CHEM763 Special Topics in Chemistry

This module comprises 32 credits which is equivalent to 80 L. You are allowed to select from the list below the topics that in total will give 80 L.

For example:
Student A chooses *X-ray Crystallography*, *Stability of Metal Complexes, Industrial Perspective of Analytical Science, Introduction to Mass Spectrometry, Introduction to Bioinorganic Chemistry and Strategies in Drug Synthesis and Design* for a total of 80 L.

Student B chooses *X-ray Crystallography, Stability of Metal Complexes, Chemical Biology and Natural Products, The Chemistry of the f-Block Elements and Introduction to Mass Spectrometry* for a total of 80 L.

TOPIC DESCRIPTORS

X-ray Crystallography: Symmetry in the Solid State [20 L]

Dr. Matthew Akerman

This course will cover both the theoretical and practical aspects of single crystal X-ray crystallography. The theoretical aspect will focus on the following concepts: lattice and unit cells, point symmetry operations using the international notation, the 32 crystallographic point groups, the 7 crystal systems, the 14 Bravais lattices, development of space groups and applications of space group symmetry. The practical component will cover crystal growth, crystal selection and crystal mounting as well as basic data collection strategies, data reduction and structure solution. The data reduction and structure solution components will be the culmination of both the practical and theoretical aspects of single crystal X-ray diffraction. The course will have a practical test.

The Chemistry of the *f*-Block Elements [10 L]

Dr Irvin Booysen

The f-block elements exhibit unique physical and chemical properties which render them ideal in an array of applications used in medicinal inorganic chemistry, nuclear reactors and superconductors. In this course we will focus on the chemistry of the lanthanides (4f block) and actinides (5f block elements). In particular, the general trends, the properties and the influential factors on the coordination chemistry will be described. In addition, the occurrence and extraction of these elements, as well as the preparation of special actinides will be highlighted. We will briefly examine the coordination chemistry of selected metals. Finally we will associate these properties with common lanthanide and actinide applications.

Recommended Textbooks

1. P. Atkins, Shriver and Atkins' Inorganic Chemistry, Oxford, 5th edition.
2. J.D. Lee, Concise Inorganic Chemistry, Chapman & Hall, any edition.

Industrial Perspective of Analytical Science

Mrs Heidi Duveskog

Education will play a pivotal role in preparing individuals and companies for change. Graduates in the workforce will need to develop cutting edge competencies and knowledge of services that will enable them to adapt to the changing nature of employment.

Excerpt from Programme for University Industry Interface (Ireland)

Course Description

The aim of the course is to highlight the multifaceted role of Analytical Science in industry and the environment. To give the participants an overview of how Analytical Science is applied across a value chain of processes and to introduce them to the various technologies and stakeholders encountered in the workplace.

This course is designed to educate the participants about careers as scientists and as industrial analytical practitioners specifically. Students are made aware of the different roles of the industrial analytical chemist/scientist. These include analyst, scientific consultant, method developer (researcher), and most importantly, problem solver.

Another focus of the course is on further development of professional transferable skills. Analytical Chemistry provides a perfect platform for this because it is involved with everyday functioning of our society. More often than not, the analytical chemist/scientist has to deal with situations where the recipient of results is a non-scientific person e.g. business manager, plant engineer, lawyers, judges, legislators or civil servants. Apart therefore from technical competence, it is important for the analytical chemist/scientist to be able to communicate their findings effectively. The ability to translate the findings into the context of the problem statement is where the value proposition lies for the stakeholders. This requires a thorough understanding of the technical component of their area of expertise (concepts such as 'detection limits' and statistical tolerances associated with results), but also includes a thorough understanding of the business component and the ability to use those results to influence decisions. The course focuses extensively on the latter role, utilizing case studies and real problems solved in industry in general and at Sasol.

Students can use the skills they have developed in other courses in their studies for problem solving, and will come away with additional ones. The entire course is structured for extensive participation and interaction.

Assessment

2 Team assignments - Peer review and feedback
1 Individual assignment

Assessment Tools

The participants will be evaluated according to the following criteria:

a. The ability to learn new concepts
b. The ability to lead and influence
c. The ability to communicate effectively
d. The capacity to analyse and synthesise information
e. To solve problems
f. Participate in teamwork
g. Concern for quality
h. The capacity to adapt to new situations
i. Work in a virtual environment

Learning Tools to be used in course

Teaching – to share/give knowledge in context
Facilitation – to activate participation and integration
Team activities – to understand and practice different team roles

Application	– to build and practise skill
Assessment	– to develop self-knowledge
Reading	– to stimulate own thinking and understanding of latest work in the field

This course is scheduled to delivered during the week as block lecture which is equivalent to 10 L

Green Chemistry [10 L]

Dr. Vineet Jeena

The long-term impact of synthetic organic chemistry on the environment cannot be understated and in recent times, many environmental groups have called for stringent control on the use of certain chemicals. These groups have argued that efforts must be made to reduce exposure to these chemicals and that subsequent disposal of hazardous chemicals may affect the natural and aquatic environment. Synthetic chemists, on the other hand, have indicated the importance of being able to carry out chemical reactions under the optimum yet environmentally unfriendly conditions. For example, in developing drugs that have anti-Hepatitis B activity, the synthetic chemists focus their attention on the amount and purity of the potential drug rather than the environmental impact of the synthetic route.

Both of the above arguments have valid points and the obvious solution would be to marry these two concepts where synthetic chemistry is developed that is environmentally friendly and produces the desired compounds in high yields and purity. The following course will embrace this 'go green' methodology through the synthesis of valuable heterocycles, some of which possess interesting biological applications.

Introduction to Mass Spectrometry (MS) [10 L]

Dr. Allen Mambanda

This section of the module covers the fundamentals of mass spectrometry as an instrumental technique. There is a wide range of different MS instruments with different methods of producing, separating and detecting the masses of the generated ions.

At the end of the lectures, the students should understand the following concepts:

1) The basic (block) components of a mass spectrometer.
2) Principles of some selected methods of ionization. (Electron Impact (EI), Chemical Ionization (CI) (two methods primarily used for gaseous samples), Electrospray methods (liquids: nanoionspray and turboionspray & APCI) and MALDI (solids).
3) Principles of ion dispersion or separation of ion by the following selected mass analyzers: (sector-based: (magnetic/electric fields); time of flight; transmission and ion traps (including an appreciation of their use as tandems or hybrids).
4) Principles of ion/charge detection and amplification in mass spectrometry (electromultipliers and multichannels).
5) Applications of mass spectrometry in analytical chemistry.

(*10 L+ a tutorial assignment + a test*)

Useful books

1. J. Throck Watson & O. David Sparkman, *Introduction to Mass Spectrometry: Instrumentation, Applications, and Strategies for Data Interpretation*, 4th ed., John Wiley, 2007.
2. Edmond De Hoffmann & Vincent Stroobant, *Mass Spectrometry: Principles and Applications,*, 3rd ed., John Wiley, 2007.

Strategies in Ligand Design and Catalyst Development [10 L]

Dr. Stephen Ojwach

This course aims to introduce students to the basic principles and fundamentals of ligand design and catalyst development to achieve a catalyst system that is efficient, active, stable and selective for a given process. In broad terms, it covers the balance between catalyst stability, activity and selectivity. The relation between complex structure and catalyst activity; the role of ligand and metal atom, steric and electronic considerations, thermodynamic and kinetic factors and hemi-lability. Selected case studies, olefin oligomerization and polymerization; chain propagation verses chain termination and isomerization; hydroformylation and hydrogenation reactions; branched and linear products. Catalyst recycling through development of immobilization-methods, multiphase operations.

Strategies in Drug Synthesis & Design [10 L]

Prof. Ross Robinson

This course will focus on the synthesis of complex organic molecules, many of which are used as pharmaceuticals. You will be exposed to the rational design of pharmaceutically active compounds focusing on issues such as drug delivery, metabolism and synthetic strategies to fine-tune biological activity. Case studies such as the anti-malarials, anti-HIV compounds and the tropane alkaloids will be reviewed to illustrate certain concepts. Modern techniques such as combinatorial chemistry will also be dealt with.

Natural Products in Drug Discovery [20 L]

Prof. Fanie Van Heerden

Many pharmaceutical drugs (morphine, aspirin) are derived from natural products, i.e. compounds that are produced by living organisms such as plants and microorganisms. In the course, you will be introduced to the different steps in the drug discovery pipeline and terms such as hit compound, a lead compound, structure-activity relationship, pharmacophore, pharmacokinetics, pharmacodynamics, clinical studies etc. The role that natural products played in drug discovery will be emphasised and you will be introduced to some South African ‘muthi plants’ and the compounds present in them. A short introduction to the biosynthetic pathways used by nature to assemble the major classes of natural products will be given.

Electron Paramagnetic Resonance (EPR) Spectroscopy [10 L]

Dr Bheki Xulu

This course aims to explain basic concepts of EPR spectroscopy and its chemical application. After completing this course students will understand basic features of EPR including the following topics:

- EPR spectroscopy: magnetic properties of electrons, quantization of angular momentum and magnetic moment; Zeeman effect, resonance condition; Selection rules for spin absorption; Construction and operation of EPR spectrometer.

- Characteristics of the EPR spectrum: intensities and number of lines; determination of the g-factor; relaxation processes, line width, EPR signal saturation.
- Hyperfine interactions.
- Hyperfine interactions, the anisotropic and isotropic components, powder spectra.
- Spin trapping.
- Simulation.