Theoretical Methods in Chemistry - 2

Prof. Nicholas Harrison
nicholas.harrison@imperial.ac.uk
http://www.ch.ic.c.uk/harrison/Teaching/teaching.html
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Aims

To provide an introduction to practical theoretical methods used in physical, inorganic and organic chemistry.

Summary

8 Lectures (4 Autumn Term, 4 Spring Term)

The following topics will be covered

- Solving linear equations - determinants
- LCAO theory and the chemical bond
- Matrices for larger systems – how modern codes work
- Matrix elements and properties
- Symmetry & Matrices
- Series summations (arithmetic and geometric progressions)
- Summing partition functions
- Thermodynamics in the quasi-harmonic approximation.

3 Problem Classes (1 Autumn Term and 2 Spring Term)

The problem classes provide an opportunity for supervised problem solving using the methods discussed in the lectures and exploited in the labs.

Autumn Term:

Week 6	06-Nov	Tue	2-5	Pippard LT (Group B)
Week 10	04-Dec	Tue	2-5	Pippard LT (Group A)

Spring Term:

Week 4	30-Jan	Tue&Thurs 2-5	Pippard LT (Group B)
Week 7	20-Feb	Tue&Thurs 2-5	Pippard LT (Group A)

3 Theoretical Methods Laboratories (1 Autumn Term, 2 Spring Term)

Three computer based projects which illustrate the concepts introduced in the lectures. The projects focus on chemical concepts and are designed to encourage self-study offering opportunities for students to explore theoretical chemistry using state of the art computational tools. Each project should occupy about 12 hours in the computer laboratory over the course of a week. Projects are assessed through a laboratory report for accuracy, originality and innovation. Laboratories are structured as supervised sessions

Chemistry Computer Room C1. 135

Autumn Term

Molecular Symmetry
2pm-5pm on Mon-Tue-Thurs and Friday

Group B:	Week 7	13th Nov.
Group A:	Week 11	11th Dec

Spring Term

Thermodynamics of MgO (Vibrations and Thermal Expansion)
11am-1pm on Mon-Tue-Thurs and Friday

Group B:	Week 5	5th Feb
Group A:	Week 8	26th Feb

Electronic Structure
11am-1pm on Mon-Tue-Thurs and Friday

Group B:	Week 6	12th Feb
Group A:	Week 9	5th March

Objectives

By the end of this course you should be able to:

- Sum the partition function of analytic systems and derive thermodynamic quantities
- Test series for convergence
- Perform basic matrix operations
- Solve the eigenvalue problem for chemical bonding in the Huckel approximation
- Analyse the band structure of simple metals and semiconductors
- Identify molecular symmetries and determine molecular symmetry groups.
- Analyse NMR spectra.

Building Upon: Theoretical Methods 1 and Quantum Mechanics lecture courses, Theoretical Methods 2 laboratory. Physical Chemistry Lecture courses including in particular Electrochemical Dynamics, Interfacial Thermodynamics, Spectroscopy and Electronic Properties of Solids.

Looking Forward to: Theoretical Methods Laboratory 2, 2nd year lecture courses in Interfacial and Statistical Thermodynamics, Electronic Properties of Solids and Photochemistry, 3rd year lecture courses in Quantum Chemistry and Symmetry and Spectroscopy.

Bibliography

1. *The Chemistry Maths Book*, Erich Steiner, OUP, 1996
2. *Experiments in Undergraduate Mathematics,* Kent, Ramsden and Wood, ICP.
3. *Mathematical Methods for Physics and Chemistry,* Mary L Boas, Wiley.