

CHEMISTRY 5660 - Computational Chemistry and Biochemistry

Dr. Paul Marshall

Fall 2026

Classes:

Mondays and Wednesdays at 12:45 pm - 2:05 pm, in **room 232 of the Chemistry Building**.

My Office Hours:

Wednesdays 2:30 - 3:30 pm in **room 274 of the Chemistry Building**. Other times by appointment.

If your preferred name is not the same as the name that appears on the university provided roster for the course, please let me know so that I can use your preferred name.

I care about the success of each student. When you have questions about the course material, questions about the subject more broadly, concerns to discuss, accommodations you need, or thoughts you want to share, please come to office hours, or we can talk after class, or we can set up a meeting or a Zoom appointment.

My e-mail is marshall@unt.edu. This is the recommended way to reach me. Sometimes my inbox gets quite full, but I do want to hear from you. If you email me and don't hear back from me within two business days, please send a follow-up email. I will appreciate the gentle reminder.

Additional Information:

The information on this page is available online via Canvas and my own web site, at <http://www.chem.unt.edu/~marshall>. Any syllabus updates will appear on Canvas.

I will use Canvas for assignments, to post downloadable copies of the lecture slides, and grade information.

Prerequisites:

Successful completion (grade C or better) of undergraduate physical chemistry CHEM 3520 (or equivalent), or concurrent enrollment, or consent of the department.

Areas to be covered

Note that these designations are provisional and depend on how the class proceeds.

- Aug 17 & 19 - **introduction**, quantum concepts and basic Linux commands
- Aug 24 & 26 - file editing, format of Gaussian input files, defining molecular geometry (1), basis sets (1)
- Aug 31 & Sep 2 - basis sets (2), defining molecular geometry (2), SMILES and InChI representations
- Sep 7 & 9 - Hartree-Fock theory, applications, visualization
- Sep 14 & 16 - electron correlation, MP2 theory, density functional theory
- Sep 21 & 23 - **HPC best practices**; vibrational frequencies and IR spectra
- Sep 28 & 30 - transition state searches and reaction mechanisms
- Oct 5 & 7 - thermochemistry and kinetics
- Oct 12 & 14 - ionization energy, orbital energies, excited states and UV and photoelectron spectroscopy
- Oct 19 & 21 - **midterm exam**; atomic charges and electron density
- Oct 26 & 28 - long range forces, van der Waals forces, solvation
- Nov 2 & 4 - coupled cluster theory, compound and high-accuracy methods for thermochemistry
- Nov 9 & 11 - the Orca program, methods for large molecules
- Nov 16 & 18 - multi-reference theory
- Nov 23 & 25 - **Thanksgiving week**
- Nov 30 & Dec 2 - overview, summary and **project presentations**
- Dec 8 - **project presentations**

Learning Outcomes

Upon successful completion of this course, students will

1. Understand basic applications of ideas from quantum theory, including operators, the Schrodinger equation, wavefunctions, expectation values, probability density and atomic and molecular orbitals.

2. Exhibit basic proficiency with the Linux operating system, in terms of file handling and editing, and aspects of the high-performance computing (HPC) environment such as job submission.
3. Create and submit runs with the Gaussian16 code and other programs, such as Orca, to obtain the geometry, energy, vibrational frequencies and energy levels of small and moderate size molecules.
4. Demonstrate appropriate behavior in a HPC environment.
5. Understand fundamental concepts in computational chemistry such as spin, correlation and symmetry, in terms of quantum theory and how to implement them.
6. Compute chemical properties and select appropriate methods for useful results for understanding thermochemistry, reaction mechanisms, and various forms of spectroscopy.

Graded work: an exam, take-home assignments and a project

There will be one exam, to be held in-person mid-semester. Approximately 5 take-home assignments, depending on how we progress, will be made. These will involve creation and submission via Canvas of data files and a short write-up (more details to be discussed in class). In the second part of the semester, we will discuss larger projects to be collected by the last class day. During Finals Week, students will make short presentations of their project work. Students will also turn in a written report based on reading assignments made in the course of the semester.

The course grades will be calculated as follows:

- Hands-on assignments – 45% (two worst graded assignment will be excluded from the final assignments for 4660. One assignment will be excluded for 5660)
- Midterm Exam – 10%
- Readings report - 10%
- Major Computational Project – 35% based on written and oral presentation. Note that there will be no final exam in the course as this course is mostly project-based.

Letter grades will be assigned based on the numerical scores: A = 90-100; B = 80-89; C = 70-79; D = 60-69.

The University has strict rules concerning the “Incomplete” grade. The incomplete grade is given only during the last one-fourth of a term/semester, and only if a student: (1) gives notice to the instructor of being required to participate in active military service; or (2) is passing the course and has justifiable reason why the work cannot be completed on

schedule. Grades of incomplete are not to be used as a substitute for “F”. The rules governing “Incomplete” are explained in greater detail in the UNT Undergraduate and Graduate Catalogs.

It is important that you turn in all assignments and attend the exam. If you have a University Excused Absence (see [UNT policy](#)) we will reschedule. I will also consider illness and/or death of a family member or close friend, provided you have documentation. Should you otherwise miss an assignment or exam, you may receive a grade of zero for the missed work unless we have discussed this ahead of time.

I have great respect for students who are balancing their pursuit of education with the responsibilities of employment or caring for children or other family members. If you run into challenges that interfere with the class, please contact me. Advanced notice is always helpful. There may be flexibility available to support your learning.

Should you have a question concerning the way that your examination was graded, or if you think that there was an error in calculating the exam score, then it is your responsibility to bring the matter to the attention of the Instructor within one week. It is your responsibility to check your examination for grading errors, and to make sure that the score was correctly calculated.

HOW TO SUCCEED IN THIS COURSE

Working the exercises and assignments, in allocated class times and outside the classroom, is really crucial. It is how you put into practice the principles from the classes. If after you work at it there is something that doesn't make sense, please raise it with me.

I promise the midterm exam will not include anything you do not see in the classroom; anything we do cover in class I consider to be fair game!

I welcome questions during class. If one student has a question about course materials or assignment, that question is usually shared by their peers. Because everyone in the course can benefit from each other's questions, please don't be shy about questions.

No-one is born with the knowledge and ideas we will gain, nor the skills to use them to solve problems and figure out new connections and conclusions. *Anyone*, provided they work at it, can learn and grow their skills and that is what I look forward to facilitating. You do not do this alone. It is normal to encounter challenges, and normal and indeed desirable to take advantage of the help we offer, including the university resources listed at the end of this syllabus and as noted here. There are many resources available to help you, including: your classmates and study groups you set up, me, and other books and the

internet. If the lectures and/or assignments do not make sense after due consideration, then do *reach out for help* from these resources. Don't wait until the last minute!

SUCCEED AT UNT

The University endeavors to offer you a high-quality education and to provide a supportive environment to help you learn and grow. And, as a faculty member, I am committed to helping you be successful as a student. Here's how to succeed at UNT: Show up. Find Support. Get advised. Be prepared. Get involved. Stay focused. To learn more about campus resources and information on how you can achieve success, go to success.unt.edu

STUDENTS WITH DISABILITIES

Many students have visible or invisible disabilities, and The University of North Texas offers accommodations that allow them to achieve their full potential. The University makes reasonable academic accommodation for all students with disabilities. Students seeking accommodation must first register with the Office of Disability Accommodation (ODA) to verify their eligibility. If a disability is verified, the ODA will provide you with an accommodation letter to be delivered to faculty to begin a private discussion regarding your specific needs in a course. You may request accommodations at any time, however, ODA notices of accommodation should be provided as early as possible in the semester to avoid any delay in implementation. Note that students must obtain a new letter of accommodation for every semester and must meet with each faculty member prior to implementation in each class. For additional information see the Office of Disability Accommodation website at <http://disability.unt.edu/Links to an external site.>. You may also contact them by phone at (940) 565-4323. A common accommodation is for ODA to provide a special environment for exams. It is important to make appointments in good time with ODA for your exam.

WELCOME TO UNT!

I am committed to creating a learning environment where diverse perspectives are recognized and valued as a source of strength. I request that all students work with me to create a class culture based on open communication, mutual respect, and inclusion.

As members of the UNT community, we have all made a commitment to be part of an institution that respects and values the identities of the students and employees with whom we interact. UNT does not tolerate identity-based discrimination, harassment, and retaliation. UNT's full Non-Discrimination Policy can be found in the UNT Policies section of the syllabus.

Technology Requirements

You can carry out the **assignments and project work** from the CCIL that we use for classes, i.e., room CHEM 232 (open 8 am - 6 pm on weekdays except 3-5 on Thursdays), other computer labs on campus, from a computer you may have access to in an assigned research lab, or from home via the university's VPN, at untvpn.unt.edu. If using a home computer, I will try to help with any software issues, but ultimately it is your responsibility to make your home system function correctly. You will need to install Cisco software to access the VPN.

UNT intends **lectures** to be in-person in the traditional manner, where we all meet in the classroom. The one **exam** will be in-person too. You turn in **assignments** remotely via Canvas, and will need a computer, smart phone or tablet for that. If the availability of equipment or the internet is a problem, take advantage of the many computer labs across campus.

Should changes in the general situation require it, or in case you or I need to quarantine, remote learning via Zoom may be used for lectures. In that situation, you will need to have a working computer with web camera, microphone and sound. A smart phone or tablet will be sufficient if it has those functions. If necessary, we would handle examinations remotely too, and applications for scanning your exam solutions into pdf format are freely available for phone and tablet.

Part of working in the online environment involves dealing with the inconveniences and frustration that can arise when technology breaks down or does not perform as expected. You can contact the Student Help Desk for help with Canvas or other technology issues.

UNT Information Technology Help Desk: [UIT Student Help Desk site](http://www.unt.edu/helpdesk/index.htm). (<http://www.unt.edu/helpdesk/index.htm>)

Email: helpdesk@unt.edu

Live Chat: <https://it.unt.edu/helpdesk/chatsupport>.

Phone: 940-565-2324

In Person: Sage Hall, Room 130

Hours and Availability: Visit <https://it.unt.edu/helpdesk> for up-to-date hours and availability.

For additional support, visit [Canvas Technical Help](https://community.canvaslms.com/docs/DOC-10554-4212710328) (<https://community.canvaslms.com/docs/DOC-10554-4212710328>)

Legal Notices

My lectures are protected by state common law and federal copyright law. They are my own original expression. Whereas you are authorized to take notes in class thereby creating a derivative work from my lecture, the authorization extends only to making one set of notes for your own personal use and no other use. You are not authorized to record my lectures, to provide your notes to anyone else or to make any commercial use of them without express prior permission from me in writing.

Test Policy

It is important to show up on time for examinations and quizzes. The only time that one has to work a test is the allotted class time. Cell phones and cell phone calculators, tablets and computers are not to be used during the examination. Calculators are allowed. Check yours is working well ahead of time. Academic dishonesty and cheating will not be tolerated. The term “cheating” includes, but is not limited to,

- (a) Use of any unauthorized assistance while taking quizzes, tests or examinations, including use of a cell phone or notes.
- (b) Acquisition, without permission, of tests, notes or other academic material belonging to a faculty member or staff member of the University.
- (c) Claiming work by someone else or AI as your own.
- (d) Communicating with another student during an exam.
- (e) Any other act designed to give a student an unfair advantage.

Academic dishonesty and cheating is not appropriate is grounds for dismissal from the course with an “F” and will be referred to the appropriate University official. Cheating on a test will result in either: (a) a score of zero on the test (this test cannot be dropped); or (b) dismissal from the course with an “F”.

For the **take-home assignments**, these are open book and do make use of your notes, books and the internet for guidance. You have permission to discuss with classmates and generative artificial intelligence (AI) for help about how to work programs. Be aware that AI is often incorrect and should be verified, and that all responsibility for correct work is on you. **All the work you submit for credit must be by you alone, and you are forbidden from copying assignments from other students, and forbidden from having AI carry out all or part of an assignment.**

ACCEPTABLE BEHAVIOR IN THE CLASSROOM

Student behavior that interferes with an instructor's ability to conduct a class or other students' opportunity to learn is unacceptable and disruptive and will not be tolerated in any instructional forum at UNT. Students engaging in unacceptable behavior will be directed to leave the classroom and the instructor may refer the student to the Dean of Students to consider whether the student's conduct violated the Code of Student Conduct. The University's expectations for student conduct apply to all instructional forums, including University and electronic classroom, labs, discussion groups, field trips, etc. The Code of Student Conduct is at deanofstudents.unt.edu/conduct.

MISSED CLASSES

Students are responsible for the material that is covered in the class lecture and during the recitation. Should a student miss a lecture or recitation class, it is the student's responsibility to get the lecture notes from other students. See above about missing quizzes and exams.

CANCELLATION OF CLASSES BY THE UNIVERSITY

The University is sometimes closed due to bad weather. Should the University be closed during an examination day, then the examination will likely be given on either the first or second class day that we are back after the University was closed.

OTHER INFORMATION

You can learn a little more about me and my research at my website www.chem.unt.edu/~marshall.

Dates

The first class will be on Monday, August 17, 2026 and the last formal class will be on Wednesday, December 2, 2026.

There are no classes over Thanksgiving week, November 23-27, 2026. The final exam period is 1 - 3 pm on Tuesday December 8, 2026, in our regular classroom.

University Course Policies

ATTENDANCE

Students are expected to attend class meetings regularly and to abide by the attendance policy established for the course. It is important that you communicate with the professor and the instructional team prior to being absent, so you, the professor, and the instructional team can discuss and mitigate the impact of the absence on your attainment of course learning goals. Please inform the professor and instructional team if you are unable to attend class meetings because you are ill, in mindfulness of the health and safety of everyone in our community.

COURSE MATERIALS FOR REMOTE INSTRUCTION

Remote instruction may be necessary if community health conditions change or you need to self-isolate or quarantine. Students will need access to the equipment listed under Technology Requirements above to participate in any fully remote portions of the class. Information on how to be successful in a remote learning environment can be found at <https://online.unt.edu/learn>Links to an external site.

ACADEMIC INTEGRITY POLICY

Academic Integrity Standards and Consequences. According to UNT Policy 06.003, Student Academic Integrity, academic dishonesty occurs when students engage in behaviors including, but not limited to cheating, fabrication, facilitating academic dishonesty, forgery, plagiarism, and sabotage. A finding of academic dishonesty may result in a range of academic penalties or sanctions ranging from admonition to expulsion from the University. Dishonesty on an assignment may lead to a score of zero for that assignment.

PROHIBITION OF DISCRIMINATION, HARASSMENT, AND RETALIATION (POLICY 16.004)

The University of North Texas (UNT) prohibits discrimination and harassment because of race, color, national origin, religion, sex, sexual orientation, gender identity, gender expression, age, disability, genetic information, veteran status, or any other characteristic protected under applicable federal or state law in its application and admission processes; educational programs and activities; employment policies, procedures, and processes; and university facilities. The University takes active measures to prevent such conduct and investigates and takes remedial action when appropriate.

ACCESS TO INFORMATION - EAGLE CONNECT

Students' access point for business and academic services at UNT is located at: my.unt.edu[Links to an external site.](#). All official communication from the University will be delivered to a student's Eagle Connect account. For more information, please visit the website that explains Eagle Connect and how to forward e-mail [Eagle Connect](https://it.unt.edu/eagleconnect)[Links to an external site.](#). (<https://it.unt.edu/eagleconnect>[Links to an external site.](#)).

EMERGENCY NOTIFICATION AND PROCEDURES

UNT uses a system called Eagle Alert to quickly notify students with critical information in the event of an emergency (i.e., severe weather, campus closing, and health and public safety emergencies like chemical spills, fires, or violence). In the event of a university closure, please refer to Canvas for contingency plans for covering course materials. Some helpful emergency preparedness actions include: 1) know the evacuation routes and severe weather shelter areas in the buildings where your classes are held, 2) determine how you will contact family and friends if phones are temporarily unavailable, and 3) identify where you will go if you need to evacuate the Denton area suddenly.

RETENTION OF STUDENT RECORDS

Student records pertaining to this course are maintained in a secure location by the instructor of record. All records such as exams, answer sheets (with keys), and written papers submitted during the duration of the course are kept for at least one calendar year after course completion. Course work completed via the Canvas online system, including grading information and comments, is also stored in a safe electronic environment for one year. Students have the right to view their individual record; however, information about student's records will not be divulged to other individuals without proper written consent. Students are encouraged to review the Public Information Policy and the Family Educational Rights and Privacy Act (FERPA) laws and the University's policy. See UNT Policy 10.10, Records Management and Retention for additional information.

STUDENT EVALUATION OF INSTRUCTION

Student Perceptions of Teaching (SPOT) is the student evaluation system for UNT and allows students the ability to confidentially provide constructive feedback to their instructor and department to improve the quality of student experiences in the course.

SEXUAL ASSAULT PREVENTION

UNT is committed to providing a safe learning environment free of all forms of sexual misconduct, including sexual harassment sexual assault, domestic violence, dating violence, and stalking. Federal laws (Title IX and the Violence Against Women Act) and UNT

policies prohibit discrimination on the basis of sex, and therefore prohibit sexual misconduct. If you or someone you know is experiencing sexual harassment, relationship violence, stalking, and/or sexual assault, there are campus resources available to provide support and assistance. UNT's Survivor Advocates can assist a student who has been impacted by violence by filing protective orders, completing crime victim's compensation applications, contacting professors for absences related to an assault, working with housing to facilitate a room change where appropriate, and connecting students to other resources available both on and off campus. The Survivor Advocates can be reached at SurvivorAdvocate@unt.edu or by calling the Dean of Students Office at 940-565- 2648. Additionally, alleged sexual misconduct can be non-confidentially reported to the Title IX Coordinator at oeo@unt.edu or at (940) 565 2759.

ACADEMIC SUPPORT & STUDENT SERVICES

Mental Health

UNT provides mental health resources to students to help ensure there are numerous outlets to turn to that wholeheartedly care for and are there for students in need, regardless of the nature of an issue or its severity. Listed below are several resources on campus that can support your academic success and mental well-being:

- [Student Health and Wellness Center](https://studentaffairs.unt.edu/student-health-and-wellness-center) (<https://studentaffairs.unt.edu/student-health-and-wellness-center>)
- [Counseling and Testing Services](https://studentaffairs.unt.edu/counseling-and-testing-services) (<https://studentaffairs.unt.edu/counseling-and-testing-services>)
- [UNT Care Team](https://studentaffairs.unt.edu/care) (<https://studentaffairs.unt.edu/care>)
- [UNT Psychiatric Services](https://studentaffairs.unt.edu/student-health-and-wellness-center/services/psychiatry) (<https://studentaffairs.unt.edu/student-health-and-wellness-center/services/psychiatry>)

[Individual Counseling](https://studentaffairs.unt.edu/counseling-and-testing-services/services/individual-counseling) (<https://studentaffairs.unt.edu/counseling-and-testing-services/services/individual-counseling>)

Additional Student Support Services

Registrar (<https://registrar.unt.edu/registration>)

[Financial Aid](https://financialaid.unt.edu/) (<https://financialaid.unt.edu/>)

[Student Legal Services](https://studentaffairs.unt.edu/student-legal-services) (<https://studentaffairs.unt.edu/student-legal-services>)

[Career Center](https://studentaffairs.unt.edu/career-center) (<https://studentaffairs.unt.edu/career-center>)

[Multicultural Center](https://edo.unt.edu/multicultural-center) (<https://edo.unt.edu/multicultural-center>)

[Counseling and Testing Services](https://studentaffairs.unt.edu/counseling-and-testing-services) (<https://studentaffairs.unt.edu/counseling-and-testing-services>)

[Pride Alliance](https://edo.unt.edu/pridealliance) (<https://edo.unt.edu/pridealliance>)

[UNT Food Pantry](https://deanofstudents.unt.edu/resources/food-pantry) (<https://deanofstudents.unt.edu/resources/food-pantry>)

Academic Support Services

[Academic Resource Center](https://clear.unt.edu/canvas/student-resources) (<https://clear.unt.edu/canvas/student-resources>)

[Academic Success Center](https://success.unt.edu/asc) (<https://success.unt.edu/asc>)

[UNT Libraries](https://library.unt.edu/) (<https://library.unt.edu/>)

[Writing Lab](http://writingcenter.unt.edu/) (<http://writingcenter.unt.edu/>)