

APPLICATIONS OF TECHNOLOGY IN TEACHING CHEMISTRY
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PAPER 1
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THE USE OF COMPUTERS IN A JUNIOR-LEVEL ANALYTICAL CHEMISTRY -
PHYSICAL CHEMISTRY LABORATORY COURSE

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ABSTRACT:

This paper describes how students use computers and computer interfaced instruments in a laboratory course. The experiments and laboratory reports are discussed. The use of word processing, numerical methods, statistical methods, graphing and other software is explained and illustrated.

I. INTRODUCTION

The American Chemical Society's Committee on Professional Training has established guidelines for undergraduate professional education in chemistry (1 - see References in Section VII of this paper). An approved program must include at least 500 hours of laboratory work in chemistry. Some experiments must involve instrumental methods of analysis and experimental physical chemistry. "Laboratory instruction should include practical experience with instrumentation for spectroscopy, separations techniques, electrochemical methods and computerized data acquisition and analysis. . . . It should give students . . . competence to . . . analyze data statistically and assess reliability of results . . . interpret experimental results and draw reasonable conclusions . . . communicate effectively through . . . written reports." (1)

There are many standard textbooks describing the theory and practice of instrumental analysis (2-6) and experimental physical chemistry (7-8). Surveys of and recommendations for the content of instrumental analysis courses have recently been made (1,9-12), and considerable revision of the traditional physical chemistry laboratory course has been proposed (13).

This paper describes an Instrumental Laboratory course (instrumental analysis - physical chemistry) which I have taught to second semester juniors for over twenty years at Clarkson University. During this period of time the experiments, instruments and nature of the experimental reports have changed. In this paper I will describe the course as I last taught it during the spring semester of 1991. In order to place the course in proper perspective, the computing

background of the students and the relevant curriculum will be described in the next two sections of this paper.

II. COMPUTERS AND COMPUTING BACKGROUND OF THE STUDENTS

Since 1983 every entering freshman at Clarkson University has been issued a personal computer. The computer was initially a Zenith Z-100, later a Zenith Z-248, and for the last few years students have been issued an IBM PS/2. The PS/2 computer has 1 megabyte of memory, a 30 megabyte hard disk and a 3 1/2 inch disk drive. MS DOS is the operating system and Word Perfect is currently provided to each student. Appropriate additional software is provided as needed.

In addition, each student receives an instructional access code which permits access to electronic mail, file transfer and printing services on a campus-wide Novell network. The network contains a Software Distribution System which permits students to download software to 3 1/2 (or 5 1/4) inch floppy disks for use on their personal computers. An instructor may supplement these services by granting access to other computing systems which contain specialized services and facilities.

All undergraduates are required to take a three credit introductory computer course as first semester freshmen. This course emphasizes programming and the use of applications software. Beginning in the early 1970's and for many years, I taught the course to chemistry majors on a PDP-8 which belonged to the Chemistry Department and an IBM main frame. In the early days there was not a great deal of applications software available and an introduction to programming in BASIC and FORTRAN was provided. The students were asked to write t-test, linear least squares and other programs they later used in their laboratory courses. Presently, our chemistry students learn to use Word Perfect and Quattro or Lotus-1,2,3 in the introductory course.

I have distributed some CAI, plotting, numerical and statistical analysis software to my students in general and analytical chemist via the Software Distribution System. Another faculty member has helped developed some molecular modelling software which is used in organic chemistry. One faculty member is using Hyperchem in his organic course using a Departmental computer.

There are terminal rooms connected to the network distributed around campus and several computers available in the chemistry laboratories.

III. CHEMISTRY COURSES TAKEN BY CHEMISTRY MAJORS

Chemistry majors learn to perform some gravimetric and volumetric analysis in the freshman chemistry laboratory course and subsequent courses. As first semester sophomores a three credit lecture course in Spectroscopy and a three credit Spectroscopy Laboratory course are required. These courses cover atomic emission and absorption

spectroscopy, fluorescence, visible-ultraviolet, infrared and mass spectroscopy and nuclear magnetic resonance. Some of the spectroscopic techniques are used in the three credit organic chemistry laboratory courses which are taken in the second semester of the sophomore year and the first semester of the junior year. The organic chemistry lecture course is taken during both semesters of the sophomore year. In the first semester of the junior year chemistry majors take two three credit lecture courses - Separations, Radiochemistry and Electrochemistry; and the first semester of Physical Chemistry. The second semester Instrumental Laboratory course is designed to illustrate principles and provide practice in techniques considered in the two first semester courses and in second semester Physical Chemistry (taken concurrently with Instrumental Laboratory).

IV. LABORATORY ORIENTATION LECTURES AND ASSIGNMENT

Instrumental Laboratory has two three-hour laboratory meetings each week. The first three laboratory sessions were used for laboratory orientation lectures.

A. First Laboratory Orientation Session

During the first session the experimental report, errors and the use of statistical and numerical methods computer programs were discussed and a problem assignment was handed out.

1. Word Processing

Students were familiar with and were expected to use a word processor in preparing the text of their reports and a plotting program for all plots. Since the preparation of tables can be tedious, students were told they could prepare tables by hand.

2. Preliminary Report

A hand-out describing the nature of the experimental report was distributed and discussed. In order to insure that each student thoroughly understood the experiment he or she was to perform, a Preliminary Report had to be prepared and turned in to the teaching assistant at least a day before the experiment was performed. The Preliminary Report contains the following:

- a. A brief statement of the Objective of the Experiment
- b. A Schematic or Block Diagram of the Apparatus (hand drawn)
- c. Basic Principles and Equations - Mathematical equations and sketches used wherever possible.
- d. An outline of the Typical Procedure in Making a Measurement with the Equipment.
- e. A list of Precautions

The Preliminary Report was no more than three pages in length and was read by the assistant prior to the student's beginning experiments. Corrections, additions and other comments were made on the Preliminary Report. If the Preliminary Report was seriously

flawed, the student was asked to re-write the Preliminary Report and submit it with their final report.

During the orientation session the Preliminary Report for a specific experiment was discussed.

3. Final Report

The final report contained the Preliminary Report (2a through 2e) plus the following:

- f. Data - The laboratory data sheets (carbon copies torn from the laboratory notebook)
- g. Summary of Results in tabular and graphical form
- h. Precision and Accuracy - t-test, least squares, estimate of random and residual error and total error.
- i. Answers to any specific questions asked in the instructions for each experiment.

4. Errors and Problem Assignment

Time was spent during the orientation session discussing random errors, residual errors, the propagation of errors, and estimating the total error. A problem assignment was distributed which provided practice in error analysis and the use of the computer programs.

5. Computer Programs

A number of computer programs were available to the students on the Novell Network's Software Distribution System. These were programs developed over a period of years specifically for this course. These programs could be downloaded to disk and used by the students on their personal computers. Also, the programs were available on computers in the laboratory. The following programs were available:

- a. t-test
Values of $x(i)$ are input. The program calculates the mean (average), standard deviations (S.D.(x) and S.D.(mean)) and the random error at the 90% level (t S.D.(mean)).
- b. linear least squares
Values of $x(i), y(i)$ are input and the program least squares fits the data either to the equation $y = ax$ or $y = ax + b$. The least squares slope and y intercept (for $y = ax + b$) are calculated. The standard deviations of the slope and intercept and standard deviation from regression are calculated. (See Figure 9 for typical program output).
- c. roots of a quadratic equation
The numerical values of A, B and C for the equation $A X^2 + B X + C = 0$ are input. The two roots are calculated and printed.
- d. Root of $f(x) = 0$
This program can be used to find a real root for any equation of the form $f(x) = 0$. A statement $y = f(x)$ is inserted in the

program. The user specifies a "reasonable" minimum and maximum value of x and the percent accuracy to which the root is to be calculated. The program finds a value of x which makes y very small or equal to zero, or indicates no root was found. (14)

- e. Simultaneous linear equations with two unknowns
The numerical values of a(1),b(1),c(1) and a(2),b(2),c(2) are input for the equation $a(i)x + b(i)y = c(i)$. x and y are calculated.
- f. A plotting program
Clarkson University has a site license for IDPS (Interactive Data Plotting System - Version 4.0 - Copyright 1986 Unicorn Micro Ware). This program permits a user to read multiple data files containing x-y pairs and plot them. The user has control of text and numeric labels, line style, markers, data display range and can select a logarithmic mode. Linear least squares lines can be generated for a given set of data. IDPS has considerable versatility in providing different kinds of plots for different kinds of printers or plotters.
(See Figures 8 and 10)
- g. Quadratic least squares
Values of X(I),Y(I) are input to the program. Least squares values of A(1), A(2) and A(3) and their standard deviations are calculated for the equation $Y(I) = A(1) + A(2) X(I) + A(3) X(I)^2$.
(See Figure 14 for typical program output)
- h. Numerical integration
This program was specifically designed to integrate current versus time data to determine the number of coulombs required to oxidize or reduce a compound in the controlled potential electrolysis experiment (see below). The time in seconds and voltage in millivolts is input together with the resistance of the standard resistor. The current is calculated using Ohm's Law. The integration is performed and includes an extrapolation to zero current. The total number of coulombs required to oxidize or reduce the compound is calculated.
(See Figure 11)

A demonstration of the use of these programs was provided in the orientation session together with some printed instructions.

In recent years a spreadsheet (Quattro Pro or Lotus-1,2,3) and other applications programs have been used in the freshmen programming course. These programs have been used by some students in preparing their final reports.

B. Second Laboratory Orientation Session

Instructions for Instrumental Analysis Experiments

In the second orientation session the printed instructions for the first six experiments were distributed and the experiments were discussed. These experiments use techniques considered during the previous semester in the Separations, Radiochemistry and Electrochemistry course. The students pair up to form a group. Up to

six groups (twelve students) can be handled in a laboratory section. (We have had as many as three sections in this course.) Each group works on a different experiment.

The six experiments in the first half of the course are:

1. Gas Chromatography - Qualitative and Quantitative Analysis and Column Characteristics (6 laboratory hours)
2. High Performance Liquid Chromatography - Qualitative and Quantitative Analysis and Column Characteristics (6 hours)
3. Liquid Scintillation Counting - Quantitative Analysis for C-14 and H-3 labelled compounds; and Activation Analysis and half-life determination of an unknown (6 hours)
4. Gamma Radioactivity - Gamma ray spectroscopy and Quantitative Analysis (3 hours)
5. Controlled Potential Electrolysis - The reduction of p-cyanoacetophenone, determination of n and identification of the reduction product using infrared and ultraviolet spectroscopy. (6 hours)
6. Polarography - Reduction of metal ions, oxidation or reduction of organic compounds, limiting currents, and quantitative analysis using conventional and differential pulse polarography. (12 hours)

Experiments 5 and 6 were devised by Professor Petr Zuman. I developed instructions for the other experiments.

C. Third Laboratory Orientation Session Answers to the Problem Assignment

The third orientation session was held during the second week of the semester. At this session the answers to the six problems handed out during the first session were discussed. At the end of the session the assignment was collected for grading.

The purpose of this problem assignment was to make certain the students were able to use the t-test, linear least squares and plotting programs and understood the concepts of error analysis and error propagation. A knowledge of this material was needed in preparing the laboratory reports.

V. SEPARATIONS, RADIOCHEMISTRY AND ELECTROCHEMISTRY EXPERIMENTS AND REPORTS

During the next seven weeks students performed the six experiments list in section IV-B. At any given time each group was working on a different experiment. At the beginning of the experiment the Preliminary Report was returned to the students and a teaching assistant and/or I would talk to the individual groups briefly about the experiments they were to start. The final report for each experiment was due one week after completion of the experiment.

Rather than describing all these experiments, one experiment - Gas Chromatography - will be described in considerable detail. Another experiment - Controlled Potential Electrolysis - will be

Mentioned more briefly.

A. Gas Chromatography Experiment

A Perkin-Elmer Sigma 2000 gas chromatograph interfaced with a computer (or data station) was used for this experiment. A flame ionization detector and a six foot OV-101 column was installed in the instrument. The instrument was controlled and monitored by the data station.

1. Qualitative Analysis and Column Characteristics

In the first laboratory period the instrument is turned on and programmed so that the retention times of a series of seven qualitative knowns (heptane, octane, nonane, decane, undecane, 4-methyl-2-pentanone and cyclopentanone) could be determined. The chromatograms of a mixture of the seven knowns, an unknown and charcoal lighter fluid or unleaded gasoline was obtained. Temperature programming was employed so that good separations were obtained and the complete elution of the sample was obtained within eight minutes. Also, the retention times were obtained for the isothermal separation of the seven component mixture. Finally, students were asked to devise a temperature programming scheme to separate hexane from heptane.

The instrument provides (via the data station) a table of peaks, their retention times, peak areas and peak heights. A plot of each gas chromatogram was obtained. Figure 1 shows the gas chromatogram obtained for the seven component mixture. The table obtained for the seven component mixture is shown in Figure 2. Figures 3 and 4 show the data obtained for the same mixture when the column was maintained at a fixed temperature. (Most figures are taken from student reports.) Figure 5 summarizes the retention time data. (N.B. Figures 1, 3, 7, 8, 10 and 12 have been added to this paper to provide participants with practice in viewing figures. While these figures add more detail to the paper, they are not essential.)

Students were given data obtained with another instrument using a different column, a thermal conductivity detector and different conditions (See Figure 6). The retention times and the order of elution of constituents were different. Students were asked to discuss and compare these two sets of data in their final reports.

Students were asked to calculate the number of theoretical plates (P) using two different equations (See Figure 7). From P the height of an equivalent theoretical plate (H.E.T.P.) was calculated. P and H.E.T.P were calculated using the Sigma 2000 isothermal elution curves for heptane and decane. The resolution was calculated using some of the data.

A plot of $\ln(\text{adjusted retention time for the isothermal data})$ vs the number of carbon atoms in the chain for the saturated hydrocarbons was used to obtain the Kovats indices for 4-methyl-2-pentanone and cyclopentanone (equal to 100 times the value of n - see Figure 8).

2. Quantitative Analysis

During the second laboratory period the chromatograms of six quantitative knowns was obtained. In addition, each student obtained the chromatogram for his individual unknown. 0.1 uL of each solution was injected. Each solution contained heptane and octane with nonane as an internal standard and decane as the diluting solvent.

Each student was asked to include a table in his final report which contained the peak height and area for each heptane, octane and nonane peak. The heptane/nonane and octane/nonane ratio of peak heights and peak areas were calculated and tabulated for the knowns and the unknown. Linear least squares fits of the peak height, peak height ratio, peak area and peak area ratio vs concentration for heptane and octane. Also, plots were made. (see Figures 9 and 10). Four least squares fits were obtained for heptane and four fits for octane. The students were expected to examine the results of each least squares calculation and decide whether there was a linear relationship (of the form $y = a x$). Each student was asked to use each fit to obtain an estimate of the number of grams of heptane and octane in the unknown. (There were four estimates for heptane and four estimates for nonane). The students were asked to give a "best estimate" of the amount of heptane and octane in the unknown and an error estimate. The "best estimate" is not necessarily the average of the four estimates. The students were expected to explain how they decided on a "best estimate".

3. Numerical and Statistical Methods Programs Used

A t-test, linear least squares and plotting programs were used for this experiment.

4. Error Analysis

Each student was asked to estimate the error in the determination of heptane and octane in the unknown. They were expected to consider:

- a. the variation of volume of sample injected,
- b. random error in peak height and peak area,
- c. effect of using height ratios and area ratios,
- d. error associated with use of the calibration curves (standard deviation in the least squares slope),
- e. error in preparing the unknown solution,
- f. any other significant sources of error.

B. Controlled Potential Electrolysis Experiment

In this experiment the controlled potential reduction of 2×10^{-3} M p-cyanoacetophenone (4-acetylbenzotrile 1443-80-7) in 10% ethanol - 0.5 M sulfuric acid is carried out in a cell with a mercury pool working electrode (cathode) and a platinum wire anode. A silver-silver chloride reference electrode is used. Nitrogen gas is used to remove and then exclude oxygen. The solution is stirred with a magnetic stirrer. The electrode reaction is:



where R is p-cyanoacetophenone and P is the product of the reaction. The nature of the product is deduced from the determination of n (the

number of electrons per molecule of R) and the ultraviolet and infrared spectra of the product (15).

1. Choice of Potential

The current versus potential curve was determined from 0 to -1.2 volts vs the Ag-AgCl reference electrode. A potential was selected in the range where the first wave showed a limiting potential.

2. Controlled Potential Electrolysis

The electrolysis was performed on freshly prepared solution. The current was determined by measuring the voltage drop across a one ohm standard resistor every 30 seconds until the current has dropped to about 5% of its original value.

For a simple electroreduction carried out (with 100% current efficiency) at controlled potential, uniform stirring and constant temperature, the current should theoretically decrease exponentially with time. A plot of $\log i$ vs. t should be a straight line. n can be calculated from the y intercept, slope and original concentration of the p-cyanoacetophenone. In practice, linear plots are sometimes not obtained. Deviations from linearity can be due to non-uniform stirring and/or a change in temperature. In addition to making the log plot, students were asked to determine the total number of coulombs of electricity required to reduce the p-cyanoacetophenone by determining the area under the current versus time curve (numerical integration - see section IV-A-5-h above).

The controlled potential electrolysis was performed during the first laboratory period. The spectra were obtained during the second laboratory period (see below).

3. Spectra of the Product

The U.V. spectrum of the product solution was compared with the spectra of p-cyanoacetophenone and acetophenone.

A portion of the solution containing the electrolysis product was neutralized with sodium hydroxide solution. The product was extracted with chloroform and evaporated to form a thin film on a salt plate. The infrared spectrum of the product was obtained using a Perkin Elmer Model 1430 Ratio Recording Infrared Spectrophotometer and Data Station.

From the determination of n and the spectra students were asked to deduce the reduction product and to write a balanced half reaction for the controlled potential electrolysis. (Four electrons are involved in the reduction process. It can be deduced from the spectra that only the CN group is reduced in this initial four-electron step (15).)

4. Computer Programs and Error Analysis

Each student was asked to plot and perform a linear least squares analysis of $\log i$ vs t . From these results, each student was expected to decide whether current decreased exponentially with time. If there was an exponential decay, n was obtained from the data. Also,

students were asked to calculate n from numerical integration of the i vs t data (see Figure 11). Values of n (number of electrons), k (in the equation $i = kC$) and i_0 (initial current) were reported and an estimate of the error in these quantities was expected.

C. The Use of Computers in the Other Experiments

Word processing, linear least squares and plotting programs were used in preparing the final report for every experiment. The t -test program was frequently used. Simultaneous equations were solved in the quantitative analysis segment of the Liquid Scintillation Counting experiment. Numerical integration was used in the coulometry experiment (Controlled Potential Electrolysis) as described above.

VI. PHYSICAL CHEMISTRY EXPERIMENTS AND REPORTS

A. Orientation Session

After the Separations, Radiochemistry and Electrochemistry experiments were completed, five weeks were devoted to the remaining experiments. A laboratory period was used to discuss and hand out instructions for the experiments. These experiments were:

7. Infrared Gas Spectrum (1 laboratory hour)

A diatomic gas (hydrogen chloride) is prepared, dried and used to fill a 10 cm infrared gas cell. The vibrational-rotational spectrum is obtained using a Perkin-Elmer model 1430 infrared recording spectrophotometer interfaced with a computer (data station). The spectrum is printed and the peaks are tabulated by the instrument. Students use this data to determine the moment of inertia and bond length using a quadratic least squares program. The analysis is based upon the harmonic oscillator - rigid rotor approximation with added terms to correct for anharmonicity, and vibrational-rotational interaction.

8. X-Ray Diffraction (3 laboratory hours)

A Norelco X-Ray recording diffractometer is used to obtain the diffraction pattern of a powdered crystalline unknown compound belonging to the cubic system. The interplanar distances are calculated using the Bragg equation. The Miller indices for each diffraction line is determined and the unit cell dimension is calculated. From the Miller indices the student determines whether the unit cell is body-centered, face-centered or primitive.

9. First Order Kinetics - The Inversion of Sucrose (3 hours)

The acid catalyzed hydrolysis of an aqueous sucrose solution to fructose and glucose was followed using a precision polarimeter. The angle of rotation was measured as a function of time for a suitably thermostated solution. The pseudo-first order rate constant was determined by a suitable linear least squares fit of the data.

10. Second Order Kinetics - Saponification of Ethyl Acetate (3 hours)

The reaction of an aqueous solution of ethyl acetate with sodium hydroxide at constant temperature was studied using an AC conductance bridge, a 1000 Hz oscillator and an oscilloscope (null detector). The rate constant for the forward reaction was determined by suitable least squares fits of the data. An

optional part of the experiment involved determining the rate at different temperatures. The activation energy could be obtained from the rate constant - temperature data using the Arrhenius equation.

11. Gas Viscosity (3 hours)

A mercury-displacement gas viscosity apparatus is calibrated at constant temperature using dry air as the viscosity standard. The viscosities of pure helium, nitrogen and argon were determined using the standardized viscosimeter.

12. Vapor Pressure of Water (3 hours)

The vapor pressure of water was measured at ten to fifteen temperatures between room temperature and 75 degrees Celsius using an isoteniscope. The average heat of vaporization is determined from a Clausius-Clapeyron plot of $\ln P$ vs $1/T$.

13. Preparation and Molecular Weight Determination of a Polymer (8 hours)

Nylon-66 is prepared, purified and dried. Solutions of various concentration are prepared using concentrated sulfuric acid as the solvent. The viscosities of pure sulfuric and solutions of Nylon-66 in sulfuric acid is determined using an Ostwald viscosimeter. The intrinsic viscosity is determined from extrapolation of suitable plots involving viscosity and concentration. The average molecular weight of the polymer is calculated from the intrinsic viscosity.

B. Infrared Spectrum of HCl Gas

An experiment like this is included in many of the physical chemistry laboratory texts (7,8,13).

The Perkin Elmer data station was programmed and used so that the infrared spectrum (Figure 12) was plotted and the peaks were tabulated (Figure 13). The data were least squares fitted to a quadratic equation (Figure 14). From the least squares constants the moment of inertia and bond length in HCl can be calculated. The degree of interaction between vibration and rotation can be deduced from the magnitude of one of the least squares constants. The standard deviations of the least squares constants can be used to determine the random error in the bond length and other quantities. The Fortran program which performs the least squares calculation also provides a crude plot.

C. Use of Computers in the Other Physical Chemistry Experiments

Word processing, the t-test, linear least squares and plotting programs were used in preparing the final report.

For the second order kinetics experiment each student was asked to write a program to convert the resistance $R(t)$ measured at time t to the concentration of ethyl acetate (x) which had reacted at time t and the logarithmic term used in the second order rate expression (and linear least squares plot). The program and a table of t , $R(t)$, x and $\ln[(a-x)/(b-x)]$ was to be included in the final report. Students have submitted programs written in PASCAL, BASIC, FORTRAN or a spreadsheet language.

While not specifically required students were encouraged to write

programs or develop spreadsheets to perform the repetitive calculations involved in many of the experiments. Hand (electronic) calculators and computers were used to perform calculations.

VII. REFERENCES

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VIII. SOME QUESTIONS

I would be interested in learning what other participants are doing at their colleges and universities. Perhaps some of you would respond to one or more of the following:

1. How are instrumental analysis and physical chemistry laboratory taught at your school?
2. Briefly describe one or more experiments which you consider to be particularly effective.
3. Describe how computers and computer software are used in these courses. Is the use of specific software optional or required?
4. What do you consider to be the strengths and weaknesses of your courses?
5. Are there any additional references you would like to add to Section VII?

IX. FIGURES (Sent as separate files)

Acknowledgment: I would like to thank Thomas O'Haver for helping to prepare the figure files.

Paper 1 - Figure 1
Gas Chromatography Experiment
Perkin Elmer Sigma 2000 elution data for 7 Component Mixture
Temperature Programming
Data as obtained directly from the Data Station printer

Paper 1 - Figure 2
Gas Chromatography Experiment
Perkin Elmer Sigma 2000 elution curves for 7 Component Mixture
Temperature Programming
Data as obtained directly from the Data Station printer

Paper 1 - Figure 3
Gas Chromatography Experiment
Perkin Elmer Sigma 2000 elution data for 7 Component Mixture
Isothermal elution
Data as obtained directly from the Data Station printer

Paper 1 - Figure 4
Gas Chromatography Experiment
Perkin Elmer Sigma 2000 elution curves for 7 Component Mixture

Isothermal elution
Data as obtained directly from the Data Station printer

Paper 1 - Figure 5
Gas Chromatography Experiment
Summary of Temperature Programmed GC Data from a Student Report

Paper 1 - Figure 6
Gas Chromatography Experiment -
Addendum from the laboratory instructions
Data obtained using the Aerograph Autoprep

Paper 1 - Figure 7
Gas Chromatography Experiment
Number of theoretical plates (P) and resolution (R)
Equations and elution curve taken from the laboratory instructions

$$P = \frac{2.35 \frac{t_r'^2 (t_r' + t_i)}{t_r}}{t_r / 2}$$

$$P = \frac{16 (t_r' + t_i)^2}{w^2}$$

$$R = \frac{t_{r2}' - t_{r1}'}{(w_1 + w_2) / 2}$$

H.E.T.P = Length of the column / P

Paper 1 - Figure 8
Gas Chromatography Experiment
Plot of ln(adjusted retention time) vs. number of carbon atoms
for saturated hydrocarbons
Used for the determination of the Kovats index for
4-methyl-2-pentanone and cyclopentanone

Paper 1 - Figure 9
Gas Chromatography Experiment
Least squares fit of peak area vs concentration for octane knowns

Paper 1 - Figure 10
Gas Chromatography Experiment
Plot of area under peak vs concentration for octane in the knowns

Paper 1 - Figure 11
Controlled Potential Electrolysis Experiment
Integration of i vs t data

Paper 1 - Figure 12
Rotational-Vibrational Infrared Spectrum of HCl gas
Obtained using a 10 cm gas cell with a Perkin Elmer Model 1430
infrared recording spectrophotometer with a data station.

Paper 1 - Figure 13
Table of HCl Gas Infrared Absorption Peak Maxima (in Wavenumbers) and
Percent Transmittance as Obtained from the Perkin Elmer Data Station

Paper 1 - Figure 14
Quadratic Equation Least Squares Output for Data From Figure 13
Y values are absorption maxima (in wavenumbers)
X values are integers (m) related to the rotational quantum numbers
(J)
See Reference 7

THE END