

Report of Discussion Group 1
Use of Computers in the Undergraduate Chemistry Curriculum

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This discussion group was well attended and many interesting and valuable problems were discussed. Some general observations of the discussion indicate that no universal method of involving students with the computer has evolved. Of course, all institutions represented in the group did not have a computer available. Some institutions had rather extensive curricula in which students were involved in computer programming, in other cases the students with a minimum of instructions used existing programs to obtain data and/or solutions to particular problems. With respect to Chemistry Departments in particular, some institutions required all majors to have the experience of work with the computer and in other cases only certain advanced students on particular research problems were involved in the use of the computer.

It was generally agreed that the use of the computer could be a meaningful experience for the student and that more involvement was necessary. One of the problems which came out in the discussion was the need for more examples where the use of the computer was required. Simple problems may be necessary for an introduction but ~~more~~ meaningful problems were necessary to point out the real value of using a computer. Whenever an example is chosen, the most rigorous or exact equation should be used and not one that involves simplifying assumptions. Programs which are used, whether written by the student or not, should be capable of taking the data in the neatest possible form -- that is, just as it is obtained from the experiment with out any prior processing.

There are many available books on the market with published programs. However, it was generally agreed by those with experience on the use of the computer that an individual was generally better off to write his own program, to use his individual logic, and to have the output in a form of his own choosing.

Below ^{is} ~~are~~ a listing of some problems which were discussed.

1. Acid-base titrations as function of equilibrium constants, concentration and other variables.
2. Polarographic equations to include viscosity for non-aqueous solvents.
3. Adiabatic flame temperatures.
4. Spectrophotometric data for mixed complexes.
5. Fitting data to involved conductance equations.
6. Least-square treatment of data.
7. Calculation of geometric parameters for various molecules.
8. Solution by trial and error of kinetic measurements.
9. Matrix operations and calculations
10. Calculations of p-orbitals which include the radial function.