtain the diskette from us: H. Huber, Institut für Physikalische Chemie, Klingelbergstr. 80, CH-4056 Basel, Tel. 061/267 38 30, EM: huber@urz.unibas.ch.

sentation of the results (Fig. 5). A further advantage of graphical results in qualitative (or semi-quantitative) methods like HMO is that the numerical accuracy of the data is not overrated.

Experience shows that the students find most interest in this group of programs. We and other authors (see *e.g.* the program MoMo, reviewed in our last column) have observed that such programs are soon used in research by graduate students who became familiar with them in their undergraduate lectures one or two years earlier.

- [1] SFIB (Schweizerische Fachstelle für Informationstechnologien im Bildungswesen / Centre suisse des technologies de l'information dans l'enseignement / Centro svizzero per le tecnologie dell'informazione nell'insegnamento), Erlachstr. 21, CH-3000 Bern 9 (Tel. 031/23 08 31; COMNET: Net1:SFIB).
- [2] Projekt-Zentrum IDA, ETH-Zentrum, CH-8092 Zürich.  
Several programs and reports of interest to teachers in chemistry are available (for a formal fee for handling), among them the 'Dialog Machine', a package of modules which helps authors to make programs and to port them to different hardware, 'ModelWorks' an interactive simulation environment for personal computers and workstations based on the Dialog Machine (by A. Fischlin *et al.* of the Systems Ecology Group of the ETH) and a survey about interfacing computers for data acquisition (H. Domeisen, 'Laborautomation mit Personal Computern', 2. überarbeitete Aufl., Jan. 1991).
- [3] A. Ventura, H. Goorhuis, 'Unterrichtsprogramme für die Informatik-Ausbildung', Institut für Informatik, ETH Zürich, 1987; A. Ventura, W. Schaufelberger, 'Die Notwendigkeit von Benutzermodellen beim Entwurf von Programmen und Geräten', Projekt-Zentrum IDA, ETH Zürich, 1988.