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THE UNDERGRADUATE MATHEMATICS PROGRAM OF STUDENTS IN CHEMISTRY. A REPORT OF A CONFERENCE SPONSORED JOINTLY BY THE ADVISORY COUNCIL ON COLLEGE CHEMISTRY AND THE COMMITTEE ON THE UNDERGRADUATE PROGRAM IN MATHEMATICS.

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REPORTED ARE THE FINDINGS AND RECOMMENDATIONS OF A PANEL ESTABLISHED BY THE ADVISORY COUNCIL ON COLLEGE CHEMISTRY (ACCC) WORKING COOPERATIVELY WITH THE COMMITTEE ON THE UNDERGRADUATE PROGRAM IN MATHEMATICS (CUPM). THE FUNCTION OF THIS PANEL WAS TO DETERMINE THE APPROPRIATENESS OF RECOMMENDATIONS FOR CHANGES IN THE UNDERGRADUATE MATHEMATICS PREPARATION OF CHEMISTRY STUDENTS. A SHORT QUESTIONNAIRE WAS SENT TO ABOUT 70 CHEMISTS REPRESENTING A WIDE RANGE OF ACADEMIC AND PROFESSIONAL ENDEAVOR. RESPONDENTS WERE ASKED TO INDICATE THE APPROPRIATENESS OF A WIDE RANGE OF MATHEMATICS COMMONLY ENCOUNTERED IN VARIOUS PROGRAMS, RELEVANT TO THREE TYPES OF CHEMISTRY CURRICULA--(1) TERMINAL PROGRAMS, (2) PROGRAMS LEADING TO CONTINUED STUDY IN CHEMISTRY OR OTHER FIELDS, NOT ORIENTED TOWARD PHYSICAL CHEMISTRY, AND (3) PROGRAMS APPROPRIATE TO CONTINUED STUDY IN CHEMISTRY OR RELATED FIELDS OF A PHYSICAL NATURE (PHYSICAL CHEMISTRY, CHEMICAL PHYSICS). IT APPEARS THAT THERE IS A BROAD AREA OF MATHEMATICS THROUGH CALCULUS WHICH SEEMS APPROPRIATE FOR ALL STUDENTS MAJORING IN CHEMISTRY, REGARDLESS OF THEIR DEGREE PROGRAM. BEYOND THIS, IF A STUDENT IS INCLINED TOWARD GRADUATE WORK IN PHYSICAL CHEMISTRY, MORE MATHEMATICS IS DESIRABLE. THE OPINIONS GATHERED PROVIDED THE BASIS FOR A CONFERENCE HELD IN ATLANTA, FEBRUARY, 1967, WITH REPRESENTATIVES FROM BOTH ACCC AND CUPM. THIS REPORT CONTAINS THE RECOMMENDATIONS OF THAT GROUP WHICH ARE DISCUSSED UNDER THE TOPIC HEADINGS (1) INTRODUCTION, (2) THE BASIC PROGRAM, (3) ADVANCED TOPICS, (4) THE ROLE OF COMPUTATION, (5) PROBABILITY AND STATISTICS, (6) IMPLEMENTATION, AND (7) ESSENTIAL COURSE CONTENT. THIS DOCUMENT IS ALSO AVAILABLE FREE OF CHARGE FROM THE ADVISORY COUNCIL ON COLLEGE CHEMISTRY, SUITE 1124, 701 WELCH ROAD, PALO ALTO, CALIFORNIA 94304. (DH)

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A Report of a
CONFERENCE SPONSORED JOINTLY
by the
ADVISORY COUNCIL
ON COLLEGE CHEMISTRY
and
THE COMMITTEE ON THE
UNDERGRADUATE PROGRAM
IN MATHEMATICS

FEBRUARY 1967

This report of the Panel on Mathematical Preparation of Chemists is one of a series designed to aid in improving the teaching of college chemistry. The Council welcomes constructive comments, suggestions, and criticisms. These should be directed to the Executive Director at the address shown below.

All persons on the Council mailing list are being sent copies of this report. A limited number of additional copies are available free of charge upon request to:

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TABLE OF CONTENTS

Advisory Council on College Chemistry

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The Advisory Council on College Chemistry is an independent group of chemists interested in achieving improvement and innovation in undergraduate chemistry curricula and instruction at the national level. The Council collects and disseminates information through the activities of standing committees on Freshman Chemistry, Curricula and Advanced Courses, Teaching Aids, Teacher Development, Science for Non-Science Majors, Two-Year Colleges and Resource Papers. Additional *ad hoc* groups act as necessary. The Council hopes to provide leadership and stimulus for imaginative projects on the part of individual chemists.

The Council is one of a group of collegiate commissions supported by grants from the National Science Foundation. The Council cooperates in intercommission activities.

I
INTRODUCTION

The segment of mathematics traditionally included in the curriculum of students majoring in chemistry has generally fitted the well-established pattern of precalculus mathematics (algebra, trigonometry, and analytic geometry), calculus, and perhaps a course in differential equations limited to problems soluble in closed form. However, the increasing competence of students coming into collegiate work from up-graded mathematics courses at the secondary-school level and the changing nature of mathematical applications in chemistry indicate that this traditional program is not adequate for the needs of most students. Furthermore, as instruction in mathematics has tended to become more abstract in order to take advantage of the better preparation of entering students, there has developed an increasingly widespread concern among chemists that the content of both the elementary and advanced courses in mathematics is too "theoretical" and not sufficiently "applied." Therefore, chemists have shied away from further courses in mathematics departments and have designed courses of their own covering topics in mathematics they feel are particularly important to modern chemistry. And to add still more to the impetus for concern, the impact of digital and analog computers in all areas of science has raised serious questions about the need for inclusion in the chemistry curriculum of both formal instruction and practice in the application of these devices.

During the past several years, the Committee on the Undergraduate Program in Mathematics, CUPM, has examined and presented recommendations on the undergraduate curriculum in many areas. Most notably, the report "A General Curriculum in Mathematics for Colleges," presented in 1965, hereafter referred to as GCMC, attempted to lay out a series of courses with several alternatives which might consitiute a broadly acceptable program of mathematical instruction. In addition, CUPM has prepared more specific recommendations for curricula appropriate to engineering and physics, biology, management and the social sciences, computing, and applied mathematics. It seemed appropriate to determine whether similar recommendations could be found which would be helpful both to chemists in advising students of an appropriate curriculum in mathematics and to mathematicians in providing them an awareness of areas which are of interest and importance to chemistry.

To this end, a Panel was established by the Advisory Council on College Chemistry which could work with a similar group in CUPM. This Panel first formulated a short questionnaire which was circulated by members of the Panel to about 70 chemists representing a wide range of institutions and professional endeavor. The questionnaire identified broad areas of mathematics which are commonly encountered in precollegiate, collegiate and graduate studies and requested the opinions of the respondents as to the appropriateness of these areas in three types of chemistry curricula:

a. a *terminal* program leading to no further formal study in chemistry or related fields,
b. a program preparing a student for *continued study* in chemistry or allied fields (biology, medicine, etc.) which are most likely *NOT* physically oriented, and
c. a program preparing a student for *continued study* in chemistry or allied fields (physics, metallurgy, etc.) which *ARE physically oriented*, e.g., physical chemistry, chemical physics, structural chemistry, etc.

The responses to this questionnaire seemed to indicate that there was a broad area of elementary mathematics through calculus and perhaps linear algebra which seemed essential for *all* students majoring in chemistry, regardless of their degree program. Beyond this area, if a student is inclined towards physically-oriented graduate work, virtually all the mathematics which can be accommodated into his program either in courses in pure or applied mathematics or through advanced physics courses is desirable. This questionnaire and the opinions of the panelists then provided the basis for a conference held in Atlanta, Febrary 18-19, 1967, with representatives of both ACCC and CUPM. The recommendations of that conference constitute the body of this report.

Participants in the conference were: Gordon Barrow, O. T. Benfey, W. H. Eberhardt, Corwin Hansch, W. T. Mooney, Charles Reilley, and Kenneth Wiberg representing ACCC; Charles Curtiss, Charles R. DePrima, Monroe D. Donsker, Robert McDowell, Henry O. Pollak, Lynn Runnels, and Robert M. Thrall, representing CUPM.

II

THE BASIC PROGRAM

The central problem in the mathematical preparation of chemists is the great diversity of chemistry and of the individuals who choose this discipline as a career. The discipline itself encompasses a very broad range of professional activities ranging from research of the highest sophistication demanding competence of the highest order in very abstract areas of mathematics to supervision of production and sales which require virtually no mathematical skills beyond the simplest algebra. Similarly, individuals entering the discipline have widely ranging talents; some think easily in highly formal and analytical terms, others think clearly in the logical symbolism of chemistry but find analytical concepts and techniques impossible to master. In many instances, an individual is attracted to chemistry because of its inherent symbolic simplicity and practicality, but then becomes disillusioned and discouraged by the analytical mathematics demanded of him in junior- and higher level work. At present, all individuals are passed through much the same program; only in advanced work is any distinction made between courses appealing to individuals with these two extremes of talent and, even then, little effort is made to accommodate them.

However, it seems essential that every student majoring in chemistry be exposed to sufficient analytical mathematics to develop the skills and mathematical maturity required of him in his undergraduate studies and also to permit him to determine for himself his interests and limitations in these areas. It is quite likely that students entering college are totally unaware of the opportunities open to them if they are able to combine an interest in chemistry with competence in sophisticated mathematics. In considering a *minimum* program for students who enter college believing they wish to follow a career in what they then believe to be chemistry, care must be exercised that the program and courses themselves are not so minimal as to either hamper the student in his further studies or to discourage him from a career in chemistry because he sees nothing to challenge or interest him in the discipline.

If it is assumed that all students in chemistry will pursue elementary course work in physics and physical chemistry, the level of mathematics required in these courses will determine in large measure the *minimum* essential skills and level of maturity. Applications in these areas include the language and techniques of elementary calculus, differentiation, integration, and the solution of simple differential equations; vectors and linear vector spaces (although the applications might not be glorified by these names), matrices, determinants, and the solution of systems of linear equations; and perhaps elementary numerical analysis as it is appropriate to the solution of simple problems and to the statistical treatment of data. This body of competence seems to be represented with reasonable compactness in the description of the courses labeled Mathematics 0, 1, 2, 3 and 4 in the CUPM "A General Curriculum in Mathematics for Colleges," GCMC.

The course labeled Mathematics 0 is a pre-calculus course, described, along with the other basic courses, in more detail in the appendix of this report. Hopefully, this course will not long be necessary as a collegiate course, but competence in these areas will be obtained in secondary schools.

The courses designated Mathematics 1, 2, and 4 constitute a basic program in calculus requiring 9-12 semester hours; the first two courses have a sound but intuitive approach, the last course provides the more "thorough treatments of limits and series and some of the more technical parts of the single variable calculus" (Quote from GCMC, page 11).

The Mathematics 3 course is a brief exposure to linear algebra requiring 3-4 semester hours and comprising a study of linear vector spaces, linear operators, matrices and determinants, transformations, and characteristic roots and vectors of a matrix.

Thus, for a student well-prepared on entrance, the sequence 1, 2, 3, 4 would provide an excellent two-year foundation for chemistry, physics, and further mathematics. For a student less well-prepared, the sequence 0, 1, 2, 3 might be appropriate and would probably serve adequately for most chemistry.

A course in mathematical probability following the lines sketched in the course designated Mathematics 2P would be most valuable and should be recommended strongly as an elective which can be taken anywhere in the curriculum after the first year depending on the student's motivation and schedule. This course should provide the background in the mathematically sophisticated notions of random variables and distribution functions appropriate to further studies in statistics and experimental design. The more specific applications to scientific problems might best be accomplished through integration into course work in chemistry where the numerical results and their significance are especially important to the student. In addition, the notions of probability, distribution functions and moments will provide a most valuable background for work in quantum mechanics, statistical mechanics and other areas of chemical physics which rely heavily on these concepts.

This basic program has been constructed primarily with the four-year college curriculum in mind. The two-year colleges face other problems associated with both terminal and transfer students. Clearly, those students preparing for transfer at the end of two years should complete the essence of this basic program; anything less than this basis will probably require additional studies at the four-year institution before the student can enter effectively into the junior-level physical chemistry course work.

Students preparing for a two-year technician program are faced with the more difficult problem of acquiring sufficient mathematical skill to handle the elementary physical chemistry required in their program and at the same time master the complexities associated with data handling and statistics. Most likely, these students will also enter the program with a lower level of high school preparation. These students might find time for only 8-12 semester hours which can be devoted to mathematics and these hours might best be used in the equivalent of Mathematics 0, 1 and 2P with a shift in emphasis of 2P away from the purely mathematical aspects of probability theory towards the more practical applications to statistics and data handling. Thus, the first year of a technician-oriented curriculum will probably be required to provide the facilities in pre-calculus mathematics and the elementary notions of differentiation and integration with numerous applications. One semester of the second year might be available for the combined probability and statistics course with much greater emphasis on actual data handling than implied in the description of the course 2P in GCMC.

III

ADVANCED TOPICS

The program suggested in the previous section constitutes a basic program for *all* chemistry majors. This program is a minimum program and students who have the abilities to carry studies in mathematics beyond the level of the basic program are urged to do so. Although the particular courses and topics are of less importance than the continuous study of mathematics either in courses in pure mathematics or in courses in mathematical physics, there are some areas which respondents to the questionnaire indicate have greater signifiance to modern chemistry than others and these topics are listed below in an order of decreasing favor.

1. *Advanced Algebra and Group Theory*

   a. A more detailed consideration of linear vector spaces, generalization to a linear combination of orthonormal functions; linear operators, linear transformations and matrices, multiplication of matrices including the direct product, diagonalization of symmetric matrices, eigenvalues and eigenvectors of a matrix, determinants, and transformations by matrices, special matrices, e.g. Hermitian, unitary, etc.

   b. Abstract group theory and representation of groups by matrices; applications to problems involving molecular and crystal symmetry, electronic structure of atoms, molecules, and crystals, molecular vibration, classification of eigenfunctions, simplification of secular equations by linear transformations, permutation groups, rotation groups in two and three dimensions.

   Many of the above topics might be touched upon in the course in linear algebra suggested as part of the basic curriculum, but some advanced study is extremely valuable, especially for students preparing for work in theoretical chemistry and chemical physics. This set of topics represents an area for which chemists feel a great need and for which specific chemistry courses have been designed in the absence of suitable courses in mathematics departments.

2. *Ordinary Differential Equations*

   A detailed study of this area, which used to be considered a proper followup course for calculus, seems most important as a basis for students pursuing a career in chemical physics where the skill in handling complex differential equations is important. Thus, this course or topic may be of much less importance to the average chemist than linear algebra, probability, etc. provided some experience in the solution of simple differential equations is included in the regular calculus course. This topic also offers and may demand considerable emphasis on numerical analysis since solution of differential equations which are not integrable by simple techniques offers one of the most powerful areas of application of computers. Topics included under this title might be

   a. Linear differential equations with constant coefficients; qualitative analysis and analytical solutions by elementary techniques, solutions by more elegant techniques, e.g., the Laplace transform, etc.

   b. Linear differential equations with variable coefficients; classification in terms of singular points, the equations of mathematical physics, (e.g., Legendre, Hermite, Bessel, Laguerre, Mathieu, etc.); Sturm-Liouville differential equation theory.

   c. Non-linear equations; classification and techniques of solution.

   d. Numerical methods of solution, relaxation techniques, etc.

3. *Partial Differential Equations*

   The same comments pertain to this topic as to ordinary differential equations: the course is likely to be most important to students pursuing a career in chemical physics. The organization of the course depends on previous experience of the students, but should include the classification of partial differential equations, the nature and importance of boundary conditions, techniques of analytical solution in terms of eigenfunction expansions, integral transforms (Fourier-, Laplace-, Mellin-, Green-function), and numerical techniques for solution.

4. *Complex Variable Theory*

   Conformal mapping, contour integration in the complex plane, residue theory; generally, the applications of complex variables to solution of differential equations and integrals which are otherwise intractable.

5. *Special Mathematical Functions and Their Properties*

   Functions such as the Gamma Function, the Error Function and the Error Integral, Legendre Functions and Spherical Harmonics, Bessel Functions and Cylindrical Harmonics, Mathieu Functions, Laguerre Functions, etc. should be incorporated wherever feasible in courses as they appear. It would be particularly convenient for chemists to see much more application of the spherical harmonics rather than the simple trigonometric functions in elementary work, i.e., problems which involve the Legendre Functions rather than just the sine and cosine functions.

6. *Integral Equations*

   Although this type of equation is not frequently encountered by chemists, some experience may be very desirable so that the techniques of handling such equations are not completely unfamiliar. This area might also encompass a more detailed study of Fourier- and Laplace Transforms, Green-functions, etc. in which the kernel of the integral equation is related to a more familiar type function.

IV

THE ROLE OF COMPUTATION

The importance of computation in chemistry and the significance of both analog and digital computers in the curriculum is subject to continuous change depending on the facilities existing at individual institutions and the motivation of faculty. The increasing availability of remote terminals in laboratories and offices and the increasing competence of many chemists in computation are clear indications of this rapidly changing role of computation.

Not long ago, courses in the use of slide-rules were found in some curricula. Although these courses are perhaps still important in some of the two-year schools concerned primarily with technician training, the desk calculator seems to have displaced the slide-rule for almost all serious calculations of practical importance and experience with such devices should be part of a chemistry curriculum. However, there seems little need for formal course work in the use of these devices; they may be incorporated into laboratories where appropriate and where instruction in their use is treated in the same fashion as that of any other laboratory instrument.

Since the analog and digital computers are far more sophisticated in both application and complexity, more formal instruction may be required for their proper integration into the curriculum. This problem has been examined in many places; most approriate to chemistry are the Westheimer Reort "Chemistry: Opportunities and Needs," 1965, and more recently, the two reports, "Computers in Higher Education," Report of the President's Science Advisory Committee, February 1967, and "Uses of Electronic Computers in Chemistry," National Academy of Sciences—National Research Council, January, 1967. Although formal courses are given in the use of computers in almost all institutions having computational facilities, informal instruction is also usually available and probably provides the best way to approach the incorporation of digital computers into chemistry. Thus, introduction to the more common language of Fortran or Algol is accomplished readily in a few hours, perhaps included as part of a regularly scheduled chemistry laboratory, and experience in its use can be obtained with practice on real problems. The more sophisticated uses of computers requiring more complete knowledge of their structure and function is best considered as an "advanced" topic included as an elective if appropriate to a student's general interest.

The use of computers for purposes other than direct computation, e.g., data handling, machine programming and instrumentation, computer-assisted-instruction, record keeping, grading, literature searching, and innumerable other applications poses a more complex problem in instruction. It seems unlikely that mastery of these applications can be achieved without considerable self-study or formal course work in machine-oriented areas. However, it seems undesirable to recommend such a course for all chemistry majors; either elective courses or seminars should serve the essential purposes of familiarizing the student with the capabilities of instruments in these areas and actual applications will require considerable dedication beyond a casual acquaintance with the computer.

V

PROBABILITY AND STATISTICS

These two terms are generally associated both in course descriptions and curricular outlines. However, a clear distinction between them is necessary and points up the need for formal instruction by mathematicians in probability and the practical application or instruction in statistics which might best be offered by more practically oriented faculty.

As visualized in GCMC, *probability* is associated with the properties of discrete and continuous random variables distribution functions and the deduction of these distribution functions from models, the properties of these distribution functions, and the deductions possible from these functions, e.g., limit theorems and statistical inference. *Statistics* is concerned with the determination of the distribution function from data, sampling theory, design of experiments, tests for consistency, and conclusions of statistical significance from the experimental data. The essential distinction in these areas is that the probability arguments proceed from clearly defined mathematical models; the statistical arguments proceed from and are intimately tied to experimental data. Thus, although the mathematical aspects of probability theory can be introduced at almost any level after some experience has been obtained with calculus, a reasonable maturity is required of the student to benefit from studies in statistics. Most elementary experiments in chemistry are designed to yield results which do not require careful statistical analysis for their interpretation. Only as a student starts to encounter more difficult questions does he become conscious of the need for accurate statistical analysis of his results. Perhaps the classic example of this argument is the freshman experiment for the stoichiometry of the reaction of copper and sulfur which is described by D. Dingledy and W. M. Barnard in the *Journal of Chemical Education. 44.* 242 (1967).

The inclusion of a course in mathematical probability in the students' program seems desirable in that it introduces him to the complexities and importance of the problem and provides a sound base for inclusion of statistical treatments in laboratory programs when and where the needs arise. Awareness of the arguments of probability also assists him in understanding many of the operations which he must perform, e.g., counting operations which are influenced not only by the number of events, but also by such factors as the "dead-time" of the counter and measurements of intensities of spectra which are influenced not only by the sample itself, but also by the "noise" in the instrument.

Furthermore, in view of the importance of biochemistry in the modern chemistry curriculum students are going to be faced more frequently with the evaluation and interruption of biochemical and biological data. Such data must almost always be subject to careful statistical analysis, and misleading results can be avoided only by clear understanding of the statistics involved.

VI

IMPLEMENTATION

A major problem in the adoption of a sound program in mathematics is the present lack of use of mathematics by chemists and the lack of use by mathematicians in their course work of sufficiently interesting and vital illustrations drawn from chemistry. Thus, the student sees little or no connection between his formal instruction in mathematics and his ultimate career applications in chemistry.

The mathematical sophistication now generally required and used in first-year chemistry is rarely greater than junior high school algebra; it is seldom that any mathematics or mathematical concepts beyond this level are used until the student reaches the third year and even here, little is used beyond elementary differentiation and integration. Only when the student reaches the senior year or graduate school is he suddenly confronted with mathematics at a higher level and by this time, unless he has followed an inherent interest in mathematics or physics, he has generally lost whatever facilities he may once have had and is neither willing nor able to retrieve them in the face of other pressures. Thus, he is handicapped in all his future studies of chemistry and choices which were at one time accessible to him are no longer available. In many instances this problem is particularly acute for students undertaking undergraduate work in small colleges where there is no faculty member sufficiently versed in advanced techniques or sufficiently aware of them to insist the student continue his mastery of the more advanced topics in mathematics.

If, as we believe, the content of elementary calculus and linear algebra is important to the understanding and practice of chemistry, its use must be made clear to the student early and throughout his contact with both mathematics an chemistry.

Our approach to instruction in chemistry must be re-examined continuously to determine in what ways we can incorporate the language and concepts of mathematical areas in which students are developing competence. Similarly, instruction in mathematics should include wherever practicable examples chosen from chemistry as well as other fields. Of major value in this connection would be a series of detailed examples paralleling those recently presented in the text by Ben Noble, "Applications of Undergraduate Mathematics in Engineering," Macmillan, 1967. Obviously, the accumulation, editing, and presentation of such problems in chemistry is a major effort; the volume in engineering required the efforts of many individuals extending over a five-year period, but its value would in all likelihood justify the effort required. The value of such a book directed jointly at the mathematician, chemist, and student would not only be that of a resource document providing appropriate examples, but also that of a "policy weapon" indicating with specific examples the needs and applicabilities of specific mathematical topics. Hence, it would have value in counselling students and in providing leverage for inclusion of mathematics courses in programs of instruction where they might otherwise be ignored.

A program is now in operation to accumulate problems appropriate for such a book. ACCC welcomes contributions and, on request to the Executive Offices at Stanford University, will supply an informal digest of those problems currently available.

VII

ESSENTIAL COURSE CONTENT

Mathematics 0: *Elementary Functions and Coordinate Geometry*

"The prerequisites for Introductory Calculus, Mathematics 1, include the two components, A and B, below.

"A. Three years of secondary school mathematics. The usual beginning courses in algebra (perhaps begun in eighth grade) and geometry account for two of these years. The remaining year should include: quadratic equations; systems of linear and quadratic equations and inequalities; algebra of complex numbers; exponents and logarithms; the rudiments of numerical trigonometry; the rudiments of plane analytic geometry, including locus problems, polar coordinates and geometry of complex numbers; and arithmetic and geometric progressions.

"B. A study of elementary functions, their graphs and applications, including polynomials, rational and algebraic functions, exponential, logarithmic and trigonometric functions; an introduction to three dimensional analytic geometry.

"The components, A and B, of the prerequisites to Mathematics 1 will normally require 3½ or 4 years of high school mathematics. It is the component B and selected topics from A for which Mathematics 0 may be needed as a college course.

"Mathematics 0. (3 or 4 semester hours). Prerequisite: at least three years of high school algebra and geometry equivalent to A above. An outline of the course is component B above." A more detailed outline is presented on page 30 of GCMC.

Although most college-preparatory courses in secondary school would be expected either to include much of this material or at the very least prepare a student to take this course immediately on enrollment in college, the two-year colleges may face more serious problems giving this course to their entering students.

Mathematics I: *Introductory Calculus* (3 or 4 semester hours)

"The purpose of this course is to introduce the ideas of derivatives and integrals with their principal interpretations and interrelations and to develop the simpler techniques of differentiation and integration for the elementary functions studied in Mathematics 0."

Two versions of this course are presented in GCMC. Either would be acceptable for chemists, but applications are of the essence and should be included wherever practicable.

Mathematics 2 and 4: *Mathematical Analysis*

Two versions of these courses are also spelled out in detail in GCMC, pages 37-41. The version introducing multivariable calculus in Mathematics 2 is probably preferable for applied work, but either course covers the essential topics needed for chemistry: real-valued functions of several variables, vectors in two and three dimensions, integration, and elementary differential equations. Mathematics 4 provides more thorough treatment and extension of these ideas and in addition introduces more precisely the notions of limits and problems of convegrence of sequences, improper integrals, etc.

Mathematics 3: *Linear Algebra*

This course is also described in detail on pages 43 and 44. In essence, the topics comprise linear equations and matrices, vector spaces, linear transformations or mappings, determinants, and problems associated with quadratic forms. The practical problem of the diagonalization of matrices deserves strong emphasis.

Applications to molecular and crystal symmetry would be especially desirable, but perhaps cannot be accommodated at this early stage in the students' maturity.

Mathematics 2P: *Probability*

This course is outlined in brief on page 35 of GCMC and reflects the philosophy described earlier in this report. An advanced course of the same basis is described on page 57 of GCMC.

The essential broad outlines of the course are

a. Probability as a mathematical system
b. Random variables and their distribution
c. Limit theorems
d. Topics in statistical inference
e. Markov chains (from the outline of the advanced course)
f. Stochastic processes (also from the advanced course)

Although it is clear that not all these topics might be covered in a single first course, the more advanced topics are listed to indicate the type of topics which are appropriate under the title of probability.