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## An Interactive On-Line Computing System as an Instructional Aid

**D**uring the past year we have been engaged in an experimental program to evaluate the effectiveness of the University of California at Santa Barbara's on-line computing system as an aid to instruction in chemistry. The system which will be described in more detail below is served by an IBM 360/75 computer to which are connected some forty or fifty consoles located both on and off the campus.

The basic philosophy which has guided the development of the on-line system has been to provide the user with a computing capability which enables him to carry out sophisticated mathematical operations in the area of classical mathematical analysis in a convenient and natural way. In addition, the programming language has been structured so that the user need not concern himself with the programming details associated with conventional languages such as Fortran. As a result, the user is able to achieve a high level of interaction with the computer in a real time sense which in turn often allows him to learn from the problem solving process itself. A second aspect of the use of the computer this way is that it allows one to develop solutions to problems directly from fundamental theory without resorting to lengthy and often tedious algebraic development. In many instances, too, models used to represent real systems can be made more realistic. This high level of human-computer interaction inherent in the system along with its ability to conveniently handle the various fundamental mathematical operations which occur in many areas of the physical sciences led us to initiate a program to explore its use in conjunction with our junior level physical chemistry course. Due to the experimental nature of the project, participation was voluntary and consequently involved only nine of the fifty or so students enrolled in the regular course. These nine students attended the regularly scheduled lectures and were responsible for almost all of the regularly assigned work; in addition, they were given extra problems that for the most part could only be solved using the on-line system. Along with this extra work, they attended informal weekly meetings where special topics and techniques were discussed.

Since the on-line system is particularly useful as the basis for a mathematical laboratory, that was the approach that was taken; the students were given prob-

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<sup>1</sup> KARPLUS, WALTER J. (*Editor*), "On Line Computing," McGraw-Hill Book Co., New York, 1968, pp. 131-78, 303-24.

<sup>2</sup> The basic interface was built by the Data Equipment Division of Bolt, Baranek and Newman, Inc., 15808 Wyandotte Street, Van Nuys, California.

lems to solve which required them to devise the mode of solution and in so doing they discovered properties of model chemical systems which they otherwise would not have seen. To assist them, however, we did provide them with a set of worked problems illustrating the use of the system along with a set of subroutines for carrying out basic mathematical operations such as integration, differentiation, solution of differential equations, and least-squares data fitting. Some examples of the use of this material are discussed in a later section of this paper.

### The On-Line System

The U.C.S.B. on-line computing system was developed over a period of years by Professor Glen J. Culler of this campus and by Professor Burton D. Fried of the Los Angeles Campus of the University of California.<sup>1</sup> The basic hardware configuration consists of an IBM 360/75 with disk storage, two million bytes of bulk core, a specially designed communications interface which handles input and output to the user consoles,<sup>2</sup> along with the usual input/output devices such as printers and card readers. The basic software system is structured to allow normal batch processing to occur in the background simultaneously with on-line usage.

The on-line user communicates with the central computer via a console having an operator-operand keyboard for input and a storage oscilloscope for output. A photograph of a console is shown in Figure 1. The

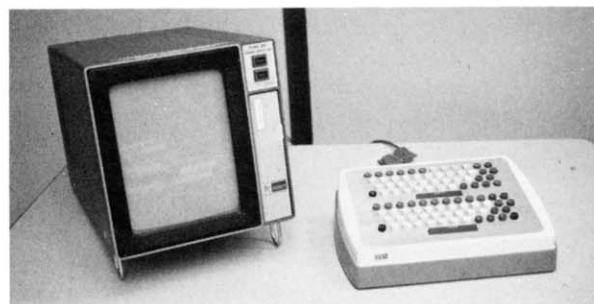


Figure 1. The on-line console with display scope and keyboard.

keyboard as shown in Figure 2 is divided into two sections; the upper consists of buttons for carrying out basic mathematical and program operations. The lower half consists of buttons which act as storage locations for data and as such represent operands. In addition, the lower half has provision for specifying numerical constants and for program punctuation. The operands may be either single numbers or they may be lists of numbers or vectors up to 124 points

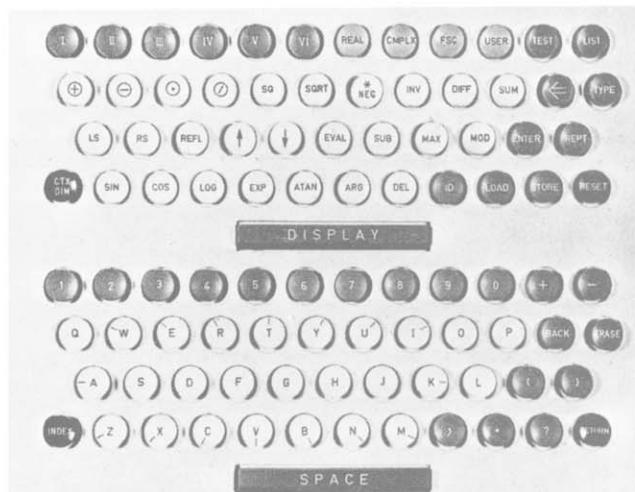


Figure 2. A detailed view of the keyboard showing the layout of the buttons.

long and hence they enable the convenient representation of functions. Some of the buttons deserve special mention. The DISPLAY key controls the output from the computer which may either be in graphical or in alphabetic form. The LIST button enables the user to specify an entire sequence of button pushes and thus create programs. TEST allows for program branching. ENTER provides for the switching between program and manual mode so as to allow data to be entered at run time, for example, or to return the control of a problem solving process to the user. The definition of the independent variables of a problem is accomplished through the use of the ID key. Pushing ID causes the computer to generate a vector of equally spaced values running over the range of  $-1$  to  $+1$ . As an example of its use, suppose one wished to calculate and display the volume of one mole of an ideal gas at  $0^\circ\text{C}$  over the pressure range of  $1$ – $10$  atm; i.e.,  $V = RT/P$  with  $R = 0.0821$ ,  $T = 273.16$ , and  $1 \leq P \leq 10$ . The following button sequence would accomplish this objective

ID (+) 1 (/) 2 (-) 9 (+) 1

Taking the operations in order, ID generates a vector running from  $-1$  to  $+1$ ;  $(+)$  1 adds 1 to every point and hence the vector now runs 0 to 2;  $(/)$  2 halves each value so that the vector is now defined between 0 and 1;  $(-)$  9 causes the vector to run between 0 and 9; and finally  $(+)$  1 gives the desired result which is a vector running between 1 and 10 thus giving a representation of the pressure over the range of interest. The remaining sequence calculates the volume by inverting the pressure vector and multiplying by the values of  $R$  and  $T$ ; i.e.,

INV (-) 0.0821 (-) 273.16

The display of the result is carried out by pushing

DISPLAY RETURN

It should be added that the calculation determined by the above button sequence is carried out in real time so that the user sees the result of his calculation instantaneously. The numerical values corresponding to the individual points can be displayed by the sequence

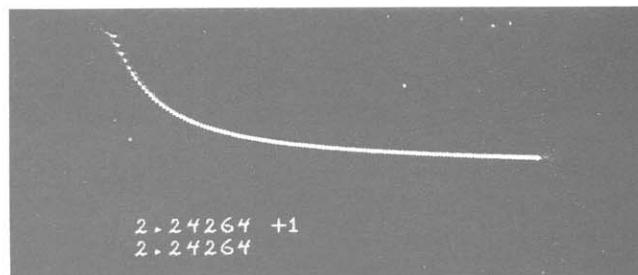


Figure 3. An example of the graphical and numeric output from the computer. The curve is the volume of an ideal gas for  $T = 273.16^\circ\text{K}$  and  $1 \leq P \leq 10$  atm. The two numeric values are the volume at  $P = 1$  and  $P = 10$  atm.

#### DISPLAY n RETURN

where  $n$  is an integer equal to or greater than 1 but not exceeding the total number of points making up the vector. Figure 3 shows the result of the above calculation along with the numerical values of the first and last points corresponding to  $P = 1$  and  $P = 10$ .

#### System Use and Applications

In thermodynamics one deals with a large number of problems involving integration and differentiation and consequently these may be handled very conveniently on the on-line system. However, in many instances the procedure for solving the problem may be quite different from the way one would do it without the computer. For example, the entropy change associated with a change in pressure of a gas can be calculated from the equation

$$\left(\frac{\partial S}{\partial P}\right)_T = - \left(\frac{\partial V}{\partial T}\right)_P$$

To evaluate  $\Delta S$  one would normally write the volume as a function of pressure and temperature, carry out algebraically the differentiation with respect to temperature treating the pressure as a constant and finally integrate the resulting expression.  $\Delta S$  would then be evaluated from the algebraic expression for the integral. Except for the simplest equations of state, the above process is difficult and tedious, and often the thermodynamics are obscured by the mathematics. To do the same problem on the on-line system, it is only necessary to set up an array of numbers representing the volume as a function of temperature and pressure over the ranges of interest. If this is done so that each column represents the volume as a function of temperature at a particular pressure and so that each row represents the volume as a function of pressure at a particular temperature, then it is only necessary to numerically differentiate down the columns to obtain an array representing  $(\partial V/\partial T)_P$ . Integration, again numerically, across the rows then yields the desired result. Note that there is no algebraic development and also that the result is obtained directly from basic theory. Figure 4 shows as a surface such an array representing  $(\partial V/\partial T)_P$  for *n*-pentane with  $1 \leq p \leq 10$  atm and  $50 \leq T \leq 250^\circ\text{K}$  obtained using the Van der Waals equation of state.

For the less mathematically sophisticated students, a number of programs of a more or less auto-tutorial type were devised. For example, one program was written to illustrate the relationship between the value of an equilibrium constant and the rates of the reactions

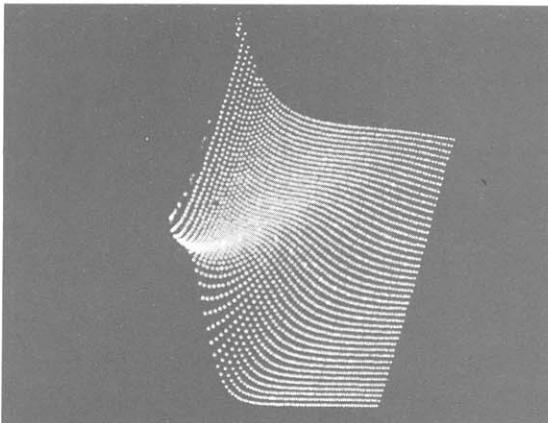


Figure 4. The surface representing  $(\partial V / \partial T)_p$  for *n*-pentane over the ranges  $1 \leq P \leq 10$  atm and  $50 \leq T \leq 250^\circ\text{K}$ . The coordinate system is a standard right-handed one with  $P$  increasing along the positive  $y$  axis,  $T$  increasing along the negative  $x$  axis, and volume along the positive  $z$  axis.

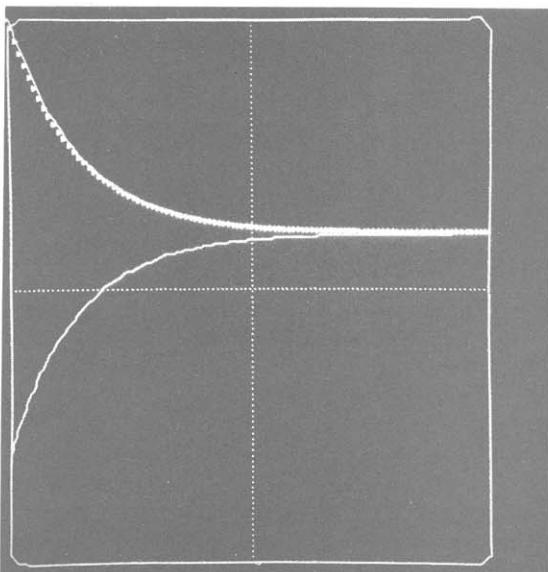


Figure 5. A display of the concentration of A and B as a function of time for the  $A \xrightleftharpoons[k_2]{k_1} B$  system. The lower curve is  $A(t)$  and the upper is  $B(t)$ .  $A(0) = 1$  and  $B(0) = 4$  with  $k_1 = k_2 = 0.035$ .

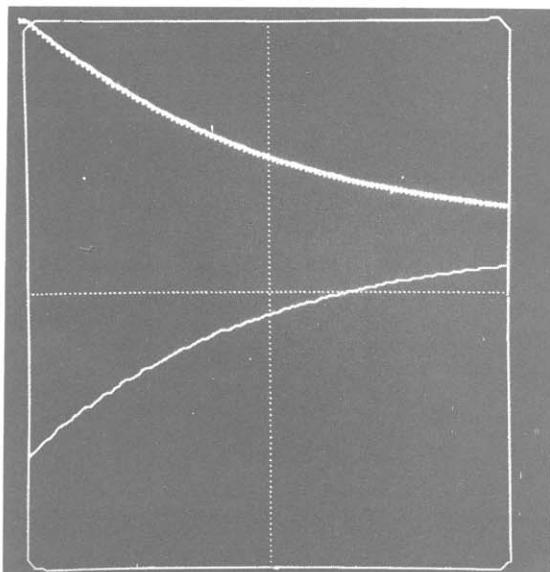


Figure 6. The same as Figure 5 but with  $k_1 = k_2 = 0.010$ .

which make up the system. The example that was used involved the simple reaction



The computer was programmed to accept the initial concentrations of A and B and the two rate constants  $k_1$  and  $k_2$ . The program then computed and displayed the concentrations of A and B as a function of time. In a write-up that went along with the exercise, the student was asked to explore the effect of different initial concentrations and different values of the two rate constants. Figures 5 and 6 are examples of the output from the program showing the concentrations of A and B as a function of time for two different sets of values for  $k_1$  and  $k_2$ . In both cases  $k_1 = k_2$ ; however, in the first case equilibrium has been achieved, with  $A(\infty) = B(\infty)$ ; in the second, the rate constants are sufficiently small so that equilibrium has not yet occurred.

The on-line system was also used to solve quantum mechanical problems. In this case, however, the students were supplied with a basic subroutine program for solving second-order differential equations based on a Runge-Kutta method. Initially, they obtained the wave functions and eigenvalues by trial and error; that is, they guessed a trial eigenvalue and determined the resulting wave function. The process was repeated with different guesses for the eigenvalue until the wave function which was obtained behaved properly at the boundaries. Figure 7 shows the first and second eigenfunctions for a Morse oscillator determined in this fashion. As soon as they had become familiar with the general properties of the Schrödinger equation, they were able to take advantage of the fact that the vector structure of the system allows the differential equation to be solved for a range of trial energies all at one time. As a consequence, a surface of trial eigenfunctions is generated corresponding to the set of trial eigenvalues. The resultant surface as shown in Figure 8 provides a graphic demonstration of the behavior of the solution with respect to assumed energy. The surface in the figure is for a harmonic oscillator

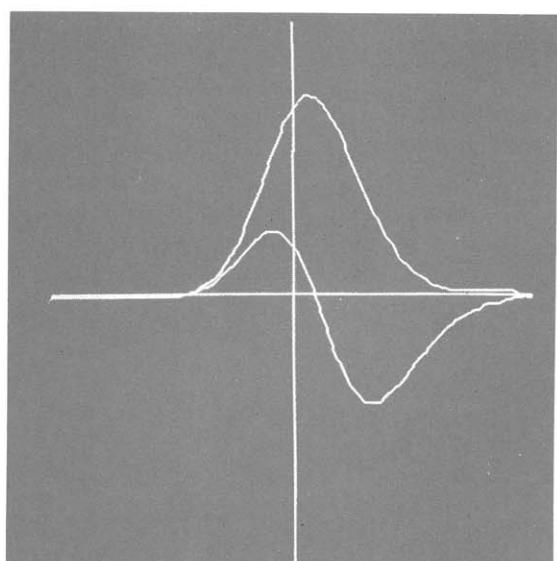


Figure 7. The first and second eigenfunctions for a Morse oscillator.

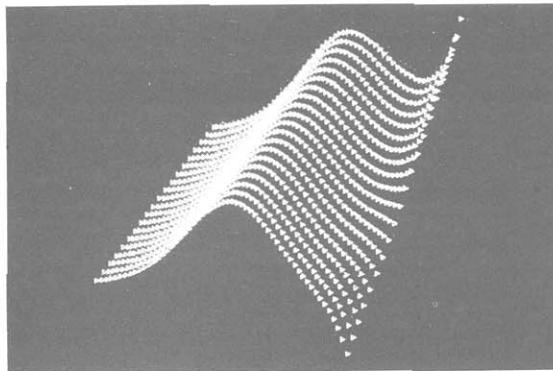


Figure 8. The surface of functions obtained by solving the Schrödinger equation for a harmonic oscillator for a range of trial energies slightly above and below the first eigenvalue.

with the vector of energies ranging from just above to just below the first eigenvalue. This same procedure can be carried out for a range of trial energies greater than that shown in the figure; the curved line in Figure 9 which oscillates negatively and positively about zero is a plot of what is effectively  $\Psi$  at infinity versus trial energy. As can be seen there are four places where it crosses the zero axis indicating that there are four energies within the range of trial eigenvalues which yield acceptable wave functions; that is, those where  $\Psi(\infty) = 0$ . The actual numerical values corresponding to the four eigenfunctions are obtained by applying the DEL operator to the function in the figure; this yields a vector of zeros where the function is non-zero and ones where it is zero. Multiplication of this vector by the vector of energies then "picks out" the energy values of interest; this result is also shown in Figure 9. Although this example was for a harmonic oscillator, the procedure has been used to study a whole class of one dimensional oscillators including the Morse, quartic and double minimum types.

On-line programs have been developed to display theoretical nmr spectra for systems of nuclei in which exchange between different magnetic environments is possible. Both the simple Gutowsky-Holm two-site

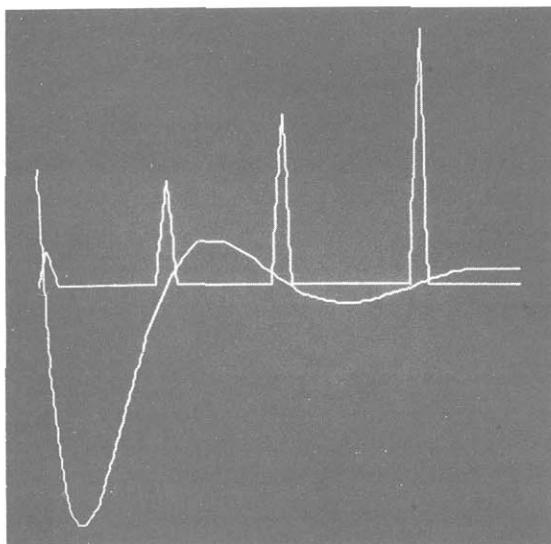


Figure 9. The curved line represents the functional behavior of  $\psi(\infty)$  for a harmonic oscillator over a range of energies which include the first four eigenvalues. The non-zero values of the other function in the figure are these eigenvalues corresponding to the acceptable wave functions where  $\psi(\infty) = 0$ .

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TWO-SITE NMR EXCHANGE.  
WHAT IS LEFT FREQ.? -5  
WHAT IS RIGHT FREQ.? 5  
HOW MANY POINTS? 101  
FREQ. AXIS COMPLETED.  
CHEM. SHIFT AT SITE 1? -5  
CHEM. SHIFT AT SITE 2?
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Figure 10. The prologue to the nmr exchange programs. By a series of such questions the parameters needed to characterize the spectrum are obtained.

exchange process and the interchange of two nuclei in a spin coupled situation have been treated. These programs operate in a conversational mode. A series of questions are displayed on the output screen to which the user replies with information about the width of the spectrum, the chemical shifts, the coupling constants and the like. The beginning of this sequence is illustrated in Figure 10. After receiving the information, the on-line system computes and displays the corresponding nmr spectrum. Figure 11 shows the output for a series of values of the half-life. Options in the program allow the student to adjust the reaction parameters so that he sees immediately the effect of these parameters on the spectrum.

In addition to these examples the on-line system has also been used to study the properties of orthogonal functions and linear transformation theory, titration curves and ionic equilibria, data smoothing, linear and non-linear least squares curve fitting as well as for a variety of other things. Figure 12 shows a Fourier approximation to a square wave summed through the first, fifth, and eleventh terms. The coefficients were calculated by direct numerical integration. Figure 13 demonstrates the use of the system to illustrate the angular dependence of the hydrogen-like atomic orbitals.

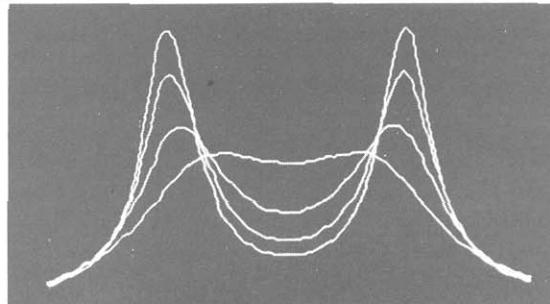


Figure 11. Several superimposed theoretical nmr spectra at different  $\tau$ -values for two-site exchange.

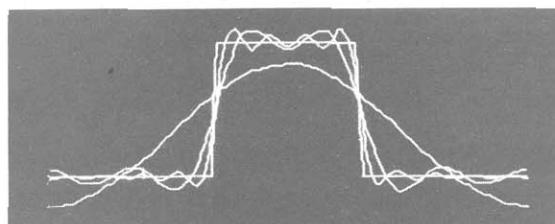


Figure 12. The Fourier approximation to a square wave summed through the first, fifth, and eleventh terms. The coefficients were determined by direct numerical integration.

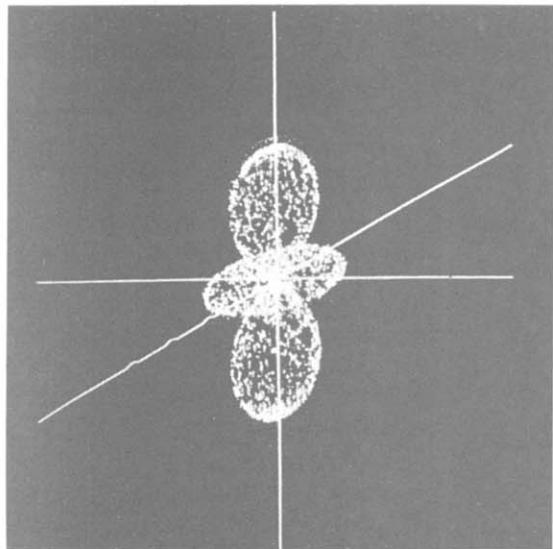


Figure 13. An example of the use of the on-line system to show the angular dependence of the hydrogen like atomic orbitals.

#### Discussion

The above examples illustrate the kinds of things that

can be done with the aid of a computer in an undergraduate chemistry course. We have found that most undergraduates are capable of learning enough of the on-line language to use it to their advantage very quickly. As a consequence, we feel that the program has been quite successful in that it has demonstrated how a computer-oriented approach to instruction can cover a wider range of topics, consider more realistic problems and more general approaches to their solution, and by the use of a mathematical laboratory approach treat each topic in greater depth than would otherwise be possible. An additional benefit which we noticed was that the use of the computer seemed to generate and maintain a higher level of enthusiasm on the part of the student than one normally experiences in the usual teaching situation.

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### SCANREC: A Computer Test Grader, Analyzer, and Record Keeping System

Within the last three years, several computer programs have become available for the scoring of exams and/or the keeping of records.<sup>1</sup>

This program is an expansion of and an addition to the program produced by Pollnow. The input may be partially or totally computer graded, or may be totally hand-graded information. The program is written in Fortran IV for the IBM 1130 computer, equipped with the 1131 disc processor, 1142 card read punch, and the 1132 printer. The program is broken up into the main line program and five subroutines; it will handle 507 tests, and proceeds at a rate of about 12 exams per minute. The program can be readily modified to handle 858 tests, and more extensive use of the disc would expand its usefulness to several thousand.

Nine option switches are employed, one to five of which may be utilized during any one compilation.

One or two answer cards per student can be read. (Up to 140 quintuple choice answers with variable point values.) Two "essay" grades (up to 99 points each) can also be simultaneously assimilated for processing with the computer-graded portions. If you prefer to fully hand-grade tests, up to twelve grades per student can be fed to the computer on a single card.

Only one answer per question is allowed, but second choice answers can be loaded into the correct answer cards for one-half credit.

Under switch option, blank answers may be ignored, and one-fourth of wrong answer values may be subtracted.

Statistics are printed for each question as to the number of times missed, the number of times the second choice answer was missed, or the question had been skipped. All values supplied to the computer for the program's operation are printed in the output.

The computer, unless directed otherwise, will update the students' records, and print out all of the information next to the students' typewritten names, in alphabetical order. Should a student not take an exam, the output is altered so as to keep his old record unchanged, and print the word "ABSENT" in place of the current test grade. If the student used the wrong identification number, the words "NO PAST RECORD" will be printed next to the identification number used, and his current test grade. Records are kept on running totals of both the percentages and T-scores for four categories of grades, *viz.*, quizzes, exams, lab, and final exam.

When the final exam is fed into the computer, the grade categories are averaged, the final grades, both percentage and T-score according to the instructor's stipulated weight basis, and the percentile ranks are computed.

A copy of this program will be supplied upon request.

<sup>1</sup> HINCKLEY, C. C., and LAGOWSKI, J. J., *J. CHEM. EDUC.*, **43**, 575 (1966). MANN JR., J. ADLIN, ZEITLIN, HARRY, and DELFINO, ALLAN B., *J. CHEM. EDUC.*, **44**, 673 (1967). YANEY, N. DOYAL, *J. CHEM. EDUC.*, **44**, 677 (1967). POLLNOW, GILBERT F., *J. CHEM. EDUC.*, **44**, 678 (1967).

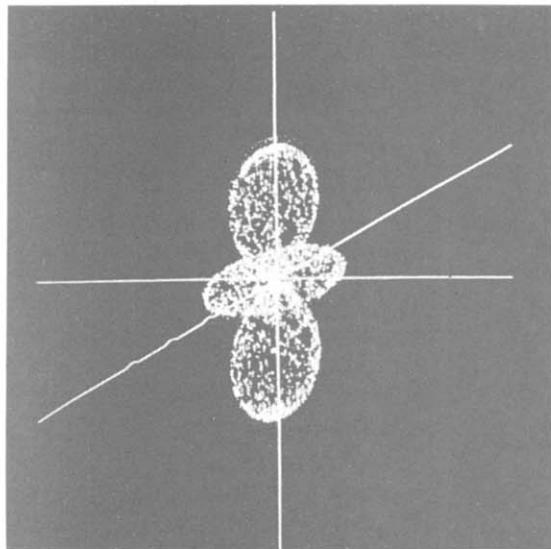


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