

MATH0042 Mathematical Methods in Chemistry

<i>Year:</i>	2021–2022
<i>Code:</i>	MATH0042
<i>Level:</i>	5 (UG)
<i>Value:</i>	15 credits (= 7.5 ECTS credits)
<i>Term:</i>	1
<i>Assessment:</i>	85% examination, 15% coursework
<i>Normal Pre-requisites:</i>	MATH0040, MATH0041
<i>Lecturer:</i>	Dr J Marshall

Course Description and Objectives

This is a course designed for second year students of chemistry, dealing with some of the mathematics useful for physical chemistry. Thus it covers series solution of ODEs, Legendre polynomials, group theory and some matrix theory. Applications of the methods to problems in Chemistry are discussed (e.g. the hydrogen atom).

Recommended Texts

Recommended books are: (i) G Stephenson, *Mathematical Methods for Science Students* (Longman); (ii) Kreysig, *Advanced Engineering Mathematics* (Wiley).

Detailed Syllabus

- Solution of differential equations in series. Regular and singular points. Legendre's differential equation.
- Solution of partial differential equations by separation of variables. Bessel's equation. Laplace's equation. Wave equation.
- Three-dimensional problems with central potential. Angular momentum. Schrödinger equation for the hydrogen atom.
- Introduction to matrices. Orthogonal and unitary matrices. Hermitian matrices. Normal modes. Functions of matrices.
- Group theory. Symmetry groups. Transformation matrices. Matrix representations of groups.

About 20 lectures are given and most but not all the above material is usually covered in this time.