



*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.*

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## CHEM 3PA3 – Quantum Mechanics and Spectroscopy 2021 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

There are no synchronous lectures. All materials will be posted online. The primary element of the course is assignments. There is a final “project” which is really just another assignment. Some, and perhaps all, assignments will be turned in during virtual office hours, and the marks 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 online, 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.

### Virtual Course Delivery

To follow and participate in virtual classes it is expected that you have reliable access to the following:

- A computer that meets performance requirements [found here](#).
- An internet connection that is fast enough to stream video.
- Computer accessories that enable class participation, such as a microphone, speakers and webcam when needed.

If you think that you will not be able to meet these requirements, please contact [uts@mcmaster.ca](mailto:uts@mcmaster.ca) as soon as you can. Please visit the [Technology Resources for Students page](#) for detailed requirements. If you use assistive technology or believe that our platforms might be a barrier to participating, please contact [Student Accessibility Services](#), [sas@mcmaster.ca](mailto:sas@mcmaster.ca), for support.

### Course Overview and Assessment

**Course Outline:** - My tentative plan is below.

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

### **Assignments - (~10): (0-80% of the final mark)**

There will be assignments roughly every week. These assignments will consist of both material to learn and questions to answer. Assignments will often be turned in, and graded, during office hours. When this is the case, the anonymity of marks cannot be ensured, but it is possible to receive greater partial credit because not only is the correctness of an answer judged, but also the depth of insight that led to the answer. Any assignment grade that is lower than your final exam/project mark will be replaced by the final exam/project mark.

### **Extra Credit: - (each 30 pages counts 1% of the final mark; up to 40%)**

It is *very* important that you do not get behind in this course. To help you do this, if you turn in problems (either that I post online, or that you find from a suitable, preapproved, source) then I will give you extra credit. For extra-credit homework, you must clearly show what problem you are solving, where that problem comes from, and your solution must be written out neatly (or typed) in meticulous detail. Style matters here; I do not give credit for sloppy work as these are graded in a snap: the TA and I just read the problem, decide what key elements the solution must have within it, and then give credit based on our ability to find those key elements. The points-per-problem is based on the number of pages I think it would take me to work the problem (1 point/expected-page). Then, if your solution is clear, neat, and convincing at a glance, you will get that number of points. Otherwise I will reduce credit for sloppiness. In general, I give very generous credit for people who attempt challenging multistage/multipage problems, because you learn more that way. For every 30 pages of work you turn in, 1% of your final grade will be a 100%, up to a maximum of 40% (1200 pages).

### **Final Exam: - (20-100% of the final mark)**

The final project/exam will have the same basic format as the assignments, but will be longer. After the exam has been given, there will be an “interview” where you can justify your answers or fix small errors.

### **Overall Grading Scheme**

If your assignment average is higher than your final exam grade, your assignment average will count 80% and your final exam will count 20%. If your final exam is higher than your assignment average, your



assignment average will count 0% and your final exam will count 100%. After this component of your grade is set, extra credit will be factored in.

### Make-up and Attendance policy

Attendance is not required. But if you do not attend office hours you will probably have a very poor mark for assignments, and your grade in the course will be determined by the final exam alone.

### 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.” Partial credit will often be given when you understand a problem and will always be given when you understand how to solve a problem. The “details” of solution are less important. In particular, if you are running out of time, it will be beneficial to you to do all but the “tedious” mathematics for as many problems as possible. Omitting (or making errors in) the arithmetic will rarely cost you more than 25% of the total available points on a problem, but if it causes you to “misinterpret” your or get the wrong answers in subsequent problems, it could be devastating. I find that working “neatly” and not skipping steps helps me avoid careless errors. In summary, 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 “get the right answer for the right reason.”

**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 on the book before class. After class, you will need to go through the lecture notes, rewriting them and adding marginal comments/questions about the material. Then you will need to work through some of the problems in the book, 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 outside of 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 in lecture that were not clear (sorry!), provide guidance on homework, 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 tend to use 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 the homework and other take-home assignments, you can use notes, books, the internet—anything you think will help you. However, what you turn in must be written in your own words. On in-class exams, you are not allowed to use any electronic aids, collaborate or copy off of other people, or look at any written materials. In some cases I will allow you to have certain electronic devices (e.g., calculators) or text-based aids (part of the exam might be “open notes”).

If you have inadvertently (or even purposely) engaged in impermissible collaboration, 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 forty-eight 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. If you know you will miss an assignment you must arrange it with me beforehand.

### **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](mailto: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.