

## Computer Aids in Chemistry

The above was the title of the Analytical Division Symposium at the RSC Autumn Meeting. The following are summaries of six of the papers presented at the Symposium, which was held at the University of Swansea on September 20th–22nd, 1983.

### Trends in Laboratory Instruments with Microcomputers

M. Hewins

*Pye Unicam Ltd., York Street, Cambridge, CB1 2PX*

The major change made in laboratory instruments in the last decade has been the incorporation of microprocessors, giving new facilities for control and operation. Typically these give: more printed results and experimental details; more information about the instrument; less staying with the instrument to change valves or temperature at set times; and the possibility of making several measurements of, for example, wavelength simultaneously. It is in these control facilities that major developments are occurring and will continue for some time to come.

During the last 10 years users and manufacturers have been exploring the benefits and limitations of microcomputing and identifying the optimum mix of facilities. The importance of this can be appreciated if you turn to 1905 and the infant motor car industry. Mass production was unknown but hundreds of small "garage shops" were making cars. Most had four wheels, but the similarities stopped there: some had steering wheels, some tillers; some had hand-brakes on the right, foot-brakes on the left; some had fixed throttles, others had dashboard throttles. The design elements were present but no combination had emerged that was suitable for the average person. Laboratory instruments are in the same position today, with the design elements present but no stabilised architecture linking them. This talk looks at the design elements and their stabilisation.

#### Changes so Far

Elements have emerged in the last decade in increasing numbers and complexity as computing power increases. Integrators, which have halved in cost in the last decade, have increased several-fold in capability, providing a group of elements that is going to become important for the control of instruments. Early integrators gave area counts only, but now they detect a peak automatically, look for base lines and separate small peaks from the shoulders of big peaks; an example of this type is the Philips CDP1. Later integrators have added further elements to the list with statistical calculations, storage of data, alternative methods of peak area measurements, etc.

Data processing (DP) provided the first group of design elements but the major role of the microprocessor is in direct instrument control. Things began simply with, for instance, a solvent programmer, produced during the late 1970s, which used a processor to control the switching period of a valve admitting varying proportions of two solvents to a liquid chromatography pump. This simple function has now become a small part of the PU-4002 pumping system, which controls the pump motor, balances out fluctuations in pumping rates and solvent mixes due to pressure, compensates for solvent compressibility, provides safety cut outs and many other features. It is a typical example of the way in which more and more complex functions are being put under processor control to self-correct changes.

In other control applications, such as the Philips Series 304 chromatograph, the processor has replaced functions previously carried out in hardware. Here, three ovens have different requirements and each has a different degree of control and accuracy, typically  $\pm 0.5\%$ . The ovens cool or warm as appropriate, and control calculations are performed once in every second. In this manner, very precise control of the ovens can be achieved at accurate temperatures and for very accurate analyses.

#### Today

Where are we now in facilities for instrument control? Most of the elements identified carry out existing tasks in new ways, giving a more reliable instrument or a less expensive product. The major developments are not here, however, but in facilities that give more control than was previously possible, allowing tasks to be performed more reliably and efficiently. The CDP1 integrator saved the time of writing down the results by printing them. Later integrators draw the chromatographic trace and label the peaks. The pumps and chromatographs are not quite so clever but give error messages, failure warnings, etc. These design elements are here to stay and new ones are appearing.

# Computer Aids To Chemistry

**L Darling-Hammond**



## **Computer Aids To Chemistry:**

*Computer Aids to Chemistry* Gaston Vernin, Michel Chanon, 1986      *Computers in Chemical Education and Research* E. Ludena, 2013-03-09 The impact of computers on all realms of Chemistry has been one of the most important factors in the development of this science during the last years In recognition of this fact in 1971 the First International Conference on Computers in Chemical Research and Education was held at DeKalb Illinois USA A second Conference took place in Ljubljana Yugoslavia in 1973 and this third Conference in Caracas Venezuela in 1976 The aim of these conferences was to provide a high level forum for the leading researchers to exchange information at the frontiers of present day computer applications to the different fields of Chemistry The present Third International Conference on Computers in Chemical Research Education and Technology whose proceedings are published in the present volume was conceived by means of a series of invited lectures as a survey of the present state of the art in some of the most relevant areas of computer applications in Chemistry      Expert Systems and Computer Aids to Decision-making, 1970-1986 Karl Schneider, 1987      **A Guide to Undergraduate Science Course and Laboratory Improvements** National Science Foundation (U.S.). Directorate for Science Education, 1979      **Resources in Education** ,1977      Wood and Cellulosics John F. Kennedy, Glyn O. Phillips, Peter A. Williams, 1987      The Education Index ,1987      Modelling of Structure and Properties of Molecules Zvonimir B. Maksić, 1987      Chemical Research Faculties ,1988      **Industrial Research Laboratories of the United States** Jacques Cattell press, 1983      **Scientific and Technical Organizations and Agencies Directory** ,1985      An Introductory Guide to EC Competition Law and Practice Valentine Korah, 1994      *Forbes* ,1992      **Annual Reports on the Progress of Chemistry** ,1993      Computer Aids in Chemistry ,1984      **East Europe (Albania, Bulgaria, Czechoslovakia, East Germany, Hungary, Poland, Rumania, Yugoslavia)** ,1967      Illinois Technograph ,1961      **The Federal Employee** ,1920      *British Education Index* ,1985      **Index of Conference Proceedings** ,1994

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