

TITLE

Bridging Mathematics and Chemistry

AUTHOR, DEPARTMENT

Lia Vas

Assistant Professor of Mathematics

e-mail: l.vas@usip.edu

url: <http://mpcs.usip.edu/faculty/vas/index.htm>

Department of Mathematics, Physics,
Computer Science and Statistics

GOALS

MAIN IDEA: To create a course relevant to chemistry majors.

SPECIFIC OBJECTIVES. To provide students with:

5. mathematical perspective of the material learned in certain chemistry courses,

8. better understanding of some mathematical techniques used in chemistry and medical imaging.

11. emphasis on **research ideas**, not just mastering various techniques or methods.

4. knowledge of mathematical methods used in certain graduate programs in chemistry (for students interested in continuing their education at graduate level).
5. hands-on examples of an interaction of two different fields.

A student interested in a career in science is likely to be a part of a research team consisting of different professionals. The material covered in the course will enable students to better interact with other members of such a team.



INNOVATIVE BECAUSE :

- **innovative in the choice of topics.**

It unites different areas of mathematics **rarely presented together in the same course** in either the mathematics or chemistry curriculum. I present them together because

- all these topics are significant for a working chemist
- they have the same underlying theme.

- **innovative in the way the topics are presented.**

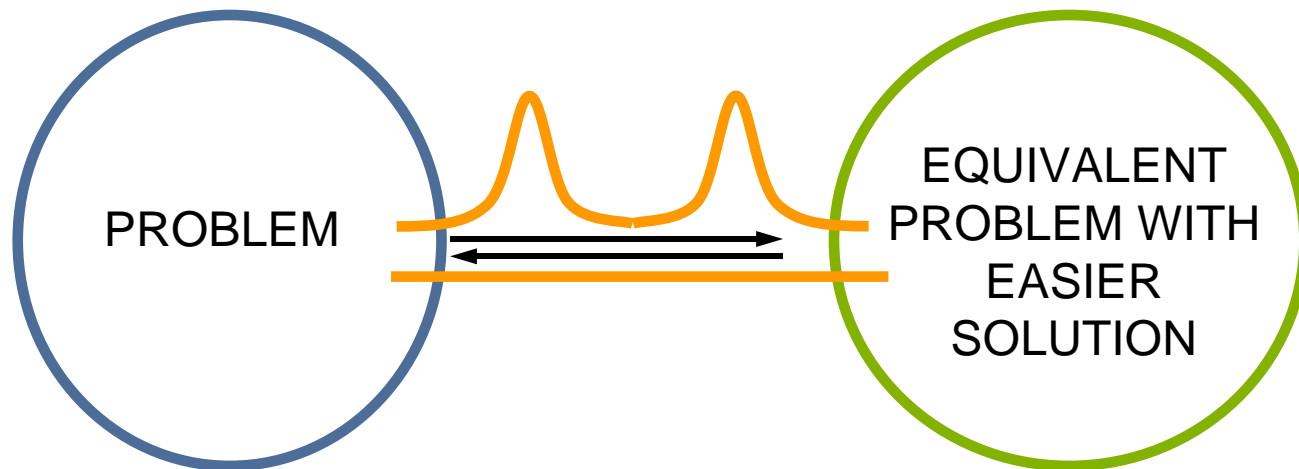
I use books written by chemists and articles and information posted at various chemistry websites to **change the way in which some topics are presented in a traditional mathematics textbook**. As a result, the students can really perceive the interdisciplinary aspect of the topics.

UNDERLYING THEME OF ALL COVERED TOPICS

It might be easier to solve a certain problem by translating it to a different field, solving it there and then translating the solution back into the original setting. This general principle of problem solving is often used in various fields and will be a useful concept for the students to acquire.

FORMULATION 1

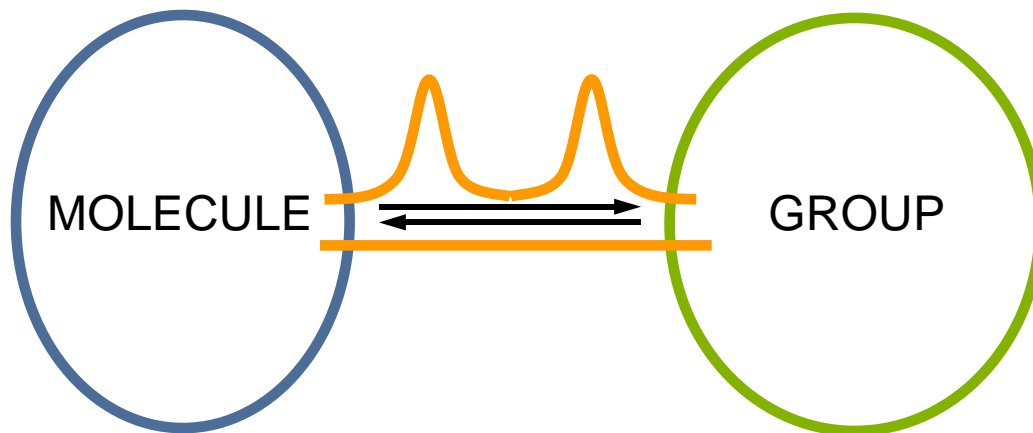
FORMULATION 2



TOPIC 1: GROUPS AND SYMMETRIES

**GEOMETRY
OF
MOLECULES**

**GROUPS OF
SYMMETRY**

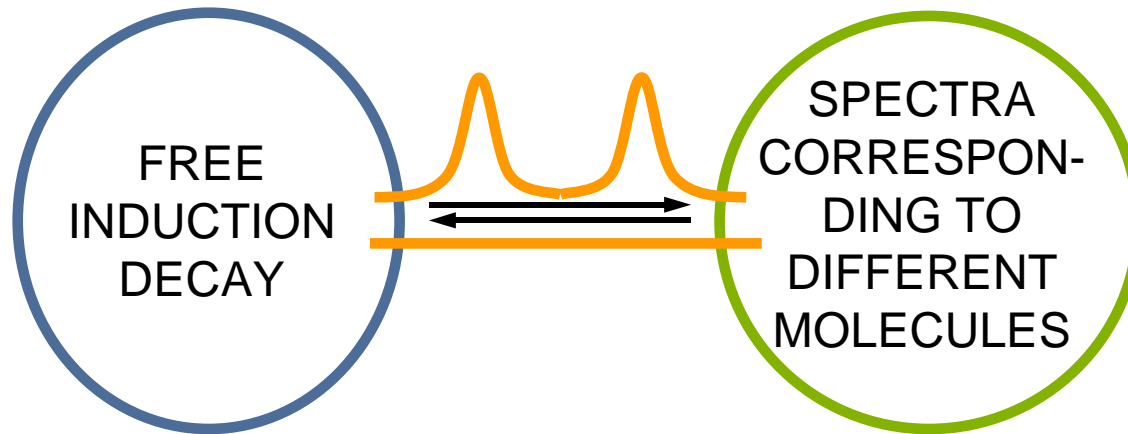


Group theory is a powerful mathematical tool used in physics, quantum chemistry and spectroscopy. In the course, I expand on the ideas from CH331 and present the **mathematical definition** of a group to the students. Students also learn the basics of topology and algebraic topology and how group theory is used to obtain information about a space of interest.

TOPIC 2: FOURIER TRANSFORM

SIGNAL

SPECTRUM

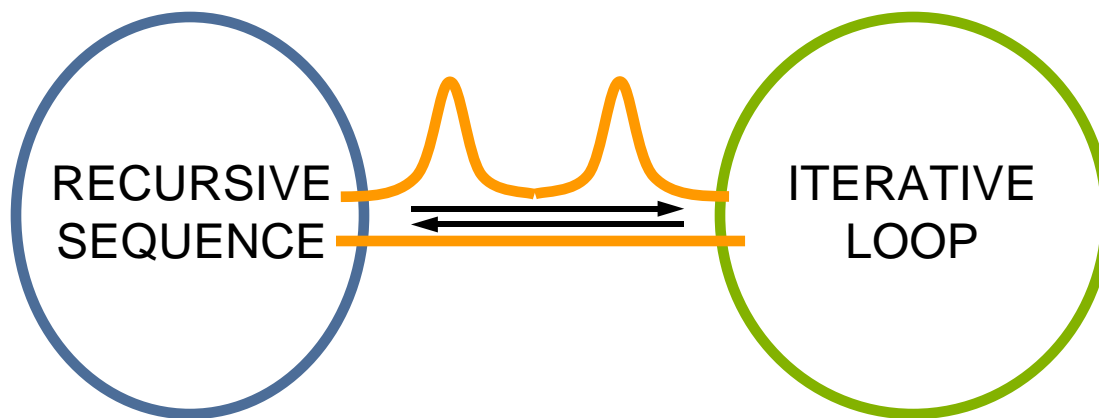


Students learn about the Fourier transform and find out how it is used in nuclear magnetic resonance and signal processing. Imaging and signal processing illustrate how the same idea (Fourier Transform) can be successfully applied to problems in various fields, ranging from physics to medicine.

TOPICS 3: RECURSIVE FORMULAE AND PROGRAMMING

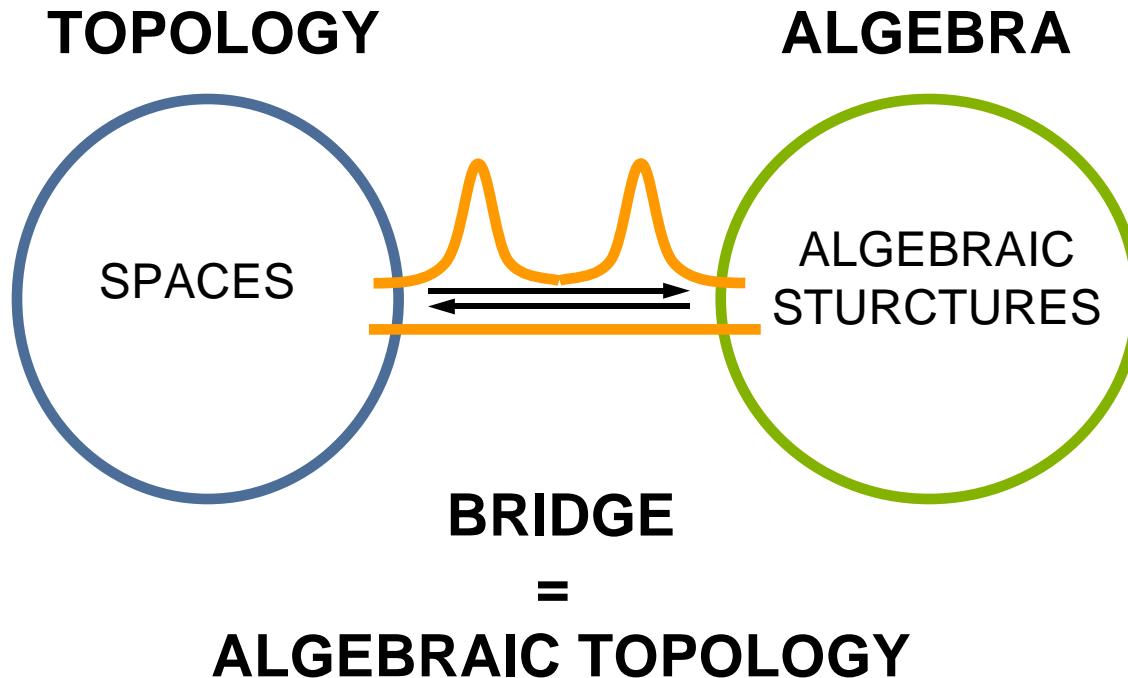
**CHEMICAL
EQUATIONS**

**COMPUTER
APPLICATIONS**



Students learn about basics of programming and write programs for TI83 calculators and programs in MATLAB that model certain chemical equations.

CONNECTION TO MY RESEARCH



In order to investigate a given topological space, we transfer the relevant information from the topological setting to the algebraic setting. We then study this information with some powerful algebraic methods. After obtaining the desired results on the space, we transfer them back to the topological setting.

OPPORTUNITIES FOR UNDERGRADUATE RESEARCH

Poster presentation based on ideas from Topic 3 with Kate Beishline (on the left) and Raeanne Napoleon on Scholarly Day.

