

**Revision of the course number: CHM521**

**Title of the course: Mathematics for Chemistry**

**Credit details: 2-0-0-0 [6]**

**Objective of the course:** Introducing basics of mathematics, which are essential for the chemistry courses during the MSc 2 year. This course could also be open to PhD students.

**Specialized Infrastructure requirement:** None

**Modular/Full semester:** Full semester

**Instructional aspects:** The topics are to be taught with examples from chemistry. Tools like Mathematica/Matlab/Octave are encouraged to be used in this course.

**Course content:** (*This will go in the "Courses of Study" book. Please note that the duration of each lecture is 50 minutes.*)

**Lecture-wise break-up: (please note that the duration of each lecture is 50 minutes)**

<b>Topic</b>	<b>Suggested no. of lectures</b>
Functions: Series expansion, Special functions (including plotting and sketching), contour plots/surfaces, maximum and minimum of functions (of one and many variables)	4
Differential Equations: First Order Linear Differential Equation (Homogenous, Non-Homogenous), Second Order differential equation, Solution by Power Series Expansion, Sturm-Liouville Problem, Eigenvalue-Eigenfunction Problems	8
Partial Differential Equations: Method of Separation of Variables, Wave Equation, Diffusion	4
Fourier Series and Transform: Sine and Cosine Series, Fourier Transforms, Power Spectra, Applications in Solving Partial Differential Equations	4
Linear Algebra: Vector Space, Hilbert Space, Inner Products, Solving Linear Equations, Matrix Inversion, Eigenvalues and Eigenvectors, Hermitian Matrices, Matrix Equations	6
Coordinate Transform: Polar Coordinates, Spherical Polar Coordinates, Elliptical Coordinates	2
<b>Total number of lectures</b>	<b>28</b>

**Suggested text and reference material:**

1. D. A. McQuarrie, Mathematical Methods for Scientists and Engineers, University Science Books
2. M. L. Boas, Mathematical Methods in the Physical Sciences, John Wiley, India
3. George B. Arfken, Hans J. Weber and Frank E. Harris, Mathematical Methods for Physicists, Academic Press (2001).
4. E. Kreyszig, Advanced Engineering Mathematics, 10 th Edition, Wiley (2018).

**Main differences suggested in this review:**

The course is now made into an introductory level course. Only essential mathematics required for taking the chemistry courses in the MSc program will be covered.



Nisanth N Nair



Debabrata Goswami

(Names and signatures of the committee members)



T. G. Gopakumar (DUGC)