Mathematics and Chemistry

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Introduction

As the Mathematical Association of America envisions the future of mathematics education, the discipline of mathematics should not be considered in a vacuum. Mathematics is an important tool for the sciences, and it is the responsibility of mathematics departments to provide undergraduates with the quantitative background that they need to succeed in their science courses. This applies to students who are only taking a few mathematics courses and are majoring in a scientific field, as well as to students who are double majoring in mathematics and science.

This study group focused on the relationship between mathematics and chemistry. The goal of this report is to help mathematics departments strengthen their programs by offering suggestions about how mathematics and chemistry can be coordinated better in the undergraduate curriculum. In particular, we would like to provide some guidelines as to how mathematics departments can work with chemistry departments to offer a variety of possible courses and programs that would benefit students in each of the disciplines.

Topics in mathematics that would benefit general chemistry students

Mathematical confidence and problem solving ability are probably the most important factors in predicting the success of students in a first-year course in general chemistry. However, knowledge and skills in the areas of basic mathematics, calculus, and 3-dimensional geometry (as described below) can be useful as a prerequisite or co-requisite to general chemistry.

Basic mathematics. It is unlikely that a student will excel in general chemistry without a solid understanding of and facility with the following elementary topics:

- unit conversions
- significant figures
- proportions and concentrations
- expressions involving exponents and logarithms
- basic trigonometry and algebra including graphing
- summation notation
- very basic probability and statistics
- applications of all of the above to word problems

Note that while there is substantial overlap between the above list of topics and what is often covered in a precalculus course, this list does not precisely correspond to the spirit or content of a standard precalculus course. In particular, most precalculus courses are not application driven and tend to focus on families of functions and their graphs, analytic geometry, and trigonometric identities, with additional material chosen from topics such as mathematical induction, the binomial theorem, matrices, complex numbers, and parametric equations. In addition, precalculus courses rarely cover such foundational topics as unit conversions, significant figures, and proportions and concentrations.

We recommend that mathematics departments consider introducing an elementary applied mathematics course as an alternative to precalculus that would be motivated by applications and cover the elementary material listed above. A course with a catalog description like the following could replace precalculus for science students (and possibly also for other students).

> **Elementary Applied Mathematics**. This course develops elementary techniques that will be useful to science students and applies them in a variety of scientific contexts. The course emphasizes word problems while covering unit conversions, significant figures, proportions and concentrations, review of basic trigonometry and algebra including graphing, exponents, logarithms, summation notation, and very basic probability and statistics.

Such a course would prepare students for Calculus, while simultaneously giving them the quantitative skills they will need for their science classes. While students who take this class rather than precalculus would have less preparation in analytic geometry and trigonometric identities, they would have much more practice with word problems, which might actually serve them better in their subsequent calculus classes. Furthermore, students often find the material in a college precalculus course reminiscent of mathematics they were exposed to in high school, but may not have learned. Indeed, the feeling of having tried unsuccessfully to learn this material in high school can discourage students from applying themselves to learn it in college. By contrast, students can become interested in a class like the Elementary Applied Mathematics described above because the techniques they are learning are motivated by and intertwined with real world applications.

Calculus. While a course in Calculus is not a formal prerequisite, students taking general chemistry would benefit from a conceptual understanding and basic facility with derivatives and integrals and their applications to the study of functions and their graphs. It is particularly helpful for students to know how to use derivatives to find the maxima and minima of a function.

Topics in 3-dimensional geometry. It would also be ideal if general chemistry students had at least a very rudimentary knowledge or experience with visualizing graphs in 3-dimensional space, 3-dimensional vector arithmetic, 3-dimensional spherical and polar coordinates.

Unfortunately, these topics are normally not introduced in the mathematics curriculum until multivariable calculus. Students with AP calculus may be taking multivariable calculus concurrently with general chemistry, and can benefit from the exposure to topics in 3-

dimensional geometry that they will see there. However, though this exposure could be helpful more generally, many students do not have the background to take multivariable calculus until their sophomore year, which will be after they have completed general chemistry. Addressing this problem would seem to require significant changes to Calculus II. *(Editor's note: See also the course area report on Calculus.)*

Mathematics courses or skills that are useful for students in chemistry courses beyond general chemistry

For organic chemistry. Students in organic chemistry would benefit from experience visualizing in 3-dimensions. This skill would most naturally be developed in a multivariable calculus course, though it could be developed in an Elementary Applied Mathematics course, or in a somewhat restructured Calculus II course.

For physical chemistry. Students taking physical chemistry would benefit from having taken courses in single variable calculus, multivariable calculus, linear algebra, differential equations with modeling, and statistics (i.e., data analysis, rather than statistical theory).

Preparation for graduate school in chemistry. Students planning to go to graduate school in chemistry are encouraged to take the mathematics courses listed above for physical chemistry. They should also have taken an introductory computer programming or computer science course which covers the basics of computer programming. Ideally, students heading to graduate school in chemistry should also have some experience using mathematical software (e.g. *Mathematica*, Maple, Sage, MATLAB, Octave, Berkeley Madonna, LSODE).

Not all mathematics departments currently offer a course teaching students how to use mathematical software packages. However, as more and more mathematical software packages are being developed which make scientific computations practical, we would like to encourage mathematics departments to offer such courses, with or without academic credit attached.

In addition to the mathematics courses listed above, students planning to go to graduate school in chemistry would find any of the following courses useful: partial differential equations, numerical analysis, a one-semester abstract algebra course covering group theory, and Fourier analysis. A course on intuitive topology and geometry, that includes an introduction to symmetry, could also be an interesting elective.

Double majors in mathematics and chemistry

Both chemistry and mathematics are demanding majors that require a lot of courses. In order to encourage double majors, both departments should be willing to compromise a little on their normal requirements so as not to make it almost impossible for students to complete the two majors while satisfying the general education requirements at their college or university. Some mathematics departments handle this problem by allowing one or two of the more quantitative chemistry courses (such as physical chemistry or computational chemistry) to also be counted as courses in the mathematics major. Chemistry departments should consider doing something similar.

For the chemistry part of a double major, students should be expected to take two semesters of each of general chemistry, organic chemistry, and physical chemistry, as well as one semester of each of biochemistry and inorganic chemistry. In addition, if possible, a student should take two semesters of analytical chemistry (quantitative analysis and instrumental analysis) and one semester of computational chemistry. We also recommend that students participate in an advanced topics seminar and/or a research-based senior thesis.

While the above courses would be normal for most chemistry majors, it would make sense to modify a ``standard" mathematics major to emphasize courses which are most useful in chemistry. More specifically, for students double majoring in mathematics and chemistry, we recommend a mathematics major consisting of the following courses. For each course listed below, the area(s) of applications to chemistry are indicated in parentheses.

- single and multivariable calculus (used in physical chemistry)
- linear algebra (used in physical chemistry)
- differential equations with modeling (used in chemical kinetics and thermodynamics)
- applied statistics (used in almost all areas of chemistry)
- analysis, advanced calculus, or Fourier analysis (used in physical chemistry and quantum mechanics)
- one semester of abstract algebra or group theory (used in inorganic chemistry and crystallography)
- probability theory (used in biophysical chemistry and Monte Carlo simulations)
- partial differential equations (used in chemical reaction kinetics, mass transport and thermodynamics)
- numerical analysis (used in computational chemistry)
- introduction to programming or computer science (used in physical chemistry)

While the above list of mathematics courses would be ideal, many smaller schools do not regularly offer either partial differential equations or numerical analysis. At such schools, additional courses in applied math, statistics, or computer science could be substituted for partial differential equations and numerical analysis

Mathematics majors concentrating or minoring in chemistry

For mathematics majors concentrating or minoring in chemistry we would recommend the mathematics major described in the double major section. The chemistry end of such a program would include two semesters of general chemistry, two semesters of organic, two semesters of physical chemistry, plus one semester of either biochemistry, inorganic, analytical, or computational chemistry together with an advanced topics seminar.

An interdisciplinary major

If an interdisciplinary option is desired, we recommend an integrated mathematics/chemistry/computer science major, requiring the following courses:

Chemistry: Two semesters of general chemistry, two semesters of physical chemistry, two semesters of organic chemistry, and one semester of either biochemistry, inorganic, analytical, or computational chemistry.

Math: Calculus through multivariable, linear algebra, differential equations with modeling, applied statistics.

Computer Science: Introduction to computer science including programming, data structures, algorithms.

Graduate school and career opportunities

Students with solid backgrounds in both mathematics and chemistry have many good options. They would be strong candidates for graduate programs in mathematics, applied mathematics, statistics, biostatistics, chemistry, crystallography, biochemistry, molecular biology, physics, biophysics, computer science, public health, epidemiology, and bioinformatics. In addition, these students would be desirable to medical schools and law schools.

Students with this background who do not want to obtain further education would have opportunities for employment in the pharmaceutical industry, the chemical industry, consulting, finance, data analytics, actuarial work, teaching. Even the National Security Agency can be interested in hiring students with bachelor's degrees and double majors in mathematics and chemistry.