CHEM 4341 Syllabus

Applied Spectroscopy (3 cr.)
Fall 2026

Instructor Information

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General Course Information

CHEM 4341 expands on the basic principles of NMR spectroscopy, IR spectroscopy, and mass spectrometry that you probably learned about in a small handful of lectures of an introductory organic chemistry course. Success determining the structure of organic molecules often depends on combining clues obtained from different analytical methods. When working with real data, you might find that different sets of data initially seem to conflict with one another. Some data might be deceiving, or we might not fully understand it. Our job is to come up with an organic structure that best fits the complete set of data provided. Sometimes more than one structure may be acceptable and receive full credit.

Course Learning Outcomes

Upon completion of the course, students will be able to:

- Explain the effect of molecular structure (e.g., resonance, presence of electronegative elements, hybridization, hyperconjugation) on the appearance of spectral features;
- Assign spectral features to specific parts of a molecule, and vice versa; and
- Most importantly, elucidate the structure of organic molecules from spectra and other analytical data.

Within each module you will find a series of *unit goals*. These usually relate to a very specific skill regarding a small unit of material. These are measurable and an important component in attaining our ultimate goal of determining the structure of organic molecules using data from different analytical techniques.

Course Delivery and Required Course Materials

This course will make use of a residential instructional mode. You should review any materials posted for particular section in Canvas (videos, readings, problems). More guidance will be provided in weekly announcements.
There is no textbook to purchase.
In class we will work through a large number of problems, which is far more valuable than "lecturing" during this valuable time together. Solutions to the problems will be posted (typically before midnight of the day of class meeting). While attendance is not required, it is strongly recommended.

Data tables.
Tables of NMR, IR and MS data, along with a periodic table, *will be provided* for use on graded in-class assignments and the final. While you do not need to memorize this data, you should aim to become familiar with the data tables as you work on homework assignments and self-study problems before the in-class assignments. *You should bring a clean hard copy of the relevant data tables to use in the class on graded assignments.*

Canvas site
The site includes:

- *Short videos* that should be viewed before attending class.
- Skeleton" Powerpoint presentations of the videos on which you might want to make notes. These do not contain annotations made during the videos or in class.
- A modest amount of *reading materials* and links to materials on other sites.
- *Self-study problems* are… what they sound like. More important, they are the types of problems that you should expect on graded assignments.
- *Practice in-class assignment* illustrate the mix of problem styles you might expect to see on grades in-class assignments. Work through as many as these as possible. Convince yourself that you can do the problems. If working through these problems reveals a misunderstanding (or an instructor error), let's deal with these concerns sooner rather than later.
- Solutions to problems worked in class.

Textbook material
There is no textbook to purchase for this course. Make use of:

- Material posted or linked on the *Canvas site*.
- For Module 1: *Any two-semester introductory organic chemistry textbook*, e.g., Solomons, McMurry, Carey, Smith, Klein, Wade, etc. *The McMurray text is available for free from Openstax.*.
- For modules 3 and 4: *Organic structures form 2D NMR Spectra* by Field, Li and Magill, is available online from the Georgia Tech Library.

Links to these resources appear in relevant points in the modules of the Canvas course.

Other texts that you might wish to consult are:

- *Introduction to Spectroscopy*; 4e and 5e, Pavia, Lampman, Kriz, and Vyvyan.
- *Spectrometric Identification of Organic Compounds;* 8e by Silverstein, Webster, Kiemle and Bryce*;* or 7e.
- *Structure Determination of Organic Compounds: Tables of Spectral Data* by Pretsch, Bühlmann, and Badertscher; available online from the Georgia Tech Library (for modules 3 and 4).

Other materials
Sharp pencils, eraser, paper, calculator, ruler.

Grading Policy

Ungraded problems on Canvas – do as many of these as you can to develop successful problem-solving strategies and confidence. If you can, collaborate with others. These problems will be very similar to those on graded in-class assignments, on which you must work alone.

Graded homework – we will distribute homework problems at the start of each module, with due dates before the end of the module. Each problem in a homework set will be graded +1 or 0. Only totally correct answers will be graded "+1". Occasionally "+½" will be assigned for an answer that is "mostly", but not fully, correct. *On homework sets, you do not need to get every question correct to get full credit*, or even do every problem. You need to score 70% on a particular homework set to receive full credit on it. The aim of the homework sets is to promote learning. The few points associated with the homework (% of the course grade) are there to incentivize exploration of the material. However, given that graded in-class assignments and the final will include problems that are very similar to the homework sets, it is still worth working through all of the problems and reconsidering problems which you did not get completely correct.

Graded In-class assignments (exams)*– the three 50-minute graded in-semester in-class assignments will generally consist of six problems.* Four of these will be focused on individual techniques; the other two will make use of data from multiple techniques to determine the structure of an organic molecule. By the time of a graded in-class assignment you will be familiar with each type of problem - from on-line problems, problems illustrated in class, and homework problems. In-class assignments will be very similar in style to practice assignments that will be provided. For example, a practice assignment might include a short answer question, two "matching" problems, a calculation, and analyses of complete data sets to determine the structure of two compounds: The graded in-class assignment will consist of the same mix of type of problem. Each problem will be graded +1, +½, or 0: "+1" for a totally correct answer, and "+½" for an answer that is "mostly", but not fully, correct. If you either: (i) miss an assignment for any reason, or (ii) do not get full credit for a question, there are options to complete the assignments at a later date. Keep reading...
In-class assignment #4 covers 2D NMR as well as MS, IR and 1D NMR to solve structures. It will consist of four questions with lots of partial credit available.

Optional "make-up and re-take" opportunities. Two "make-up and re-take" sessions are scheduled: One before Thanksgiving, and one during the scheduled final exam period for the course. During these sessions you may:
(1) Make-up a missed in-class assignment.
(2) Rework any individual questions from previous in-class assignments for *which you did not receive full credit* (i.e., +½ or 0). The "re-take" questions will be *similar in style* to the ones on the original in-class assignment, *but with different data, and therefore different answers*. The highest grade on each question (+1, +½, or 0) from the original in-class assignment or either of the optional "make-up and re-take sessions" will contribute to your final grade. Note that multiple attempts are not additive, only the single highest score counts. There is no benefit to

re-doing questions on which you have already scored full credit. Note that it will be up to you to keep a record of which questions you want to work on during the "make-up and re-take sessions".

In-class assignment 1	Using basic information from **IR, MS and NMR** to determine structures (Module 1)	*20%*
In-class assignment 2	**IR and MS** (Module 2, plus use of basic principles of NMR to determine structures)	*20%*
In-class assignment 3	**1D NMR** ((Module 3, plus use of MS and IR to determine structures)	*20%*
***Make-up and re-take opportunity (1)*:**	***OPTIONAL Make-up and re-take opportunity (1):*** You can make-up a missed in-class assignment (1-3) from earlier in the semester and/or choose to do individual questions for which you did not receive full credit on the original in-class assignment.	–
REQUIRED **Final Period** **(2 hr 50 min)**	**In-class assignment 4: 2D NMR** ((Module 4, plus use of MS, IR and 1D NMR to solve structures)	*30%*
	OPTIONAL Make-up and re-take opportunity (2): You can make-up a missed in-class assignment (1-3) from earlier in the semester and/or choose to do individual questions for which you did not receive full credit on the original in-class assignment.	–
Homework	Six homework assignments (HW 1-4 1% each; HW5-6: 3% each)	*10%*

In-class assignment 4, administered during the final exam period, is required. Whereas earlier assignments are focused primarily on single techniques and building problem-solving skills, In-class assignment 4 integrates a lot that we have learned. No single technique allows for the determination of the structure of complex organic molecules, so this integration across all techniques is really important. That said, the focus of in-class assignment four is on the material from the latter part of the course. The expanded time available during the final exam period for this 100 point assignment is helpful.

Semester % score is sum of:
0.6 x % questions 1-18
0.1 x % HW
0.3 x % Final

Typical grade cut-offs in the course have been:
A: 90%+
B: 80%
C: 70%
D: 60%

An “A” performance typically requires demonstration of a consistently high level of success in determining the structures of organic molecules using spectroscopic and other data. A grade of “B” generally requires a high level of success in the interpretation of data from individual experimental techniques and good success in solving structural problems. A lower level of success in interpreting data from individual techniques and determination of complete structures might result in a “C” or a “D”.

Returned work and regrade requests. All assignments will be graded and returned as soon as possible. *If you want any work considered for a regrade you must make a written request by email within one week of the graded work being made available to you. Work will not be regraded after this deadline. The request should specify which question(s) you wish to be regraded, and a rationale.* Remember, only *totally* correct answers will be graded “+1”. You have an opportunity to re-do in-class problems on which you scored “+½” or “0” in one of the “make-up and re-take” sessions, and only the highest grade on that question counts.

Course Policies

The *Transparency in Learning and Teaching* framework informs the relationship between *course objectives, unit goals*, *instructional strategies* and *assessment*. Clearly articulated course objectives and unit goals are components of a strong internal structure to a course. They are the foundations for the design of both the *instructional strategies* (how the class is structured and delivered) and the *assessments* (how you are graded). I want to be clear about each of these features so that everyone is on an equal footing. If you ever have a question, please do not hesitate to ask.

Instructional strategies in the course include the use of short videos and modest reading assignments, These are followed by exploration of the material and application of what we have learned through activities that are either (1) online, or (2) in-class. While these activities are ungraded, you should complete each one. These are largely self-paced. It is okay to get the wrong answer in these activities, you can revisit the course material and re-try the activities until you get the right answer. With more practice I think that you will have more success with the activities, develop your own strategies to succeed, and build confidence. For each graded assignment you will find practice questions that have been used in previous years. All of these activities are meant to prepare you to succeed on the graded assessments.

Assessments in the course includes: (1) Relatively "low-stakes" homework sets that are designed to encourage you to keep up with the course and lay a foundation to succeed on “higher stakes” assignments; (2) graded in-class assignment that both examine specific skills, and also require integration of these skills; and (3) the final.

Application of what you learn from individual pieces of data is a first step in the determination of molecular structures based on data from a set of different techniques. Real success comes from an integration of all that you have learned from each piece of data and weighing the evidence from different techniques. Real data (the real world) is often "messy". *Often you will need to reconcile what might appear, at first sight, to be conflicting pieces of data. You will need to work out how different clues about structure relate to one another.* The only way that I know to do this is to challenge yourself, and one another, by working through as many problems as possible - individually, in small group discussions, and in class.
Making a start… We all come into this class with different levels of preparation. I believe that for most students a significant portion of the first module of the course will be a review of concepts covered in their introductory organic courses (i.e., CHEM 2311 and 2312/3 at Georgia Tech, or their equivalent elsewhere). But you might not be confident in your recall of material from these courses, which is entirely reasonable and understandable. The aim of the first module is to give you an opportunity to re-familiarize yourself with this material as a foundation for the remainder of the course.

Learning through doing and sometimes learning through failing. We learn by doing. Success in this class absolutely relies on working through problems. Some problems are formulaic with a single recommended approach to developing a solution, while others can be addressed using a variety of different approaches. Most problems, but not all, have a single solution.

It's okay to "fail" so long as we learn from our mistakes, and so long as the environment provides pathways for equitable opportunities to eventually demonstrate mastery. By providing lots of practice problems the hope is that you gain familiarity and develop problem solving approaches before being challenged on a graded assignment. However, it might be that you are unable to master a particular concept before completing a scheduled graded assignment. This might come from a lack of time based on your own academic preparation, other academic or non-academic obligations, or unforeseen challenges (e.g., health). So, my aim is to provide all students with flexibility and options to revisit those graded assignments on which they did not receive full credit.

In other words… The aim of this approach is to provide flexibility by allowing you multiple opportunities to demonstrate mastery of key concepts. While the journey through material over the semester is important to building expertise, your grade depends on demonstration of mastery of concepts at some point in time, not necessarily on a pre-determined schedule. If you have mastered a type of problem early in the course – great, move on. If you have not quite mastered a particular type of problem early in the course, this instructional approach gives you opportunities to continue to engage with that material and to demonstrate expertise later in the course without suffering negative consequences.

Attendance and/or Participation
Attendance is not required other than for exams. However, most students will realize significant benefit from: (1) attending every, and (2) maintaining regular study habits to make sure and steady progress through the course material.

Academic Integrity
Georgia Tech aims to cultivate a community based on trust, academic integrity, and honor. Students are expected to act according to the highest ethical standards. Review Georgia Tech's Honor Code and the student Code of Conduct.

Any student suspected of cheating or plagiarism on a quiz, exam, or assignment will be reported to the Office of Student Integrity, who will investigate the incident and identify the appropriate penalty for violations.

Core IMPACTS
This is not a Core IMPACTS course

Accommodations for Students with Disabilities
If you are a student with learning needs that require special accommodation, contact the Office of Disability Services (404-894-2563) as soon as possible to make an appointment to discuss your special needs and to obtain an accommodations letter. Please also e-mail me as soon as possible in order to set up a time to discuss your learning needs.

Student-Faculty Expectations Agreement
At Georgia Tech, we believe that it is important to strive for an atmosphere of mutual respect, acknowledgement, and responsibility between faculty members and the student body. The Student-Faculty Expectations articulate some basic expectations that you can have of me and that I have of you. In the end, simple respect for knowledge, hard work, and cordial interactions will help build the environment we seek. Therefore, I encourage you to remain committed to the ideals of Georgia Tech while in this class.

Prerequisite
A year-long (two-semester or three-quarter) introductory course in organic chemistry (e.g., at GT, CHEM 2311 and 2312/3) or equivalent.

Collaboration, Group Work, and Use of Generative AI
Collaboration outside of class – including on graded homework assignments – and discussion in class are both highly encouraged. Work on exams must be your own.
Generative AI might be useful to you in generating summaries of course materials. *However, it is prone to frequent and significant errors when applied to problem solving.*

Extensions, Late Assignments, & Re-Scheduled/Missed Exams
All homework will be due by the announced deadlines (the schedule will be published on Canvas). Assignments submitted up to 24 hours after the deadline will receive half credit.

If you will miss an exam due to illness, please let the instructor know as soon as possible. Attempts will be made to provide an option to take a make-up exam. If this cannot be arranged prior to the next class meeting, a student will need to make use of the scheduled "make-up and re-take" sessions.

Inclement Weather and Digital Learning Days
The instructor will communicate modifications to the schedule as soon as possible. To the extent possible we will make use of digital delivery to maintain the schedule of topics in the class.

Student Use of Mobile Devices in the Classroom
Students may make use of mobile devices in the classroom *for course related purposes only*. Devices may not be used during the exam periods.

Institute-approved absences
Institute-approved absences will be honored upon presentation of documentation from the Office of Student Life/Dean of Students Office. If the absence covers the due date of an assignment or an exam, you will receive an extension to the day after the approved absence.

Re-grading of assignments
Exams will be graded and returned as soon as possible. If you want any work considered for a regrade – *within one week of the work being returned to you* – you must: (1) make a **written request by email,** the request should specify which question(s) you wish to be regraded, and a rationale; and (2) **hand the exam paper at a class meeting**. Work will not be regraded after these deadlines.

Campus Resources for Students

Undergraduate Student Academic Success Resources:
A list of resources for undergraduate students' academic success and information about advising can be found at Success at Tech.

Student Well-Being:
At Georgia Tech, we are concerned about your overall physical, social, and mental well-being. A comprehensive list of wellness related resources has been compiled and maintained by the Office of the Vice President for Student Engagement and Well-being (student-resource-guide . More resources on supporting student well-being are available through the Learning Well Initiative.

List of Topics

This list is subject to minor changes. The final list will be provided on Canvas by the first day of classes and this syllabus will be updated accordingly.

1. **Foundations: An introduction to NMR, IR and Mass Spectrometry**
   This should be a review, and slight expansion, of material you likely encountered in an introductory course in Organic Chemistry.
2. **Infrared Spectroscopy**
3. **Mass spectrometry**
   This module focuses on electron impact ionizatio**n**
4. **1D NMR spectroscopy**
5. **2-D NMR spectroscopy**
   This module focuses on COSY, HETCOR, INADEQUATE and HMBC. Other 2D techniques will also be introduced.