UNIVERSITY OF
KWAZULU-NATAL

School of Chemistry

Honours 2010

General Information Document

Dr WE van Zyl
(Honours Coordinator)

January 2010

HONOURS CLASS 2010

Welcome! The staff wishes to congratulate you for choosing to do your Honours degree at the UKZN School of Chemistry (Westville Campus) in 2010, and for meeting the minimum academic requirement we implement for enrolment.

Employment statistics clearly indicate that successful completion of an Honours degree in Chemistry will make you significantly more marketable and with better remuneration and perspectives within the chemical industry, be it in the private-, government-, or education sectors. Indeed, the Honours degree is the minimum requirement to be considered a qualified chemist, and to register as a professional scientist.

The School of Chemistry on the Westville Campus has recently undergone a dramatic make-over. This included acquiring state-of-the-art facilities and infrastructure for teaching and research. The laboratory, lecture room, and computing facilities as a stand-alone unit for the exclusive use of Honours students is among the largest and best equipped in the country. We also have an excellent fleet of experienced and energetic staff to guide and teach you along the way.

Honours is tough! – Deal with it! The Honours degree we offer is significantly more difficult and challenging than any Chemistry course or undergraduate degree you ever enrolled in.

What makes it difficult? Here are some of the reasons: You will be introduced to many new topics in Chemistry that you vaguely or never heard of before and the course materials will grow rapidly, relentlessly and with an increased intellectual challenge. It is therefore imperative to stay on top of your game from the first hour of Day 1. You will be expected to be at the School from approx. 8 am to 5 pm, Monday to Friday, during which time you will be either engaged in lectures or practicals. Many former successful Honours graduates will tell you effective “time management” was among the hardest challenges to confront. You will be expected to set your priorities straight, a lot will come down on your plate: from pracs to lectures to study-time to library visits to report writing and related assessment mechanisms, and many more; YOU need to figure how to best spend your time and energy for optimal returns (i.e. marks).

Many of you may consider furthering your education through a research-based MSc degree with one of many research-active staff within the School; indeed, the School strongly encourages applications for postgraduate studies at this level. Take note that the entrance requirement for MSc studies at the School is an average of >60% for your Honours degree as a whole, as well as 60% earned separately in the research project (CHEM791). It therefore makes good sense to work hard and smart right from the start!

Finally, take heart of the fact that many students have achieved the goal of an Honours degree before you, and many more will achieve it after you, but now it is your turn to shine. Make the best of it!

Dr WE van Zyl
Honours Coordinator

HONOURS 2010 INDUCTION PROGRAMME 3RD TO 9TH FEBRUARY 2010

LECTURE CONTENT (STARTS 08H40)	PRACTICAL COMPONENT (STARTS 14H10)
Wednesday 3 Feb.: **Mr Dilip Jagjivan and Dr Phil Coombes** NMR Topspin (software) Data interpretation	Wednesday: **Dr P Coombes** NMR: H and C nuclei only. Interpretation. 2-D
Thursday 4 Feb. **Dr P Coombes and Dr M Bala** SciFinder ChemOffice (Chemistry Drawings)/ Freeware downloads Cambridge Crystallographic Structural Database (CCSD)	Thursday **Dr P Coombes** NMR: H and C nuclei only. Interpretation.
Friday 5 Feb. **Prof Martincigh** Use of a Laboratory Notebook; How to Write a Scientific Report; Time Management	Friday **Dr W.E. van Zyl** Safety lab, solvent pre-drying, solvent drying, Na wire pressing, freeze-thaw-degassing, Schlenk tubes, Schlenk lines. Tour.
Monday 8 Feb. **Prof Martincigh** Practical aspects of HPLC (and GC) Basic Analytical Procedures and Data Manipulation.	Monday **Dr M. Humphries and Prof B.S. Martincigh** Class to be divided in half for today and tomorrow. FT-IR +ATR: Skill in using one method, theory of other methods. KBr; Nujol mulls; thin films. UV-vis
Tuesday 9 Feb. **Prof B. S. Martincigh** Presentations (Oral and Poster)	Tuesday **Prof Martincigh and Dr Humphries** FT-IR and UV-vis (same as Mon. programme)

GENERAL

THE COURSE

The aim of the Honours Programme in Chemistry is to introduce students to advanced studies in analytical methods, inorganic-, organometallic- and supramolecular chemistry, organic chemistry and physical chemistry; to enable students to specialize in various areas of chemistry; and to introduce students to the process of scientific research. In the first semester, the course consists of core modules in each of the Analytical, Inorganic, Organic and Physical Chemistry sections, as well as a practical component over 2 weeks, with 1 week of assessment for each section. A selection of elective topics in these general areas, as well as a 12 week research project, is given in the second semester. The core modules in the first semester each consist of 30 lectures, whereas elective topics amounting to 80 lectures are chosen for the second semester.

The titles of the topics offered are given below, and detailed course outlines are provided further in this document.

FIRST SEMESTER COURSES

Course (Code)	Topic	Lecturer	No. of lectures
Analytical Chemistry (CHEM741)	A1. Sample Preparation and Speciation A2. Electroanalytical Techniques A3. Mass Spectrometry	Prof A. Kindness Dr C. Ngila Dr B. Moodley	10 10 10
Inorganic Chemistry (CHEM711)	I1. Organometallics in Catalysis I2.Organometallics and Materials Chemistry I3. Supramolecular & Nanomaterials Chemistry	Prof H.B. Friedrich Dr V.O. Nyamori Dr. W. E. van Zyl	10 10 10
Organic Chemistry (CHEM721)	O1. Stereochemistry O2. Synthesis in Action & Mechanisms of some Pericyclic Reactions O3. Selective reactions and protection	Dr P. H. Coombes Prof F. Shode Dr N. A. Koorbanally	10 10 10
Physical Chemistry (CHEM731)	P1. Molecular Symmetry P2. Gas and Solution Kinetics P3. Photochemistry	Prof T.A. Ford Prof S. B. Jonnalagadda Prof B. S. Martincigh	10 10 10

SECOND SEMESTER COURSES

A full list of elective courses will become available during the course of the first semester. Students will be advised of the full range of available topics before they are asked to make their selections. Courses may be withdrawn due to insufficient student numbers.

LECTURES
All first semester lectures will take place at 08h40 and end at 10h20 each day from Monday to Friday. A separate lecture timetable will operate during the second semester.

PRESCRIBED AND/OR RECOMMENDED TEXTBOOKS
These will be indicated by the lecturers responsible for teaching each course.

TUTORIALS
Although tutorials are not formally scheduled for Honours courses, lecturers may wish to use some of their scheduled lecture periods for tutorial purposes. The actual distribution between formal lectures and tutorials in each course will be at the discretion of the lecturer responsible.

PRACTICAL COMPONENT
Practical work in each of the four sections Analytical, Physical, Inorganic and Organic Chemistry will be held during the first semester. This amounts to 10 workdays for each section, with the following 5 workdays allocated for assessment. The specifics of the Practicals will be given to you by the lecturer in charge of each section.

The schedule for the first semester practical work can be summarized as follows:

WK 1	WK2	WK3	WK4	WK5	WK6	WK7	WK8	WK8-12	WK13	WK114	WK15	WK16
INDUC	INDUC	ANAL	ANAL	ANAL	ORG	ORG	ORG	PHYS	PHYS	INORG	INORG	INORG
				*			*		*			*

*Indicates the week during which the assessment of that section will take place. NOTE: In some cases the weeks may be broken up due to Public Holidays.

The First week, INDUC, is the Induction week during which a number of core practical principles will be presented, following the Induction lectures in the morning.

WEEK	Starting date	Finishing date	Section	Assessment dates	Day of assessment
1,2	Wed 3 Feb	Tues 9 Feb	Induction (5)	N/A	N/A
2,3,4,5	Wed 10 Feb	Tues 23 Feb (10)	Analytical	24/2 – 2 March	1 March
5,6,7,8	Wed 3 March	Tues 16 March (10)	Organic	17/3 – 24 March	23 March
8	Thurs 25 March	Friday 26 March (2)	Physical	CONT...	CONT...
8,9,10,11	27/3 – 5/4 VAC	VAC	VAC	VAC	VAC
11,12,13	Tues 6 April	Thurs 15 April (8)	Physical	16/4 – 22/4	21 April
13,14,15,16	Fri 23 April	7 May (10)	Inorganic	10/5 – 14/5	13 May

Assessment: Days 1-3 = preparation, Day 4 = assessment, Day 5 = lab clean-up.
*22 March Human Rights Day; 2 April Good Friday; 5 April Family Day; 27 April Freedom Day; 1 May Workers Day. The exact date of assessment within that week will be provided by the lecturer(s) at a later stage. ** Graduation ceremonies take place during 19-23 April whereby students can take the afternoon off, as applicable. *** Need to start poster before this assessment.

ASSESSMENT OF PRACTICAL COMPONENT:

Analytical:
Viva (oral exam) (50%)
Lab notebook (30%)
Practical effort & attitude (20%)

Organic:
Written Report (50%)
Lab notebook (30%)
Practical effort & attitude (20%)

Inorganic:
Poster (50%). Introduction to poster to be given on individual basis. Your supervisor is not a co-author.
Lab notebook (30%)
Practical effort & attitude (20%)

Physical:
Oral presentation (50%)
Lab notebook (30%)
Practical effort & attitude (20%)

Students will be expected to provide themselves with two hard-covered A4 notebooks (one for Analytical and Inorganic and the other for Physical and Organic) which will be used for reporting the experimental results of all experiments. The notebook should be available for inspection at all times.

NOTE:
No students in lab area for ANY REASON after 17h30 without consent of Honours Coordinator, and only then in presence of another student working in lab.
No student allowed to work in lab over weekends.
Students receive computers virus free -- keep them that way!

CHEM791:
In the second semester students will undertake a research project selected from a number of projects offered by members of staff. During the second quarter of the academic year, students will be presented with descriptions of the projects and will be asked to make their first, second and third choices. Assignment of projects to students will be made before the end of the first semester, and every effort will be made to accommodate students' preferences. Some selections of projects may be restricted, as they may require one of the elective lecture courses to be taken in the second semester as a co-requisite. Students are strongly advised to consult with prospective supervisors regarding course pre-requisites before making their final choices. On completion, students will report the results of their research findings by means of a written report and an oral presentation. The oral presentations will take place during the week immediately following the end of lectures in October.

CHEM781:

A number of elective courses will be available in the second semester. Note that a course will only be offered if there is >40% attendance. As an example, if the whole Honours class has 16 students, a minimum of 7 students need to attend a course (44%), while 6 students (38%) would be insufficient, these students then need to find another course. Each student needs to take 4 electives and usually 5-6 different courses are eventually given (out of a potential 10 or so on offer).

EXAMINATIONS

One three-hour examination will be written in each of the four first semester core modules during June, and a combination of ninety-minute (1h30) and three-hour (3h) examinations, depending on students' choices, during November.

PROGRESSION TO SECOND SEMESTER

The rules for the award of a Bachelor of Science Honours degree are summarized in the Faculty of Science and Agriculture handbook (2010). To be allowed to progress to the second semester, the student should be on course towards meeting all the requirements of these rules.

PLAGIARISM

Plagiarism is defined as the submission or presentation of work, in any form, which is not your own, without acknowledgement of the source(s). It is an attempt to deceive the reader that the work or ideas presented are your own, whereas in fact they are the work or ideas of others. With regard to essays, reports and dissertations, a simple rule should be used when deciding if it is necessary to acknowledge sources. If you obtain information from an outside source, that source must be acknowledged. Another rule to follow is that any direct (verbatim) quotation must be placed in quotation marks and your wording should indicate clearly that the item is not your own work and the source cited immediately. The mere inclusion of the source in a bibliography will not be considered sufficient acknowledgement. This applies to all work contributing to assessment, including laboratory reports and projects. All assessed work must be your own individual effort. Copying of laboratory reports, for example, is plagiarism. You may share data, where appropriate, but the calculations, answers to assignment questions and the discussion of results must be your own work. Work referred to from Internet sources must also be acknowledged as above, with the web address (URL) of the source included, and the date on which it was accessed.

DEPARTMENTAL SEMINARS

In order to familiarise students with the work of the various research groups in the School and in those at other universities, seminars are arranged regularly in alternate weeks, usually on Thursdays from 11h25. These seminars are considered to be a vital part of class activity. Attendance at the seminars throughout the year is mandatory for all Honours students and is monitored through the maintenance of an attendance register. Active participation at the seminars is strongly encouraged. Notices advertising the seminars will be posted regularly, check your email daily!

LITERATURE REVIEWS

In the other alternate weeks, literature reviews will take place. During these exercises, Honours students will be asked to discuss selected papers from the chemical literature, assigned to them by a member of staff.

OTHER ACTIVITIES

Attendance at other School activities, such as the Annual Bayles Lecture, etc., is compulsory for all Honours and post-graduate students in the School.

The School also takes part in the annual SACI colloquium toward the end of the year (2nd semester); it was held at DUT in 2009. Each student is required to present either a poster or an oral presentation on his/her research project (CHEM781).

ASSESSMENT OF THE HONOURS COURSE

The final mark for the course will be made up of contributions from each module as shown in the table below.

SEMESTER I			
Module	Marks for Each Module		% of Final Mark
	Component	%	
Analytical Chemistry (CHEM741) (16 credits)	Exam	80	12.5
	Practical	20	
	Total	100	
Inorganic Chemistry (CHEM711) (16 credits)	Exam	80	12.5
	Practical	20	
	Total	100	
Organic Chemistry (CHEM721) (16 credits)	Exam	80	12.5
	Practical	20	
	Total	100	
Physical Chemistry (CHEM731) (16 credits)	Exam	80	12.5
	Practical	20	
	Total	100	
SEMESTER II			
FOUR Chemistry Elective COURSES (CHEM781) (32 credits)	Class mark Exam **Total**	20 80 100	25 (of which the 4 courses contribute 25% each)
Project (CHEM791) (32 credits)	Report Oral General impression **Total**	70 20 10 100	25
OVERALL			
Final Mark (128 credits)			100

CHEMISTRY HONOURS 2010
COURSE OUTLINES FOR FIRST SEMESTER

ANALYTICAL CHEMISTRY

A1. Sample preparation and speciation
Prof A. Kindness (10 lectures)
This course will deal with sample preparation with respect to its influence on speciation and its role in instrumental analysis.

A2. Electroanalytical techniques
Dr J. C. Ngila (10 lectures)
This course covers principles and applications of electroanalytical techniques. These include potentiometry, polarography and voltammetry used widely by analytical, physical, organic and biological chemists for fundamental studies. The studies involve oxidation and reduction processes in various media, adsorption processes and electron transfer mechanisms at chemically modified electrode surfaces. At the end of the module, students will learn trace analytical applications based on stripping voltammetry (cathodic and anodic stripping) which is a powerful tool that is significantly used for the determination of metals and organic substances in different matrices including water, soil food, pharmaceutical and different environmental samples. The Laboratory exercise will introduce the students to electrochemical analyzer instrument and how to apply the technique for analysis in various sample matrices.

A3. Mass spectrometry
Dr B. Moodley (10 lectures)
This course will serve as an introduction to the technique of mass spectrometry and its use as an analytical tool. It will focus on GC-MS and LC-MS (ion trap) as these instruments are present in the department and students will be using them for various analysis. Students will learn about the fundamental principles of mass spectrometry, the workings of these 2 instruments and interpretation of mass spectra.

INORGANIC CHEMISTRY

I1. Organometallics in Catalysis
Prof H.B. Friedrich (10 lectures)
The course aims to introduce the student to synthetic organometallic chemistry. Emphasis will be on various ligand systems. The modes of coordination of the ligands, synthetic techniques and how they can be functionalized to influence the reactivity (stoichiometric and catalytic) of the complex will be discussed. The use of NMR and IR to monitor reactions of complexes (beyond characterisation) will be discussed. Finally, students will learn the techniques of handling air and moisture sensitive compounds and of growing quality crystals suitable for single crystal XRD.

I2. Organometallics and Materials Chemistry
Dr V. O. Nyamori (10 lectures)
The course is intended to introduce the shaped carbon nanomaterials (SCNMs) and visualize material science at the nanoscale i.e. constitutes a bridge between molecules and infinite bulk systems. Various kinds of SCNMs, their synthesis and reactor designs will be covered. Emphasis will be on carbon nanotubes (CNTs) and use of organometallic catalysts in the chemical vapour deposition (CVD) method. The role of the metal, carbon source and heteroatoms on CNTs synthesis will be covered. The students will also learn to interpret and characterize SCNMs with the help of TEM, SEM, XRD and TGA. The electronic and mechanical structure of CNTs and how they relate to their actual and potential applications will also be explained.

The course also is aimed at defining and explaining what are liquid crystals (LC) materials. Types of LC, mesophases and gives some organometallic examples. The course also will briefly look at some of the current applications of LC.

I3. Supramolecular and Nanomaterials Chemistry
Dr W. E. van Zyl (10 lectures)
The course is designed to highlight some of the (inorganic) topics currently at the frontier of chemical research which are predicted to have a major technological impact for many decades to come. This course is quite *descriptive* in nature because most of the concepts and topics covered are recent discoveries where, unlike classic/traditional inorganic chemistry, coherent theories still need to emerge, be tested by experiment, and mature.
By the end of the course, students should have a better appreciation of the main principles and applications that underpin advances in supramolecular- and nanomaterials chemistry.

Interpret and apply fundamental aspects of **solution-phase** supramolecular chemistry, including acceptor-receptor concepts, supramolecular self-assemblies, the hydrogen bond and metallophilicity, non-covalent synthesis, macromolecular coordination chemistry and metallorecognition; coordination-driven self-assembly; the chemistry of dithiophosphonates and dithiocarbamates; gold-heteroatom interactions. Explain and comment on aspects of **solid-phase** supramolecular chemistry, including crystal engineering, reticular synthesis, metal-organic frameworks (MOFs) and porous materials, luminescent materials.
Interpret and apply fundamental aspects of nanochemistry, including synthesis methods and properties of nanomaterials, sol-gel chemistry, polyhedral oligosilsesquioxanes (POSS) and carboranes, gold nanoparticles and some of its many applications.

ORGANIC CHEMISTRY

O1. Advanced ^{1}H NMR: Determination of Stereochemistry by Spectroscopic Methods (Claydon Chaps 11, 15, 32)
Dr PH Coombes (10 lectures)
An extension of the NMR spectroscopic techniques studied in 2nd & 3rd year, this course focuses on the use of ^{1}H NMR in determining the stereoscopic aspects of complex molecules. Among the topics covered are: the role of the Karplus equation in determining a dihedral angle from the coupling constants of the protons involved, the effect of ring size, elemental electronegativity and π systems on coupling constants, how homotopic,

enantiotopic and diastereotopic protons are related in terms of ^{1}H NMR, and the use of the nuclear Overhauser effect (nOe) in structural elucidation.

O2. Synthesis in Action & Mechanisms of some Pericyclic Reactions (Claydon Chaps 25, 35, 36)
Prof F Shode (10 lectures)
Synthesis is one of the powerful tools organic chemists use to make desired compounds for various reasons. To achieve a successful synthetic operation, mechanistic understanding of organic reactions is important in the design and execution. In this part of the course, synthesis of some important industrial chemicals as well as the mechanisms of some pericyclic reactions will be presented and discussed.

O3. Selective reactions and protection; Free radical reactions
Dr N. A. Koorbanally (10 Lectures)
For an organic chemist to predict the precision of chemical reactions with respect to attack at a particular position in a molecule and/or production of constitutional isomers or stereoisomers, the knowledge of selective reactions is important. In this course, chemoselectivity, regioselectivity, and stereoselectivity will be discussed using specific examples. The use of protection groups in chemical synthesis enables the chemist to selectively react one functional group in the presence of other reactive groups. Some examples of the application of protection groups in synthesis will be discussed.
Finally, free radical chemistry will be discussed in light of its application in organic synthesis.

PHYSICAL CHEMISTRY

P1. Molecular Symmetry
Prof T. A. Ford (10 lectures)
Symmetry elements and symmetry operations will be introduced, illustrated by reference to the structures of some common compounds. This will lead on to the concept of the point group, described using the Schoenflies notation. Character tables will be discussed, and their use in understanding the symmetry properties of molecular vibrations and of atomic and molecular orbitals will be demonstrated.

P2. Gas and solution kinetics
Prof S. B. Jonnalagadda (10 lectures)
Theories of reaction rates, including bimolecular collision theory and absolute reaction rate theory will be introduced. The calculation and interpretation of the thermodynamic properties of the activated complex will then be discussed. This will be followed by an introduction to solution kinetics. The similarities and differences between gas and solution phase reactions will be described, in particular the role of the solvent. Classes of reactions will then be introduced, including diffusion- and activation-controlled reactions for neutral species. A review of theories of reactions will be presented, in particular the double sphere and single sphere models for reactions between charged species. The course will end with a discussion of electrorestriction, the kinetic salt effect and the effect of ionic strength on the rates of reactions between charged species, and charged and neutral species.

P3. Photochemistry
Prof B. S. Martincigh (10 lectures)
In this course the basic concepts of photochemistry will be reviewed, and the principles of absorption and emission of radiation discussed. The experimental techniques appropriate to photochemistry will be described, along with some important photochemical processes found in nature. Some commercial applications of photochemistry will also be discussed.

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WE van Zyl
Honours Coordinator
January 2010