

# 6201 (Mathematical Methods in Chemistry)

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| <i>Year:</i>                  | 2014–2015   |
| <i>Code:</i>                  | MATH6201  |
| <i>Level:</i>                 | Intermediate  |
| <i>Value:</i>                 | Half unit (= 7.5 ECTS credits)                          |
| <i>Term:</i>                  | 1   |
| <i>Structure:</i>             | 3 hour lectures per week.<br>Weekly assessed coursework |
| <i>Assessment:</i>            | 90% examination, 10% coursework                         |
| <i>Normal Pre-requisites:</i> | MATH6105, MATH6106                                      |
| <i>Lecturer:</i>              | Dr L Louder   |

## *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.
- Three-dimensional problems with central potential. Separation of variables. Angular momentum. Hydrogen atom.
- Introduction to matrices. Orthogonal and unitary matrices. Normal modes and matrices. Functions of matrices.
- Elementary group theory related to ideas of symmetry.
- About 20 lectures are given and most but not all the above material is usually covered in this time.