Nanyang Technological University
Division of Chemistry and Biological Chemistry

Academic Year	AY2020-21	**Semester**	2
Course Coordinator	Tan Howe Siang, Loh Zhi Heng		
Course Code	CM1804		
Course Title	Mathematics for Chemistry		
Pre-requisites	MH1802: Calculus for the Sciences		
No of AUs	2		
Contact Hours	2 hours per week (2 hours of Lecture)		
Proposal Date	6 January 2020		

Course Aims

This course aims to

- ensure students acquire the mathematical skills and analytical capability to read higher level core physical chemistry courses which cover topics such as quantum chemistry, spectroscopy, kinetics, and thermodynamics
- equip students with adequate mathematical reading skills so that they can read and understand related mathematical content in the basic and popular scientific and engineering literature
- equip students with mathematical communication skills so that they can effectively and rigorously present their mathematical ideas to mathematicians, scientists and engineers.

Intended Learning Outcomes (ILO)

Upon the successful completion of this course, you (as a student) would acquire the mathematical competence and understand their applications to associated chemical problems. You will be able to:

Cartesian and Spherical Coordinates (CSC)

1. transform functions between the Cartesian and Spherical Coordinate system;
2. use the appropriate coordinates when solving problems with the corresponding symmetry and perform coordinate transformations;
3. visualize the shapes of atomic orbitals given their mathematical functions;
4. perform double or triple integral to determine surface areas and volumes in 3D space;

Complex numbers (CN)

5. manipulate complex numbers using Euler's formula and de Moivre's theorem to solve related problems;

Summation, Series and Expansion of Functions (SSE)

6. express functions in terms of a power series;
7. apply power series to obtain meaningful approximate solutions to problems in chemistry;

Vectors (V)

8. perform vector multiplications to solve related problems;
9. apply the concept of basis sets and use it for the expansion of functions;
10. perform transformation of basis vectors;

Linear Algebra and Matrices (LAM)

11. demonstrate understanding of the concepts and properties of matrices through solving problems;
12. perform simple matrix operations;
13. determine eigenvectors and eigenvalues of a given matrix and use them to solve related problems;
14. apply the above-mentioned concepts to solve problems in chemistry (such as rate kinetics, optics, and applied quantum mechanics problems);

Fourier Transform (FT)

15. recognize the use of Fourier Transforms and be able apply it whenever appropriate; and
16. apply FT to understand molecular spectroscopy: Fourier Transform Infrared (FTIR) and Nuclear Magnetic Resonance (NMR) Spectroscopy

Course Content

Cartesian and Spherical Coordinates (CSC)

Polar and spherical coordinates; Change of variables in double and triple integrals; Jacobians.

Complex numbers (CN)

Polar representation of complex number; de Moivre's theorem; Euler's formula.

Summation, Series and Expansion of Functions (SSE)

Maclaurin and Taylor series; Applications to chemical problems.

Vectors (V)

Vector multiplications; Basis Sets; Transformation of basis vectors.

Linear Algebra and Matrices (LAM)

Determinants; Matrix operations; Matrix diagonalization; Eigenvector and eigenvalue; Coupled rate equations; Applications to other selected topics in quantum mechanics and optics.

Fourier Transform (FT)

Fourier Transform Equations; Fourier Transform Infrared Spectroscopy; Free Induction Decay in NMR spectroscopy.

Assessment (includes both continuous and summative assessment)

Component	Course LO Tested	Related Programme LO or Graduate Attributes	Weighting	Team/Individual	Assessment Rubrics
1. Final Examination	All	Competence, written communication	60%	Individual	Point-based marking (not rubrics based)
2. Continuous Assessment – Component 1 (Weekly Assignments / Quiz)	All	Competence	12%	Individual	Point-based marking, automated marking (not rubrics based)

3. Mid Term 1	BAS / DIF	Competence	14%	Individual	Point-based marking (not rubrics based)
4. Mid Term 2	DIF / INT	Competence	14%	Individual	Point-based marking (not rubrics based)
5. Total	100%				

Formative feedback

[Component 2] Formative feedback is given through discussion within tutorial lessons as well as interactive, computer based hints and pointers in the online assignments/weekly assignments.

[Component 3, 4] Feedback is also given after each midterm on the common mistakes and level of difficulty of the problems.

Learning and Teaching approach

Approach	**How does this approach support students in achieving the learning outcomes?**
Derivation of formulas and demonstrating problem solving (Lecture and Tutorial)	Train students to be independent learners who are able to derive ideas/concepts from first principles and take ownership of their own learning. Help students understand the motivation behind mathematical theorems, definitions and formulas. Develop the train of thought in problem solving and presentation skills in presenting mathematical solutions.
Problem solving (Lecture)	Develop competence in solving chemical problems using mathematical skills.

Reading and References

Applying Maths in the Chemical & Biomolecular Sciences. An example based approach, Godfrey Beddard. Oxford University Press, 1st edition (2009), ISBN-13: 978-0199230914.
Mathematical Methods for Physics and Engineering: A Comprehensive Guide, K. F. Riley, M. P. Hobson, S. J. Bence. Cambridge University Press, 3rd edition (2006), ISBN: 0521861535.

Course Policies and Student Responsibilities

Absence Due to Medical or Other Reasons

If you are sick and unable to attend your class (particularly the mid-terms), you have to:

1. Send an email to the instructor regarding the absence and request for a replacement class.
2. Submit the original Medical Certificate* to administrator.
3. Attend the assigned replacement class (***subject to availability***).

* The medical certificate mentioned above should be issued in Singapore by a medical practitioner registered with the Singapore Medical Association.

Academic Integrity

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values.

As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Course Instructors

Instructor	Office Location	Phone	Email
Tan Howe Siang	SPMS-CBC-03-06	6316 2987	howesiang@ntu.edu.sg

Planned Weekly Schedule

Week	Topic	Course LO	Readings/ Activities
1,2	Cartesian vs. Spherical coordinates.	CSC 1, 2	#
2,3	Atomic orbitals. Double and triple integrals	CSC 3, 4	#
4,5	Power Series	SSE 6,7	#
5,6	Complex numbers. Vector multiplications	CN 5, V 8	#
7	Basis sets. Transformation of basis vectors	V 9, 10	MT1,#
8	Matrices	LAM 11, 12	#

9	Eigenvectors and eigenvalues	LAM 13	#
10	Applications of matrices in chemistry	LAM 14	#
11,12	Fourier transform	FT 15	MT2,#
12,13	Applications to Chemistry and Spectroscopy	FT 16	#

MT* Mid-term - to be conducted off regular curriculum time (in the evenings or Saturdays)
Pre/Post-lecture online assignments

CBC Programme Learning Outcome

The Division of Chemistry and Biological Chemistry (CBC) offers an undergraduate degree major in Chemistry that satisfies the American Chemical Society (ACS) curricular guidelines and equips students with knowledge relevant to the industry. Graduates of the Division of Chemistry and Biological Chemistry should have the following key attributes:

1. Competence

Graduates should be well-versed in the foundational and advanced concepts of chemical science, be able to evaluate chemistry-related information critically and independently, and be able to use complex reasoning to solve emergent chemical problems.

2. Creativity

Graduates should be able to synthesize and integrate multiple ideas across the curriculum, and propose innovative solutions to emergent chemistry-related problems based on their training in chemistry.

3. Communication

Graduates should be able to demonstrate clarity of thought, independent thinking, and sound scientific analysis and reasoning through written and oral reports to audiences with varying technical backgrounds. They should also be able to effectively engage other professional chemists in collaborative endeavours.

4. Character

Graduates should be able to act in responsible ways and uphold the high ethical standards that the society expects of professional chemists.

5. Civic-mindedness

Graduates should be aware of the impact of chemistry on society, and how chemistry can be applied to benefit mankind. They should also be aware of and uphold the best chemical safety practices.