FAS syllabus CHEM 224 – Winter 2026

1. General Course Information

Course: **CHEM 224**
Course title: Mathematical Tools for Chemical Problems
Pre-requisites: Chem112
Semester and year: winter 2025
Number of credits: 3.0
Learning hours: 36
Modality: On campus
Classroom accessibility: [redacted]
Course Instructor: Jean-Michel Nunzi
Contact Information: nunzijm@queensu.ca
Office Hours & Location: [redacted] - virtual appointment preferred
Teaching Assistants: Zikai Zhu
Contact Information: zhu.jikai@queensu.ca

2. Course Description

This course introduces and reinforces mathematical methods needed to understand quantum chemistry, spectroscopy, thermodynamics, kinetics, etc.
Subjects covered include introduction to complex numbers; calculus; differential equations; vector spaces and vector algebra; matrices and determinants. Throughout the course an effort is made to illustrate mathematical concepts with chemical problems.

3. Topics

Complex Numbers and Functions
– complex numbers and arithmetic, functions of complex variables
Topics from Calculus
– derivatives, chain rule, implicit functions, Leibnitz rule
– partial differentiation, total differentials, exact and inexact differentials
– integrals and integration
Differential Equations
– definitions, simple solution methods
– boundary conditions and eigenvalues
– solution by series
– partial differential equations and separation of variables
Vectors, Vector Spaces and Vector Algebra
– geometric vectors
– vector spaces, inner products
– functions as vectors and orthogonality
– Fourier series

Operators and Matrices
– matrix algebra
– determinants
– linear equations
– matrix eigenvalue problems

4. Course Learning Outcomes

On successful completion of this course, students will be able to:

1. Translate chemical problems into mathematical language, determine which mathematical tools are useful for which problem.
2. Use the mathematical methods (especially linear algebra and (multivariate) calculus) that are most relevant for chemical problems.
3. Interpret chemical phenomena through mathematical modelling.
4. Identify which types of chemical problems can be understood using mathematical tools and apply the appropriate tools.
5. Identify, and correct, imprecise and incorrect mathematical reasoning and statistical fallacies.
6. Present mathematical concepts and tools required for quantum chemistry and spectroscopy courses.
7. Explain how mathematical models are used in chemistry.

5 Important University Dates

Please visit the Faculty of Arts and Sciences Sessional Dates website for all academic deadlines.

6 Land Acknowledgement

Queen's University is situated on the territory of the Haudenosaunee and Anishinaabek.
Ne Queen's University e'tho nón:we nikanónhsote tsi nón:we ne Haudenosaunee táhnon Anishinaabek tehatihsnonhsáhere ne onhwéntsya.
Gimaakwe Gchi-gkinoomaagegamig atemagad Naadowe miinwaa Anishinaabe aking.

7 Equity, Diversity, and Inclusivity

Queen's University recognizes that the values of equity and diversity are vital to and in harmony with its educational mission and standards of excellence. It acknowledges that direct, indirect, and systemic discrimination exists within our institutional structures, policies, and practices and in our community. These take many forms and work to differentially advantage and disadvantage persons across social identities such as race, ethnicity, disability, gender identity, sexual orientation, faith, and socioeconomic status, among other examples. In this class I will work to promote an anti-discriminatory, anti-racist and accountable environment where everyone feels welcome. Every member of this class is asked to show respect for every other member.

8 Recommended Course Textbook

Course Textbook	Edition(s)	Publisher	For Purchase	Cost	At Queen's Library?
John E. Straub - MATHEMATICAL METHODS for MOLECULAR SCIENCE - Theory and Applications, Visualizations and Narrative	# 1 - 2022	University Science Books - AIP	Amazon	$78	No

9 Copyright of Course Material

Course materials created by the course instructor, including all slides, presentations, handouts, tests, exams, and other similar course materials, are the intellectual property of the instructor. It is a departure from academic integrity to distribute, publicly post, sell or otherwise disseminate an instructor's course materials or to provide an instructor's course materials to anyone else for distribution, posting, sale or other means of dissemination, without the instructor's express consent. A student who engages in such conduct may be subject to penalty for a departure from academic integrity and may also face adverse legal consequences for infringement of intellectual property rights.

10 Queen's Email

The university communicates with students via Queen's email. Please check your email regularly to ensure you do not miss important information related to your course.

11 Course Feedback

At various points during the course, you may be asked to take part in a variety of feedback activities, such as surveys and questionnaires. This feedback enables the teaching team to improve the course. All surveys are anonymous and are directly related to activities, assessments, and other course material.

12 Weighting and Alignment with Course Learning Outcomes (CLOs) - dates

Assessment	Alignment with CLOs	% Weighting	date
Take home 1	all	5	[redacted]
Quiz 1	all	5	
Mid term	all	30	[redacted] Week
Take home 2	all	5	[redacted]
Quiz 2	all	5	
final	all	50	April
Total			100%

13 Descriptions of Learning Activities and Assessments

Week	Topic and Readings	Activities	Learning outcomes
1-2	Review of Functions and Derivatives and Integrals	• Quiz #1 • Assignment #1 • Mid-term	1,2,6,7
3-4	Multivariable calculus and Taylor Series	• Quiz #1 • Assignment #1 • Mid-term • Final	1-3,6-7
5	Complex numbers	• Assignment #2 • Mid-term • Final	1-4, 6-7
6-7	Orthogonal functions and Fourier Series	• Quiz #2 • Assignment #2 • Final	1,2,6-7
8-10	Matrices, determinants, linear systems, eigenvalues	• Quiz #2 • Final	1,2,5-7
11-12	Numerical Methods	• Final	1-3,5-7

Note that the learning outcomes are not achieved chronologically. They are general and will be stressed during many of the twelve weeks. We have thought carefully about the correspondence between learning outcomes and the mathematics presented in weeks 1 to 12. When a new type of chemistry problem is presented, we shall begin by (Learning outcomes 1,7), explaining how to translate it into mathematical language, explaining how to apply the required mathematical tools (Learning outcomes 2,4,6) and how to interpret the results (learning outcomes 3,5).

14 Proctored Exams

Timing of Final Examinations

Once the exam schedule has been finalized, the exam date will be posted on your SOLUS account. The exam dates for each term are listed on the Faculty of Arts and Science webpage under "Important Dates." Student exam schedules for the Fall Term are posted on SOLUS immediately prior to Thanksgiving and on the Friday before Reading Week for the Winter Term. Students should **delay finalizing any travel plans until after the examination schedule has been posted**. Exams will **not be moved or deferred** to accommodate employment, travel/holiday plans or flight reservations. For information regarding what is considered

extenuating circumstances and qualifications for Academic Consideration, please visit the Faculty of Arts and Science's Academic Consideration webpage.

If you are unable to attend an exam and receive approval for a deferred proctored exam, a further deferral of that exam will not be accommodated.

15 Class Attendance

Your presence and participation in class contributes to the knowledge and skills that you will develop throughout this course. I expect that you attend class regularly, participate in class conversations and learning activities. These types of activities provide active engagement, promote a deeper understanding of the course content, and contribute to your success in this course.

16 Building a Classroom Community

University is a place to share, question, and challenge ideas. Each student brings a different set of lived experiences. You can help to create a safer, more respectful classroom community for learners by following these guidelines:

- Make a personal commitment to learn about, understand, and support your peers.
- Assume the best of others and expect the best of them.
- Recognize and value the experiences, abilities, and knowledge each person brings to the course.
- Acknowledge the impact of oppression on other people's lives and make sure your words and tone are respectful and inclusive.
- Encourage others to develop and share their ideas.
- Pay close attention to what your peers say/write before you respond. Think through and re-read what you have written before you post online or send your comments to others.
- Be open to having your ideas challenged and challenge others with the intent of facilitating growth.
- Look for opportunities to agree with one another, building on and intentionally referencing peers' thoughts and ideas; disagree with ideas without making personal attacks, demeaning, or embarrassing others.

17 Name/Pronoun

If, for whatever reason, you wish to change how your name appears in onQ and/or on class lists, please follow these steps. You may also use this process to add your pronouns to the appearance of your name.

1. Log into SOLUS.
2. Click on Personal Information tab.
3. Click on the Names tab
4. Click on the Add New Name tab
5. Choose Preferred from the Name Type drop down menu
6. Enter the name you would like to appear in onQ and/or on class lists.

7. Click Save.

Please allow 24 to 48 hours for your name to be registered within the system. If you have further questions or concerns, please contact ITS at Queen's University.

18 Academic Support

All undergraduate students face new learning and writing challenges as they progress through university: essays and reports become more complex; effectively incorporating research into writing becomes more important; the types of assignments become more diverse; managing your time and developing the skills you need to read and think critically gets more challenging. I encourage students to contact Student Academic Success Services (SASS). SASS offers many different ways to receive support:

19 Accommodations for Disabilities

Queen's University is committed to working with students with disabilities to remove barriers to their academic goals. Queen's Student Accessibility Services (QSAS), students with disabilities, instructors, and faculty staff work together to provide and implement academic accommodations designed to allow students with disabilities equitable access to all course material (including in-class as well as exams). If you are a student currently experiencing barriers to your academics due to disability related reasons, and you would like to understand whether academic accommodations could support the removal of those barriers, please visit the QSAS website to learn more about academic accommodations or start the registration process with QSAS by clicking ***Access Ventus*** button at **Ventus | Accessibility Services | Queen's (queensu.ca)**

VENTUS is an online portal that connects students, instructors, Queen's Student Accessibility Services, the Exam's Office and other support services in the process to request, assess, and implement academic accommodations.

To learn more go to: https://www.queensu.ca/ventus-support/students/visual-guide-ventus-students

20 Academic Consideration for Students in Extenuating Circumstances

Academic Consideration is a process for the University community to provide a compassionate response to assist students experiencing unforeseen, short-term extenuating circumstances that may impact or impede a student's ability to complete their academics. This may include but is not limited to any extenuating circumstance (illness, bereavement, traumatic event, injury, family emergency, etc.) which is short-lived, begins within the term, and will not last longer than 12 weeks - see Academic Consideration webpage for details (https://www.queensu.ca/artsci/undergraduate/student-services/academic-consideration)

Each Faculty has developed a protocol to provide a consistent and equitable approach in dealing with requests for academic consideration for students facing extenuating

circumstances. For more information, undergraduate students in the Faculty of Arts and Sciences should consult the Faculty's webpage on Academic Consideration in Extenuating Circumstances and submit a request via the Academic Consideration Request Portal. Students in other Faculties and Schools who are enrolled in this course should refer to the protocol for their home Faculty.

Students are encouraged to submit requests as soon as the need becomes apparent and to contact their instructor and/or course coordinator as soon as possible once academic consideration has been granted. Any delay in contact may limit the options available for academic consideration. While we encourage instructors to accommodate, each instructor has discretion in deciding whether or how to apply the Academic Consideration. For more information on the Academic Consideration process, what is and is not an extenuating circumstance, and to submit an Academic Consideration request, please see the Faculty of Arts and Science's Academic Consideration website. ASO courses include links to information on **Academic Consideration** on your **Course Homepage** in onQ.

Please see the Teaching Team page for contact information for your instructor and TA(s), where relevant.

For more information, please see the Senate Policy on Academic Consideration for Students in Extenuating Circumstances.

21 Queen's Policy Statement on Academic Integrity

Queen's University is dedicated to creating a scholarly community free to explore a range of ideas, to build and advance knowledge and to share the ideas and knowledge that emerge from a range of intellectual pursuits. Each core value of academic integrity, as defined in the Senate Academic Integrity Policy, gives rise to and supports the next.

Honesty appears in presenting one's own academic work, whether in the context of an examination, written assignment, laboratory or seminar presentation. It is in researching one's own work for course assignments, acknowledging dependence on the ideas or words of another and in distinguishing one's own ideas and thoughts from other sources. It is also present in faithfully reporting laboratory results even when they do not conform to an original hypothesis. Further, honesty is present in truthfully communicating in written and/or oral exchanges with instructors, peers and other individuals (e.g. teaching assistants, proctors, university staff and/or university administrators).

Trust exists in an environment in which one's own ideas can be expressed without fear of ridicule or fear that someone else will take credit for them.

Fairness appears in the proper and full acknowledgement of the contributions of collaborators in group projects and in the full participation of partners in collaborative projects.

Respect, in a general sense, is part of an intellectual community that recognizes the participatory nature of the learning process and honours and respects a wide range of opinions and ideas. However, "respect" appears in a very particular sense when students attend class, pay attention, contribute to discussion and submit papers on time; instructors "show respect by taking students' ideas seriously, by recognizing them as individuals, helping them develop their ideas, providing full and honest feedback on their work, and valuing their perspectives and their goals" ("The Fundamental Values of Academic Integrity", 3rd Edition, p. 8).

Ultimately, responsibility is both personal and collective and engages students, administrators, faculty and staff in creating and maintaining a learning environment supported by and supporting academic integrity.

Courage differs from the preceding values by being more a quality or capacity of character – "the capacity to act in accordance with one's values despite fear" ("The Fundamental Values of Academic Integrity", 3rd edition, p. 10). Courage is displayed by students who make choices and integrous decisions that are followed by action, even in the face of peer pressure to cheat, copy another's material, provide their own work to others to facilitate cheating, or otherwise represent themselves dishonestly. Students also display courage by acknowledging prior wrongdoing and taking proactive measures to rectify any associated negative impact.

All of these values are not merely abstract but are expressed in and reinforced by the University's policies and practices.