

We recognize and acknowledge that McMaster University meets and learns on the traditional territories of the Mississauga and Haudenosaunee nations, and within the lands protected by the "[Dish With One Spoon](#)" wampum, an agreement amongst all allied Nations to peaceably share and care for the resources around the Great Lakes.

CHEM 3PA3 – Quantum Mechanics and Spectroscopy

2022 Winter Term

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Course Description

Three discoveries from the 20th century revolutionized the way we understand our world. The first was the theory of relativity (1905, 1916). The second was development of the quantum theory of matter (1900-1935). The third was the discovery of DNA (1953). Of these three discoveries, quantum theory has had, by far, the largest impact on modern life. Indeed, quantum theory has revolutionized physics and chemistry: most of the “interpretative” tools of chemistry from before 1900 had to be revised (or more often, totally discarded) after the discovery of quantum mechanics.

I believe that everyone—even students in the humanities—should know something about the three seminal scientific discoveries of the 20th century. I will introduce you to quantum theory, as it pertains to atoms, molecules, and materials. My main goal is to elucidate how quantum mechanics helps chemists understand chemical bonding and interpret spectra.

Course and Learning Objectives

The “obvious” objective is for you to learn something about quantum mechanics, as it pertains to chemistry. The more subtle, important, and difficult objective is for you to learn to ask questions and then solve. Learning quantum mechanics requires cultivating analytical and mathematical reasoning skills at a high level; by the end of this course, you will hopefully be more capable of “thinking like a chemist.”

Make-up and Attendance policy

Most course content will be made available online. Attendance at in-person components is largely optional, except that assignments are graded in one-on-one sessions (either virtually or physically, depending on the university’s protocols). Marks for assignments will reflect not only the correctness of the answer but the depth of insight that led to the answer.

Materials & Fees

Required Materials/ Resources

- Materials will be posted the course web site, <https://qchem.qcdevs.org/>, including the textbook by my colleague Randy Dumont. I do not follow any book especially closely, and the documents, notebooks, and videos I put online are the authoritative reference for the course.

Delivery

You will require a computer that meets the performance requirements [found here](#).

Assessment: Mondays, 2:30-5:30 (HH 305)

Tutorial: Tuesdays, 2:30-3:20 (HH 305)

However, until further notice, these meetings will be hosted on Microsoft Teams. The Monday time slot has been (re)allocated to assessment. Everyone will be given a ~20 minute timeslot, and will meet with either Rik (the TA) or me (the instructor). Your assignment will be reviewed, discussed, and marked.

Virtual office hours: Tuesday: 3:30-4:30 [However, in general I will stay online as long as necessary.]

Virtual office hours: Friday: 5:30-6:30 [However, in general I will stay online as long as necessary.]

For now, all office hours will be virtual. Rik and/or I will be available (by request) for chats on MSTeams, but the primary mode of communication will be through GitHub.

Course Overview and Assessment

Course Outline: - My tentative plan is below.

1. Introduction to GitHub, Python, Jupyter, etc.
2. From Newton to Schrödinger
3. The Particle in a Box
4. The Harmonic Oscillator
5. Elementary Spectroscopy
6. Vibrational Spectroscopy
7. The Rigid Rotor and Rotational Spectroscopy
8. The Born-Oppenheimer Approximation
9. The One-Electron Atom
10. Many-Electron Atoms
11. Hartree-Fock Theory and Ab Initio Methods
12. Diatomic Molecules
13. Polyatomic Molecules

This is an absurd amount of material. We will move quickly. Do not get behind. If (when) I wish to modify the schedule/content, I will notify you in class and/or online.



Marking Scheme

This course will be graded unconventionally, motivated by an instructional philosophy called [Mastery Learning](#). The basic idea is that you will be assessed based on whether you learn a topic and the depth with which you learn it. This is a flavor of [specifications grading](#) that is adapted for a system, like McMaster, where I am required to give you a letter grade, and not merely a pass/fail mark. The basic intention is that your mark will reflect how far you have managed to ascend [Bloom's Taxonomy of Learning](#) as [it](#) relates to Quantum Chemistry.

Your course mark will consist entirely of assignments. There will be a final three (maybe just two) assignments that will be due, and defended, during the final exam period. Assignments will be submitted, and marked for *correctness* (often automatically) using [GitHub Classroom](#). Assignments will be marked for *mastery* via in-person (or one-on-one virtual) interviews (~20 minutes). The interview will also assess knowledge/understanding/mastery of the course material.

By default, all assignments are due at 11:59pm on Sunday.

The marking scheme for assignments is below. It is intended that the “default” grade (corresponding to a B work) is an S.

- U Unsuccessful.** The assignment was either not submitted or it did not fulfill the objectives of the assignment, typically because it did not pass the (automatic) tests. Alternatively, the student was unable to fully explain the thought processes they used to complete the assignment. Alternatively, the student failed to demonstrate knowledge of the relevant course material.
- S- Marginal.** The assignment was submitted on time and fulfilled the objectives. The student fully understands the thought processes required to complete the assignment, but seems to have been working near the edge of their ability. The student demonstrates knowledge of the relevant course material, but does not demonstrate knowledge of its larger context, importance/significance, or the ability to apply it to new problems. (Lose one extra point.)
- S Successful.** The assignment was submitted on time and fulfilled the objectives. The quality of the assignment was high (beyond merely marginal). The student not only understands the thought processes required to complete the assignment but demonstrates appropriate engagement with the assignment. The student not only demonstrates knowledge of the course material, but understands its larger context and importance, and how it could be applied/extended.
- S+ Excellent.** The assignment was submitted on time and exceeded the objectives. The quality of the assignment was exemplary, to the extent that it could be used as a model for others. The student demonstrates mastery of the thought processes required to complete the assignment, and understands how the assignment could be improved or extended. The student demonstrates knowledge of the course material, understands its larger context and importance, and can apply the material. Moreover, the student has engaged with the topics independently, and evinces a nuanced understanding of the material. (Gain one extra point.)

Extra Points

You **lose** extra points by receiving an S- on an assignment (minus one point), asking for a one-week extension on an assignment (minus one point), or redoing an assignment (minus two points). To accommodate your busy schedules, when you make your GitHub account and send me your username by a private message in MSTeams, you will get 4 extra points.

You **gain** extra points by receiving an S+ on an assignment (plus one point). You can also gain extra points by working example problems. These example problems should be written beautifully, at an exemplary S+ level, as Jupyter Notebooks or as Markdown or Markedly Structure Text documents, and submitted as pull requests to the GitHub repository for course content. That way you can help future students with the course material. The basic idea is that a contribution equivalent to completing an extra assignment at the S+ level will earn you +1 point.¹ In addition, when you notice typographical errors in the course material, you can correct them and submit a pull request, and will usually receive some extra marks for this. Please consult with me about what sorts of extra credit problems/assignments/examples are most helpful. In general, any contribution you make that improves the course for future generations of students will be rewarded commensurate with the magnitude and excellence of the contribution.

Final Mark

The final mark is assigned based on the fraction of the assignments you completed successfully and based on the number of “extra points” you have earned. To receive an A or a B, you must complete all assignments successfully. To receive an A, you must accumulate at least half of the available “extra points”. Because S+ grades are intended to be rare rewards for exceptional performance, earning an A (let alone an A+) will usually require doing some extra credit work.

Final Mark	# of unsuccessful assignments total number of assignments	# of "extra" points total number of assignments
A+	0	Greater than 1.0
A	0	Between 0.75 and 1.0
A-	0	Between 0.5 and 0.75
B+	0	Between 0.25 and 0.5
B	0	Between -0.25 and 0.25
B-	0	Less than -0.25
C+	Between 0.0 and 0.15	Greater than 0.0
C	Between 0.0 and 0.15	Between -0.5 and 0.0
C-	Between 0.0 and 0.15	Less than -0.5
D+	Between 0.15 and 0.3	Greater than 0.0
D	Between 0.15 and 0.3	Between -0.5 and 0.0
D-	Between 0.15 and 0.3	Less than -0.5
F	Greater than 0.30	

¹ For each page (~50 lines, but there is great variation based on difficulty and relevance), you will receive ~0.05 extra points.



Make-up and Attendance policy

Attendance is not required. But it is your responsibility to master the material and to attend office hours or other dedicated sessions for your assessments to be graded. As described above, it is possible to turn in assignments late (-1 extra point) or repeatedly (-2 extra points). The final assignments cannot be turned in late.

General Remarks/Advice

It is more important to have the “right ideas” than it is to get the “right answer.” In a course such as this one, it is more important to “think correctly” than to “work accurately.” In assessments, I’m looking to see if you (a) understand the problem, (b) understand how to solve a problem, (c) can solve the problem, and (d) can interpret the solution and describe its implications. It is better to “get the wrong answer for the right reason” than to “get the right answer for the wrong reason.” Of course, the goal is to “understand the right answer and obtain it by correct implementation of an appropriate (sometimes even elegant) strategy.”

Don’t get behind. The volume of material in this course is staggering. It will require a daily commitment from you. Probably most of you are smart enough so that you have been able to get by studying just the night before the test. That ends here. You will need to read and take notes. You will need to go through online material, rewriting it and adding marginal comments/questions. You will need to work through problems beyond those that are assigned, and think critically about the material. This course will probably require a larger commitment of time and mental energy than any course you have ever taken before. I will try to follow the registrars’ guideline, which suggests that you should spend approximately 10 hours/week (beyond the 3 hours assigned for lecture) working on the lecture material. Some weeks, you may find the course content easy (in which case you will probably need less time). Other weeks, you will find the course content very difficult, and you will need to budget your time accordingly.

Ask questions. Please visit me during office hours. (I get lonely.) I will clarify points that are not clear (sorry!), provide guidance on assignments, and more generally “shoot the breeze”, “chew the fat”, etc.. More generally, *I will do everything in my power to try to help you through this course.*

Don’t be afraid to criticize/comment on the course. In general, my teaching methods are flexible, and I will adapt them to your needs. What you learn is not negotiable. How you learn is entirely negotiable. I’ve designed this course based on what my opinions of what will work. I expect to change things during the term based on feedback and suggestions from you. I’m even open to totally detonating the course structure and building anew from the rubble. Thus, it is important that you make suggestions and/or tell me about portions of the course that need improvement. (Even if I do not agree with your suggestion, I will try to come up with an alternative approach that addresses your concerns.) If you feel uncomfortable giving feedback in person, slide a note under my door, get someone else to talk to me on your behalf (preserving your anonymity, if you wish), or come and talk to me yourself but raise your concerns in the third person: for example, “I don’t feel this way, but some of the people in class think your lectures are about as exciting as watching ice sublime.”

Learn good study skills. Many of you have never studied except the night before the test. Indeed, when I went to university I never studied until the night before the test. I never started a homework assignment until the night (or even the morning) before it was due. I *cruised* to A’s. But when I hit P-chem, I hit the wall. I had to study every day. Now, some of you (maybe most of you) are smarter than I am. Some of you will still be able to study just the night before the exam. Some of you will be able to start homework assignments

the morning they're due. But many of you will not. My advice for managing this course (and any other challenging course) is:

1. Prepare for lectures beforehand. Review the notes from the previous lecture and read the relevant sections of the book before the next lecture. Maybe work through some examples. Usually my lectures will only cover what I consider to be the difficult bits; I will leave the easy portions of the material for you to learn on your own. [30 minutes/class]
2. Take notes. Even though I will sometimes post my own notes or give a reference for a lecture's material, you should take notes. You will remember the lecture better if you take notes. After all, if the material goes in your eyes and ears, and out your hand, it must have gone through your brain. Especially for online material, it is very tempting to just "view" the material and not to really interact with it. It is very important to engage with the material. I recommend structured notetaking of some sort. I recommend the Cornell system, but if you are a fan of Zettelkasten, that's fine too. (Zettelkasten is just a little more involved, but it is better if you plan a career in chemistry.) If you've never learned structured notetaking then learning *any* type of structure notetaking will greatly increase your productivity in not just this course, but all others.
3. Review lectures afterwards. After each lecture, you will have a semi-legible scrawl of notes, scribbled down a breakneck pace. Rewrite them neatly. Expand them by incorporating material from the book and copying down examples from the lecture/text/tutorial, taking care to include all the steps in the problem (even the ones that were left out by the textbook's authors or me). To help you with this, I will try to provide a copy of my lecture notes online, but this takes a huge amount of time for me, and I will not be able to do it for every lecture. [~4 hours/week]
4. Work example problems. At university, assignments are "minimal." This is the smallest possible number of problems, which will be sufficient for the smartest person in the class. Everyone else will need to work additional problems. My advice is to look at the end-of-chapter exercises after each class. For problems that you know how to work, you will not learn much by attempting them. Instead, try to work on problems that, if they showed up on a test, would cause you problems. I usually would work problems 1, 5, 9, 13, Then I would go back through the problems, and make sure that I could also work the problems I skipped. If I thought I could work those problems, then I would skip them. If I was not sure, then I would work the problem. Usually I ended up working about half the problems. [~4 hours/week]
5. Think critically about the material. Try to imagine why a topic we covered in class is useful and where it might be applied. Think about where it might fail to apply. Write your own problems related to the lecture/reading material and solve them. Imagine how I might test a topic in class on a quiz or exam. Inventing practice problems, combining them with other course materials to make practice quizzes, then working and solving the quizzes is the most effective study strategy for this, and any other, course. [~2 hours/week]
6. <https://www.scotthyoung.com/blog/2019/02/15/memory/>
7. <https://www.scotthyoung.com/blog/2018/12/24/why-cram/>



Paul's Draconian Academic Integrity Policy

I have absolutely no tolerance for cheating. On assignments, you can use notes, books, your classmates, the internet—anything you think will help you. **However, what you turn in must be written in your own words.** On in-person exams, by default you are not allowed to use any electronic aids, collaborate with anyone in any way, or look at any written materials. Exceptions to this default will be clearly communicated.

If you have inadvertently (or even purposely) cheated in any way, you should come to me. Together we will work out a remedy that is fair to you and the rest of the class. (If you self-report I will endeavor to ensure that you are not “harmed” by your actions. In fairness to your classmates, however, I must also ensure that you do not benefit from them.) If I catch you cheating, I will not say anything for 48 hours—this is your chance to come to me and confess your transgression. If you do not raise the matter of your own accord, I will check with the appropriate Dean and if it is your first offense, you will receive a zero for that assignment/exam/worksheet/extra-credit problem. This will be registered as your “first offense” with the Dean. If it is your second offense, then the matter will be referred to the faculty council and I will argue forcibly that you should receive a zero for the course and that your behavior should become part of your permanent academic record. See <http://www.mcmaster.ca/policy/academic.htm>.

If you have observed a classmate engaging in cheating, it is your responsibility to report this behavior to me. On the one hand, you should want to do this because the presence of anomalously high grades in the class will stimulate me to increase the difficulty of the course and skew any curves I may choose to impose, adversely affecting your grade. On the other hand, if I observe that you saw someone cheating, but you do not report it to me within forty-eight hours of the event, then I will consider you an accomplice in the activity, and you will be subject to sanctions based on your involvement. A typical sanction will be to halve your score on the assignment in which you were an accomplice to the cheating and make that grade ineligible to be dropped.

If you actively aid a cheater (as by making your paper available), then you will be subject to the same sanctions as the cheater themselves. Again, you have forty-eight hours to confess your transgression.

The 48-hour rule is designed to allow you to discreetly bring matters related to academic integrity to my attention. In addition, it is designed so that in cases where cheating has many participants (ranging from observers, to abettors, to cheaters), every person has a chance to “come clean” and avoid severe sanctions.



Policies and Procedures – (McMaster's Official Legalese)

Requests for Relief for Missed Academic Term Work

[McMaster Student Absence Form \(MSAF\)](#): In the event of an absence for medical or other reasons, students should review and follow the Academic Regulation in the Undergraduate Calendar "Requests for Relief for Missed Academic Term Work".

MSAF Course Specific Information

I will not give make-up assignments. But I will be flexible.

Academic Accommodation of Students with Disabilities

Students with disabilities who require academic accommodation must contact [Student Accessibility Services \(SAS\)](#) at 905-525-9140 ext. 28652 or sas@mcmaster.ca to make arrangements with a Program Coordinator. For further information, consult McMaster University's [Academic Accommodation of Students with Disabilities](#) policy.

I will work with students with documented disabilities, and more generally with students who have temporary disabilities or other factors that inhibit their ability to perform at a high level. My goal is be maximally supportive of my students, and to treat everyone fairly. This means that while I am eager to accommodate all of you, I hold the same high expectations for all of you.

Academic Accommodation for Religious, Indigenous Or Spiritual Observances (Riso)

Students requiring academic accommodation based on religious, indigenous or spiritual observances should follow the procedures set out in the [RISO](#) policy. Students should submit their request to their Faculty Office **normally within 10 working days** of the beginning of term in which they anticipate a need for accommodation or to the Registrar's Office prior to their examinations. Students should also contact their instructors as soon as possible to make alternative arrangements for classes, assignments, and tests.

Courses with An On-Line Element

Some courses may use on-line elements (e.g. e-mail, Avenue to Learn (A2L), LearnLink, web pages, capa, Moodle, ThinkingCap, etc.). Students should be aware that, when they access the electronic components of a course using these elements, private information such as first and last names, user names for the McMaster e-mail accounts, and program affiliation may become apparent to all other students in the same course. The available information is dependent on the technology used. Continuation in a course that uses on-line elements will be deemed consent to this disclosure. If you have any questions or concerns about such disclosure, please discuss this with the course instructor.

Online Proctoring

Some courses may use online proctoring software for tests and exams. This software may require students to turn on their video camera, present identification, monitor and record their computer activities, and/or lock/restrict their browser or other applications/software during tests or exams. This software may be required to be installed before the test/exam begins.



Academic Integrity

You are expected to exhibit honesty and use ethical behaviour in all aspects of the learning process. Academic credentials you earn are rooted in principles of honesty and academic integrity.

It is your responsibility to understand what constitutes academic dishonesty.

Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: “Grade of F assigned for academic dishonesty”), and/or suspension or expulsion from the university. For information on the various types of academic dishonesty please refer to the [Academic Integrity Policy](https://secretariat.mcmaster.ca/university-policies-procedures-guidelines/), located at <https://secretariat.mcmaster.ca/university-policies-procedures-guidelines/>

The following illustrates only three forms of academic dishonesty:

- plagiarism, e.g. the submission of work that is not one’s own or for which other credit has been obtained.
- improper collaboration in group work.
- copying or using unauthorized aids in tests and examinations.

Authenticity / Plagiarism Detection

Some courses may use a web-based service (Turnitin.com) to reveal authenticity and ownership of student submitted work. For courses using such software, students will be expected to submit their work electronically either directly to Turnitin.com or via an online learning platform (e.g. A2L, etc.) using plagiarism detection (a service supported by Turnitin.com) so it can be checked for academic dishonesty.

Students who do not wish their work to be submitted through the plagiarism detection software must inform the Instructor before the assignment is due. No penalty will be assigned to a student who does not submit work to the plagiarism detection software. **All submitted work is subject to normal verification that standards of academic integrity have been upheld** (e.g., on-line search, other software, etc.). For more details about McMaster’s use of Turnitin.com please go to the [McMaster Office of Academic Integrity’s](#) webpage.

Conduct Expectations

As a McMaster student, you have the right to experience, and the responsibility to demonstrate, respectful and dignified interactions within all our living, learning and working communities. These expectations are described in the [Code of Student Rights & Responsibilities \(the “Code”\)](#). All students share the responsibility of maintaining a positive environment for the academic and personal growth of all McMaster community members, **whether in person or online**.

It is essential that students be mindful of their interactions online, as the Code remains in effect in virtual learning environments. The Code applies to any interactions that adversely affect, disrupt, or interfere with reasonable participation in University activities. Student disruptions or behaviours that interfere with university functions on online platforms (e.g. use of Avenue 2 Learn, WebEx or Zoom for delivery), will be taken very seriously and will be investigated. Outcomes may include restriction or removal of the involved students’ access to these platforms.



Copyright and Recording

Students are advised that lectures, demonstrations, performances, and any other course material provided by an instructor include copyright protected works. The Copyright Act and copyright law protect every original literary, dramatic, musical and artistic work, **including lectures** by University instructors.

The recording of lectures, tutorials, or other methods of instruction may occur during a course. Recording may be done by either the instructor for the purpose of authorized distribution, or by a student for the purpose of personal study. Students should be aware that their voice and/or image may be recorded by others during the class. Please speak with the instructor if this is a concern for you.

Research Ethics -NA

Extreme Circumstances

The University reserves the right to change the dates and deadlines for any or all courses in extreme circumstances (e.g., severe weather, labour disruptions, etc.). Changes will be communicated through regular McMaster communication channels, such as McMaster Daily News, A2L and/or McMaster email.