The following courses were part of my B.Sc. (Hons) degree, the complete syllabus can be accessed here: http://du.ac.in/du/uploads/old-ug-courses/04082010_chem.pdf

Paper 4-MACT 101: Mathematics - I

THEORY **Marks: 100**

Unit I: Recapitulation:

Fundamentals. Mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Mathematical series: Power series, Maclaurin, Taylor series, convergence (e.g. pressure virial equation of state, colligative properties).

Pythagoras theorem in three dimensions. Trigonometric functions, identities.

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations), differentials, higher order derivatives, discontinuities, stationary points, maximum minimum problems, inflexion points, limiting values of functions: L'Hôpital's rule, combining limits.

Unit II: Integral calculus:

The process of integration, odd and even functions, indefinite integrals, standard integrals, methods of integration (e.g. integrated rate law for second order reaction), numerical integration
(Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data),

probability distributions (gas kinetic theory) and mean values. Calculus of the trigonometric functions.

Calculus with several independent variables: Functions of several independent variables, change of variables, relations between partial derivatives (e.g. change in pressure for small changes in volume and temperature), total differentials, chain rules for partial differentiation, Euler's theorem, exact and inexact differentials (thermodynamics), line integrals.

Recommended Texts:

1. McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
2. Mortimer, R. *Mathematics for Physical Chemistry.* 3rd Ed. Elsevier (2005).
3. Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
4. Yates, P. *Chemical Calculations.* 2nd Ed. CRC Press (2007).

Paper 12-MACT 302: Mathematics - II

THEORY **Marks: 100**

Differential equations: differential equations with separable variables, series solution, numerical solutions of differential equations. Newton' laws of motion. The linear harmonic oscillator: Linear differential equations with constant coefficients.

Partial differential equations: separation of variables. The wave equation. Schrödinger's equation.

Multiple integrals. Changing variables. Vector derivative operators. Multiple integrals involving other coordinate systems (spherical polar). Maximum and minimum values of functions of several variables.

Stationary points, imaginary and complex numbers, complex plane, Euler's formula and polar form of complex numbers, complex conjugates, modulus of a complex number.

Operators: operator algebra, linear operators, eigenfunctions and eigenvalues, commutators of operators, Hermitian operators.

Vectors and coordinate systems: Unit vectors (application in solid state), addition and subtraction of vectors, multiplication of vectors. Vector calculus. Vectors and coordinate systems in three dimensions (Cartesian, spherical polar and their interconversion).

Determinants. Matrix algebra, Simultaneous equations: method of substitution and elimination, consistency and independence. Homogeneous linear equations. Simultaneous equations with more than two unknowns (e.g. spectrophotometry), Cramer's rule, matrix inversion, orthogonal and unitary matrices, matrix eigenvalues and eigenvectors, diagonalization of a matrix.

Recommended Texts:

1. McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
2. Mortimer, R. *Mathematics for Physical Chemistry.* 3rd Ed. Elsevier (2005).
3. Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
4. Yates, P. *Chemical calculations.* 2nd Ed. CRC Press (2007).

Paper 6-CHHT 204: Analytical Methods in Chemical Analysis

THEORY **Marks:100**

Unit I: Qualitative and Quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q, and T test, rejection of data, and confidence intervals.

Paper 8-PHCT 201: Physics-I

THEORY **Marks: 100**

Unit I: Mathematical Physics: Scalar and vector products, polar and axial vectors, triple and quadruple products.

Unit II: Vector calculus:

Scalar and vector fields, differentiation of a vector, gradient, divergence, curl and Δ operations and their meaning, idea of line, surface and volume integrals, Gauss and Stokes' theorem.

Recommended Texts:

1. Spiegel, M. R. *Vector Analysis* Schaum's Outline Series. McGraw-Hill Book Co.: Singapore (1974)
2. Beiser, A. *Concepts of Modern Physics* McGraw-Hill Education (2002).
3. Resnick, R., Halliday, D. & Krane, K. S. Physics Vol. I and II 5th Ed. John Wiley & Sons (2004)
4. Serway, R. A. & Jewett, J. W. *Physics for Scientists and Engineers* 6th Ed.

Paper 24-CHHT 618: Applications of Computers in Chemistry

THEORY Marks: 100

Unit I: Recapitulation of computer basics:

PC hardware, operating systems, data storage and backup, networks, information technology. Basic operations using windows.

Unit II: Computer programming:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

BASIC programs for numerical differentiation and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method), numerical solution of differential equations.

Conceptual background of molecular modelling: Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

PRACTICAL: Numeric modelling, numerical curve fitting, linear regression, numerical differentiation, integration. Numerical solution of differential equations.

Recommended Texts:

1. Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).
2. Venit, S.M. *Programming in Basic: Problem solving with structure and style.* Jaico Publishing House: Delhi (1996).
3. Engel, T. & Reid, P. *Physical Chemistry* 2nd Ed. Pearson (2010). Chapter on Computational Chemistry.

The following courses were part of my M.Sc. degree, the complete syllabus can be accessed here: http://www.nitj.ac.in/chemistry/MSc_Chemistry_Syllabus.pdf

L	T	P	C
0	0	4	2

CY-571 Computational Skills, Graphics & Simulation Lab

1. **Programming in C Language:** Introduction, writing programmes in C language, Exercises in C language. Features of C++ and Visual C.

2. **Introduction to Web and Internet:** LAN and E-mail, Importance of Internet; Types fo search engines: Basic components of browsing page; importance of networks; networking personal computers; importance of E-mailing, search engines in chemical sciences.

3. **Computer Graphics:** Computer-aided design, Presentation graphics, Computer art, Entertainment, Education and training, Visualization, Image processing, Graphical user interfaces.

4. **Numerical Methods and Simulation:** Numerical methods in chemistry, Mathematical modelling of reactions and their simulation, Analysis and synthesis of chemical systems.

5. **Computer Animation:** Design of animation sequences, General computer animation, Kinematics and Dynamics.

REFERENCES:

1. C Programming: Absolute Beginner's Guide**.** Greg Perry, Dean Miller.
2. Let Us C. Yashavant P. Kanetkar, Ashutosh Pandey.
3. Programming: Principles and Practice Using C++. Bjarne Stroustrup.
4. Jumping into C++. Alex Allain.

L	T	P	C
3	1	0	4

CY-631 Analytical Principles and Instrumental Methods of Analysis

1. **Data Analysis:** Uncertainties, Errors, calibrations, Mean, Standard Deviation, Least square fit.

REFERENCES:

5. Instrumental Methods of Analysis, Willard, Merritt, Dean and Settle, CBS Publisher and Distributors.,1986.

L	T	P	C
0	0	4	2

CY-597 SUMMER TRAINING IN RESEARCH LAB

This was part of my M.Sc. degree, where I did a research project in a Computational Biophysics & Soft Matter research lab in a separate research institute (Indian Institute of Science Education & Research).
I worked on a computational chemistry project which involved: a) working with UNIX systems on a super computing cluster; b) Installing and configuring chemistry software packages; c) Writing python and bash scripts for calculating various chemical and molecular properties.
More details (including project report, presentation and certificate) are here: https://github.com/tanu-rana/Graduate-Summer-Internship

L	T	P	C
0	0	16	8

CY-600 PROJECT

This was my one-year masters research project which was a partial extension of the above summer project. It was partially computational and partly experimental. Just mentioning here, the computational chemistry aspects (leaving out the experimental other half):

- Was responsible for writing programs in python and C++ (for atomic/molecular systems) which in turn ran on a remote supercomputing Linux cluster.
- Did computational studies of MoS_2 Quantum Dots using Molecular Dynamics and Monte Carlo Simulations using GROMACS and GAUSSIAN. Used other molecular chemistry software packages for visualization and trajectory analysis.