RHODES UNIVERSITY

Where leaders learn

DEPARTMENT OF CHEMISTRY

HONOURS

2021

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CHEMISTRY HONOURS – 2021
Head of the Department: Prof R Klein (r.klein@ru.ac.za)
Course Coordinator: Mrs Joyce Sewry (j.sewry@ru.ac.za)

1. GENERAL CONDITIONS

1. Admission to the final examinations of the Honours course is subject to satisfactory performance in all parts of the course during the year.
2. The Chemistry Department expects all Honours students to act as Demonstrators and Tutors (as part of their bursary obligations, or for payment, as appropriate). Demonstrating and tutoring provide valuable teaching experience. Funding for tutoring & demonstrating is determined annually by the university.
3. Permission is needed to study any other courses during the year or to take up any other form of employment.
4. Honours students are expected to be on campus every day, as per Rhodes University Covid-19 protocols during RU terms. A leave of absence must be applied for through the Chemistry Administration office in case of illness or other emergency as noted in the student disciplinary code.

• DP REQUIREMENTS

Chemistry Honours students

1. Must participate in ALL chosen lectures, and must submit ALL assessments.
2. Must attend ALL seminars in the Chemistry Department.
3. Must work on the project while not in lectures.
4. Must submit all submissions by the relevant dates.
5. Must attain a subminimum of 50% is in the research project and theory respectively.

• FINANCIAL ASPECTS

Each student is responsible for financing his or her studies.

Fees for Honours (2021):

Tuition Fee R46 490

Residence Fees range from approximately R65 000 to R75 000

Other minor administrative fees may apply, such as Application Fee of R100.

International Levy and payment options, please refer to fees booklet for 2021 at www.ru.ac.za/fees

• HONOURS RESOURCES

All resources for the Chemistry Honours course should be available on RUConnected: You will have access to this site once you have registered.

https://ruconnected.ru.ac.za/course/view.php?id=8357

2. PROGRAMME FOR ORIENTATION WEEK

3-5 March 2021

(ALL DATES ARE PROVISIONAL AND CHANGES MAY BE MADE TO THE PROGRAMME)

Wednesday 3 March

9:00	General outline of the Honours Course (Mrs Sewry; Prof Klein) By ZOOM
10:00	**Introduction to the Review Essay and research projects with all staff to be led by Prof R Klein*** (See also the attached handout on Writing a Scientific Report, Appendix 2.)
14:00	An introduction to Computer facilities and registering to use Scifinder Scholar. See a video on RUConnected by Prof Lobb on access these facilities.

<u>*POINTS FOR DISCUSSION</u>

What is meant by "RESEARCH"?
What is expected in an Honours Project?
Starting a project
Lab notebooks
Writing up
Seminar with East Cape Universities
Responsibilities of a Supervisor
Responsibilities of the Student
Practical problems
Psychological problems

Thursday 4 March

Prepare a 2-page essay on yourself and your undergraduate studies.

Contact staff to finalise lecture and essay topic choices. (See email addresses later in this document)

NB You will NOT be able to choose a topic unless you have spoken to the supervisor

14:15 Virtual Library tour.

Please see Links below that are on the Library Website under Tutorial Videos:

Virtual Tour
Please watch Search All Tutorial - English
Please watch Search All Tutorial - isiXhosa
Please watch My Library Account Tutorial Video
Finding eBooks via the Rhodes Library
Please watch Meet Your Librarian

Friday 5 March

9:00 Submit final choices of topics, projects and essays; find link on RUConnected

09h30 - 11h00 Tutor Training by Zoom: Prof Klein and Mrs J Sewry

16:00 STAFF ONLY Meeting (finalizing of Honours programme and project and essay allocations).

17:00 Hand in your essay on yourself by email to chemistry@ru.ac.za

Monday 8 March

8:00 **Lectures begin for all honours students**

A DRAFT Timetable will be provided as early as possible. This is likely to be changed from time to time. See RUConnected for the Timetable

Honours students also to start on their essays.

3. PROGRAMME FOR 2021

Important activities

PLEASE NOTE: Because of the Coronavirus pandemic, students will start the academic year virtually, and thus will be expected to do a more of their lecture topics and their essay in the first term. This will give them more time in the laboratory when they are allowed back on to campus, as guided by the Rhodes University Phased return of students guidelines, as well as National Lockdown regulations.

Dates To be Confirmed (TBC) for activities below

Summary of important dates (by Term):

- Oral presentation of project plan will take place once students are back on campus.

  (Each student will have been given key papers related to his/her project. Please read these papers carefully and prepare a short talk (10 min maximum) **on your plan for the project.**

  (see the attached Appendix on "Giving an Oral Presentation")

- Safety test (Friday of first week of lectures)
- Hand in 1st draft of essay (end of 1st Term)

Second term:

- 1st draft of essay back from supervisor (beginning of 2nd term)
- Oral presentation of essays (***provisionally*** 2 weeks before SWOT week)
- Mid-year research group project seminars (Last week of 2nd term, arranged within research groups)
- Final version of essay (Last day of lectures in 2nd Term)
- Tutor refresher (TBC)
- Mid-year exam (TBC)

Third term:

- Collect June scripts

Fourth term:

- Hand 1st draft of project (1st day of 4th Term)
    - Hand in Final version of project report (13 September)
    - Project seminar (***provisionally*** l4 October)
    - Final Honours examinations (November; dates to be determined by Registrar's division)

4. STAFF OF THE DEPARTMENT OF CHEMISTRY

Academic Staff:

Prof Rosa Klein (RK)
Head of Department

Prof Rui Krause (RuiK)

Dist Prof T Nyokong (TN)

Prof Kevin Lobb (KAL)

Prof Philani Mashazi (PNM)

Dr Vincent Smith (VS)

Mrs Joyce Sewry (JS)

Emeritus Prof Gary Watkins (GW)

Dr Theo Geswindt (TG)

Prof John Mack (JM)

Dr Jonathan Britton (JB)

5. DETAILS OF THE HONOURS COURSE

Purpose and characteristics

The Bachelor of Science (Honours) Degree is a postgraduate specialisation qualification, characterised by the fact that it prepares students for research based postgraduate study. This qualification typically follows a Bachelor's Degree, and serves to consolidate and deepen the student's expertise in a particular discipline,

and to develop research capacity in the methodology and techniques of that discipline. This qualification demands a high level of theoretical engagement and intellectual independence. In some cases, a Bachelor of Science (Honours) Degree carries recognition by an appropriate professional or statutory body. Bachelor of Science (Honours) Degree programmes must include conducting and reporting research under supervision, worth at least 30 credits, in a manner that is appropriate to the discipline or field of study. Honours is an NQF Exit Level 8 qualification, with a minimum 120 credits, of which 120 credits (~1200 notional hours) have to be at NQF level 8, and includes approximately 30 credits of supervised research. Approximate credit breakdown of the course:

	Credits(hours)	Comments
Research Project	35(350)	~20 h per week for 3 terms
Review Essay	5(50)	~5 h/week for 1½ terms
Theory	80(800)	For each hour of lectures, at least 4 h self-study

COURSE STRUCTURE

(A) Theory: Lecture topics (15 topics to be chosen):

Topics are selected by the student from the list attached, subject to the approval of the Chemistry staff, to ensure a well-rounded curriculum. Students should consult the project topics for recommendations on lectures needed.

The topics vary from year-to-year depending on staff availability and their interests, and on the number of students selecting the topic.

(B) An introductory research project:

This is done during the first three terms under the supervision of a member of staff in a field selected by the student from projects offered by staff members. Students are required to give short talks on their projects at a Departmental seminar in September or October. One or two of these talks will be selected for an oral presentation at a joint SACI (South African Chemical Institute) seminar with the three other Higher Education Institutions in the Eastern Cape, Nelson Mandela University (NMU), Walter Sisulu University (WSU) and University of Fort Hare (UFH).

(C) A review essay:

An essay of approx. 5000 words (20 x A4 pages), on a topic not associated with the project, is written in the first and second terms under the supervision of a staff member (other than the one concerned with the project). The first draft of the essay must be kept and the final mark will take the first draft into consideration.

Joint Honours: Chemistry/Another Science subject

It is possible, at the discretion of the departments concerned, for students to do Joint Honours in Chemistry and another subject. For Joint Honours, each of the component subjects must make up at least 40% of the total course. The composition must be specified in writing and agreed to by the Heads of both Departments. Joint Honours will only be available as an option to students who achieve a 1st class pass for their Chemistry 3 course.

Modules from other courses?

With permission from the Heads of Departments (HoDs) of both Departments, it is possible to swap up to 3 elective modules in Chemistry with modules from the Honours Course of another Department, provided the Credit value is approximately the same.

6. COURSE ASSESSMENT

(Total marks 800)

ONE 3-hour paper is written in June. This examination serves as a guide to students and staff as to whether satisfactory progress is being made. Where progress is not satisfactory, candidates may be advised to spread the Honours degree over two years, or to withdraw.

Students who obtain less than 50% on any question(s) answered, are required to re-write the question(s) early in the third term. However, the marks obtained during the first session will count.

The final examinations are written in November. There are **three 3-hour papers**. Each paper covers the material dealt with in FIVE of your topics; (see list under LECTURE TOPICS). You are required to answer FOUR of the questions in each paper. As in all examinations, equal time, in this case 45 minutes, should be allocated to each answer. An option of up to two modules that are evaluated by continuous assessment may be taken per paper. For **continuous assessment** modules, the relevant time per module will be deducted from the 3 hour examination time, where this option is taken up.

Component	Sub-component	Marks	% of total mark
June theory exam		40	5 %
Project:		Total:200	25 %
	Presentation	50	
	Written report	150	
Essay:		Total: 110	13.75 %
	Presentation	20	
	Essay hand-in	90	
Theory:	12 modules: 4 each in 3 papers	12 x 37.5 = 450	56.25 %
TOTAL		**800**	**100 %**

7. LECTURE TOPICS (A)

FIFTEEN topics must be chosen from the list below (a detailed explanation of the topics is given on the pages which follow). It is impossible to allow a perfectly free choice of topics. The topics are thus listed in **FOUR** groups (see below). A **maximum of FOUR topics from each paper and a maximum of THREE continuous assessment** topics must be chosen. No more than **ONE** additional topic in each section may be selected initially and the final **FIFTEEN** must be confirmed *in writing* before the end of May. A maximum of OUR topics will be answered in each exam paper. Complete the form at https://forms.gle/58cHn2miPvZenEa28

Details of topics follow below the table. (NOTE: Some more topics might be added when the new staff member arrives.)

Paper 1 Max 4	RuiK2	Biological Interactions of Nanoparticles
	VS1	Solid State Properties of Materials
	PNM1	Intelligent nanomaterials and their applications
	GW2	Vibrational spectroscopy
	RK3	Advanced retrosynthesis and Green Chemistry

Paper 2 Max 4	PTK1	Asymmetric synthesis
	RuiK3	Potholes and Pitfalls in Advanced Synthetic Strategy
	JM2	Porphyrinoid chemistry
	PNM2	Design and development of biosensors
	JS1	Introduction to Chemometrics
	GW3	Inorganic reaction mechanisms
	RK1	Pericyclics and multicomponent reactions

Paper 3 Max 4	PTK2	Strategies in drug synthesis and design
	DSK1	Physicochemical Properties in Drug Design
	RUIK4	Medicinal Chemistry, Drug Discovery and Drug Delivery
	TG1	Advanced kinetic analyses
	KAL1	NMR spectroscopy
	JM3	Optical spectroscopy
	GW1	**Symmetry and group theory**

Continuous Assessment Max 6	**VL1***	**Industrial Perspective of Analytical Chemistry**
	RK2*	**Introduction to Research Methods**
	KAL3	Molecular Modelling: Interactions and Dynamics
	JS2	Service-Learning In Chemistry
	JM1	Molecular Modelling: molecular symmetry and TD-DFT
	RuiK1	Supramolecular Chemistry in Medicine (with V. Smith)

- Topics in the last block are examined by various “in course” (continuous) assessments.
- Topics indicated in **bold** are required modules.
- A minimum of two examinable topics are required per paper, and a minimum of three continuous assessed courses are required in total.
- A student who selects continuous assessment modules and does NOT submit assignments etc., or drops out mid-way from the course will get the mark they obtained UP TO THAT POINT, which could be zero. This is equivalent to selecting the module to write in the exam and not writing anything

One paper in another major subject

It is possible for up to five Chemistry topics to be replaced by an equivalent amount of material in another subject, by arrangement with the Heads of Departments concerned. In this case the degree remains Chemistry Honours. Alternatively, some Chemistry topics may be chosen in an Honours degree in another subject. All such combinations must be specified in writing and approved by the Heads of both Departments concerned. A full joint Honours will only be available as an option to students who achieve a first class pass for 3rd year chemistry.

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DETAILS OF LECTURE TOPICS

PAPER 1

PROF R KRAUSE (ROOM F42)

RuiK2 Biological Interactions of Nanoparticles

Drug delivery is becoming increasingly important the treatment of disease as well as in diagnosis. The mode of delivery whether oral, nasal or via injection can dramatically affect product stability, patient compliance and treatment efficacy. In addition, the active ingredients are often only a small part of the medicine and we need to consider how these components interact. In each of these aspects, nanomaterials have emerged as potentially useful components in drug delivery.

They can be used to improve targeting, aid the kinetics and distribution of the medicine, and protect sensitive components from degradation. However, they also represent a risk through unwanted biological interactions. This module will look at how nanoparticles interact with human organs, and how these interactions can be used beneficially to improve drug delivery.

DR V J SMITH (ROOM S35)

VS1 The Solid State Properties of Materials

Solid state properties are key to understanding the physical behaviour of materials and to ensure optimal physical form. Moreover, the selection of optimal form is a critical aspect in the development of new materials (pharmaceutical or other). In this course we will cover the various aspects of solid state characterisation of materials.

Dr P MASHAZI (ROOM F44)

PNM1 Intelligent nanomaterials and their applications

There is a current global trend growing in the application of nanomaterials in various industries. The interest has been sparked by the intrinsic properties that nano-sized and nano-structured materials exhibit. Various interests in the application of nanomaterials look into solutions these materials may provide into current day challenges. These materials can be intelligently designed to target specific applications.

The examples are that these materials are investigated for their potential as vehicles for targeted drug delivery, enhancement of electrical signals in sensor applications, visualisation in point-of-care diagnostic tests, heterogeneous catalysts for industrial applications (such as catalytic converters, carbon monoxide oxidation, etc.), miniaturized systems for space applications, the list is endless. The module will look at different types of nanomaterials, their design for targeted applications, properties and their effect when tested for these specialized applications.

PROF G M WATKINS (ROOM S42)

GW2 Vibrational spectroscopy

A non-mathematical introduction to infrared and Raman spectroscopy and instrumentation. The application of some techniques employed in the assignment problem. (Some knowledge of Group Theory, covered in GW1, is necessary for this topic.)

PROF R KLEIN (ROOM F38)

RK3 Advanced retrosynthesis and green chemistry

In September 2015 the United Nations adopted the Sustainable Development Goals. As chemists we can make a substantial contribution to the changes which are necessary to address climate change, poverty alleviation and sustainability in general. This course will look at the application of retrosynthesis as a tool to highlight opportunities to use bio-derived compounds as renewable resources in synthesis, and the application of a set of green chemistry metrics to assess our synthetic processes.

PAPER 2

PROF PT KAYE (ROOM S41)

PTK1 Asymmetric synthesis

An introduction to the principles of asymmetric synthesis and a survey of current methodologies for the synthesis and analysis of chiral compounds.

PROF R KRAUSE (Room F42)

RuiK3 Potholes and Pitfalls in Advanced Synthetic Strategy

The module will outline and discuss several organic syntheses including total syntheses as a way to learn from published literature. The focus will be on strategic planning and how strategy is often adapted during a project. The module will rely on aspects such as “Catalysis on Organic Chemistry” and “Asymmetric Synthesis” taught in other modules, and will draw on literature examples. It will help you to identify potential problems when planning your own syntheses and how to overcome them. It will also assist you in reading existing literature to “see” the hidden strategies that were applied in each case.

Prof J MACK (NIC G28)

JM2 Porphyrinoid chemistry

The synthesis, characterization, properties and applications of phthalocyanines will be explored with a strong emphasis placed on their use in nanotechnology. The module is designed to provide students contemplating a career in chemistry with examples of how the theory learned during undergraduate chemistry courses can be applied in a research and development environment to solve practical problems and create new industrial and biomedical products.

Dr P MASHAZI (ROOM F44)

PNM2 Design and development of biosensors

Early detection of pollutants and pathogens in environmental, biological and industrial samples is a subject of international interest. The surveillance and control of the spread of these harmful substances that may be harmful to humans, microorganisms and the environment will be discussed. This will then highlight the need for systems that may be effective and accurate in detecting and/or monitoring the levels of these undesirable substances from the various samples. In the environment and biological systems these hazardous substances possess a big threat to human and animal health. Therefore to improve the quality of life for humans, detection and monitoring of these hazardous substances at an early on-set of infection or contamination is important. The detection and monitoring systems are important for effective and timeous treatment and as early warning systems. The material covered in this module will be the systems currently used and those that are under development by various institutions for detection and monitoring of the substances harmful to the environment and biological systems. The design and development issues arising from the semi-commercial systems will also be discussed whilst highlighting the

successes of other systems. Different techniques will be discussed and their impact in the cutting-edge of the bio/sensor technologies to impact the future in industrial applications

MRS JD SEWRY (ROOM S36)

JS1 Introduction to chemometrics

"Chemometrics is the chemical discipline that uses mathematical and statistical methods, (i) to design or select optimal measurement procedures and experiments, and (ii) to provide maximum chemical information by analysing chemical data." Matthias Otto.

The course does an overview of basic statistics and then looks at experimental design and finding optimal conditions

PROF G M WATKINS (ROOM S4)

GW3 Inorganic reaction mechanisms

An introduction to some inorganic reaction mechanisms: square planar and octahedral coordination complexes and redox reaction mechanisms.

PROF R KLEIN (F38)

RK1 pericyclic reactions and multicomponent reactions

This course will provide an overview of the types of pericyclic reactions and introduce some of the important applications of these processes in modern chemical synthesis.

PAPER 3

PROF PT KAYE (ROOM S41)

PTK2 Strategies in drug synthesis and design

A survey of fundamental principles in drug design and synthesis, illustrated with examples drawn from classic and contemporary medicinal chemistry.

NB: STUDENTS SELECTING THIS COURSE ARE ADVISED TO ALSO TAKE **DSK1**.

Dr DS KHANYE (T06)

DSK1 Physicochemical Properties in Drug Design

Approximately 40% of nominated clinical drug candidates fail to reach development and markets due to poor physicochemical factors. As a result pharmaceutical companies are faced with a major challenge of delivering their products to the markets on time, ultimately, fail patients who are in desperate need of important drugs to alleviate illness. In this course, physicochemical properties such as solubility, permeability and chemical stability of compounds will be discussed in the context of structural properties such as molecular weight (MW), H-Bonds, lipophilicity (log P or log D7.4), polar surface area (PSA), acidity or basicity (pKa), shape and flexibility of compounds. These concepts will be illustrated by examples drawn from various medicinal chemistry sources.

NB: STUDENTS SELECTING THIS COURSE ARE ADVISED TO ALSO TAKE **PTK1**

PROF R KRAUSE (ROOM F42)

RuiK4 Medicinal Chemistry, Drug Discovery and Drug Delivery

Medicinal Chemistry is a field at the interface between medicine and organic chemistry, and this module will introduce students to aspects of drug discovery and drug delivery.

The focus is on drug optimization and how different systems of drug delivery can be used to deliver drugs do to the human body and what the human body does to the drugs. This module will explore drug design, targeting, pharmacokinetics and dynamics, and tools and techniques in drug delivery.

Dr T Geswindt (ROOM F43)

TG1 Advanced Kinetic Analyses

In general, chemical kinetics stems from the fascinating scope of the macroscopic physical properties that chemical systems exhibit in the non-equilibrium state. These range in complexity from ligand exchange under well controlled experimental conditions, oscillating chemical reactions, pattern or structure formation and bifurcation. It is an exciting time in the field of chemical kinetics considering that, in principle, with modern computers and a fair knowledge of programming numerical algorithms, even the most complex system of differential equations can be solved. The role that chemical kinetics fulfils in nature is a testament to the importance of a detailed understanding of kinetics. This module explores the various intricacies of more complex (redox) reactions, and how to solve these systems using a combination of geometrical and numerical analyses

PROF KA LOBB (ROOM S40)

KAL1 NMR spectroscopy

The practical application of 1D and 2D Fourier transform NMR techniques commonly used to determine the structures of organic molecules. Where applicable, theoretical aspects of modern NMR techniques will be described using a largely non-mathematical approach.

Prof J MACK (NIC ROOM G28)

JM3 Optical spectroscopy of aromatic π-systems and transition metal complexes

The use of crystal field theory, ligand field theory and/or molecular orbital theory to analyze optical spectral data (including circular dichroism, magnetic circular dichroism and emission spectroscopy in addition to electronic absorption spectroscopy) of aromatic π-systems and transition metal complexes is explored, with a strong emphasis placed on the information that can be derived on molecular structure and properties.

PROF G M WATKINS (ROOM S2)

GW1 Symmetry and Group Theory

(NOTE: this is a required topic for all students.)

Symmetry and point groups. The methods of group theory are applied to simple molecules with reference to hybrid orbitals and in the interpretation of vibrational and electronic spectra. (This is a largely non-mathematical introduction to the subject)

CONTINUOUS ASSESSMENT

These topics will not have questions in the formal examinations, but will be assessed throughout the year.

VISITING LECTURER Dr Heidi Duveskog, Director of Contextualize (Pty) Ltd

VL1: Industrial Perspective of Analytical Chemistry

The course highlights the multi-faceted role of Analytical Chemistry in Industry and the Environment, giving an overview of how Analytical Chemistry is applied across a value chain of processes. The module introduces the various technologies and stakeholders encountered in the workplace, including working hands-on with tools like video conferencing. This addresses an understanding of the technical component of their area of expertise (concepts such as 'detection limits' and statistical tolerances associated with results), as well as the business component and the ability to use results to influence decision making. Participants will have the opportunity to work through case studies to see how these components come

together to establish core competencies within industry. Assessment will be by continuous assessment, with peer review and feedback (from team projects and presentations).**This course is compulsory.**

PROF R KLEIN (ROOM F38)

RK2 Introduction to Research Methods. (NOTE this is a REQUIRED topic for all students)

The aims of this course are to explore techniques which are not covered in undergraduate practical courses as well as encourage students to develop skills in synthetic experiment design, and in critical analysis of experimental outcomes. The course will combine theoretical principles with practical experimentation in the context of equipment and opportunities available within the department. Assessment will be by continuous assessment

Prof K Lobb (ROOM S40)

KAL3 Molecular Modelling: Interactions and Dynamics

Compared with the previous course this is also a practical course but with a focus on medicinal chemistry. Construction of models is addressed followed by a general background to molecular mechanics and ab initio methods, with focus on molecular mechanics and conformational searching. QM/MM methods are also included. The algorithms used in docking small molecules to active sites of enzymes are presented, followed by practical aspects of working with the docking software and the analysis of results. The course finishes with some molecular dynamics (Continuous assessment will involve the completion of a small project in lieu of an exam question.

MRS JD SEWRY (ROOM S36)

JS2 Service-Learning in Chemistry

This course will entail one lecture on an Introduction to Service Learning. Thereafter, the students will have to work in groups and do the Service-Learning module, working with the Mobile Science Lab (MSL). The idea is that the chemistry students will work in groups of 2 or 3, with staff of the MSL. Together, they will identify relevant practicals for schools. The students will make a video of the practical being performed. The video will then be available for distribution to the Makhanda schools, and for use by the MSL

Prof J MACK (NIC G28)

JM1 Molecular Modelling: molecular symmetry and TD-DFT calculations

Density functional theory (DFT) can be used to derive optimized geometries for newly synthesized molecules such as phthalocyanines, porphyrins and BODIPY dyes, which in turn can be used to carry out time-dependent density functional theory calculations (TD-DFT) so that trends in the optical and redox properties can be identified. The course will provide hands on experience with calculations of this type, which will enable students to use a rational approach in identifying target compounds for synthesis work.

Dr V Smith and Prof R Krause (ROOM S36 and F42)

RuiK1 Supramolecular Chemistry (hosted jointly with Dr Smith) – Continuous Assessment

Defined as the “Chemistry beyond the molecule”, supramolecular chemistry explains how molecules and ions join together in fascinating structures using only intermolecular forces. These entities can be small to enormous and have many applications from explaining why lizards can stick to walls, to data-storage and nano-devices that can deliver medicines like futuristic machines.

In this module we will explore some of the recent developments in supramolecular chemistry with a focus on techniques that you can use to identify and construct your own supramolecules.

The module is driven by YOUR interests using experiments, literature, and discussions.

ON THE LAST PAGE OF THIS BOOKLET IS SPACE FOR YOU TO PLAN YOUR CHOICES .

8. RESEARCH PROJECT (B)

Introduction:

The project is intended to be an introduction to the methods of research and will thus cover as many of the following aspects as possible:

1. searching literature
2. planning experiments
3. setting up and calibrating apparatus
4. preparing, purifying and characterizing samples
5. using as many different techniques as possible to study the problem on hand
6. analysing the results of experiments
7. collating the results of different experiments
8. discussing the results in terms of theory and previous work
9. writing a report on the project as a whole
10. presenting a seminar on your research

A list of the projects being offered is supplied below. You should discuss all projects of interest with the members of staff concerned before making your final choice.

The final Research Report should be concise and care should be taken with both grammar and spelling. The report should put through Turnitin before submitting an electronic copy to your supervisor. The Turnitin report must also be submitted. A full list of references, should be included. Help given by other persons in addition to the supervisor should be acknowledged. Marks for the project make up 25% of the final Honours mark. It is expected, however, that students should spend **all** of their working week, outside of time spent on lectures, tutorials and demonstrating (*i.e.* approximately 25-30 hours per week for three terms) on their project. This should be done during normal working hours, when staff are available for consultation, and for safety reasons. Other work such as reading for lecture topics, essays, prac and tutorial marking etc., should be done in the evenings. The presentation will be assessed by staff and will count for 50 of the 200 marks.

SEMINAR ON INTRODUCTION TO YOUR RESEARCH PROJECTS (No Assessment)

RESEARCH PROJECT DATES:

Practical Work	Start:	Once on campus
	End:	End of 3rd term (AT THE LATEST)
Presentation of project plan		TBC
Hand in first draft		1st day of 4th Term
Hand in final version		1st Friday of October
Mid-year research group seminar		Last week of 2nd term
End of research project group seminar		Beginning of October
Presentation to Department		End of September/Beginning of October

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- **RESEARCH PROJECT (SHORT TITLES) 2021**

PLEASE NOTE: Please indicate your first choice and second choice. These MUST be from different supervisors. (https://goo.gl/forms/UBY2QaKJCKlOwnEj2)

	Dr J Britton
JBp1	Photonic crystals
JBp2	Dye-sensitized solar cells
	Dr T Geswindt
TGp1	The chemical origin of steam nano-bubbles
TGp2	Functionalization of polymeric supports with aliphatic (poly)amines in the use of PGM separation
	Prof R Klein
RKp1	Multicomponent reactions
RKp2	Catalysis
RKp3	Green chemistry
	Prof RW Krause
RuiKp1	Pyrrolo- marine alkaloids
RuiKp2	Mass Spectrometric tools for Stromatolite chemistry
RuiKp3	Stimuli-Responsive Liposomes.
RuiKp4	A low-cost DSSC
	Prof J Mack
JMp1	BODIPY nanoparticle conjugates
JMp2	Cyclodextrin inclusion complexes
JMp3	AzaBODIPY encapsulation micelles
JMp4	BODIPY-embedded nanofibers
	Dr P Mashazi
PNMp1	pH-sensitive nanosize liposomes
PNMp2	Enzymatic properties of nanomaterials
PNMp3	Octa-carboxylic acid MPcs
	Professor T Nyokong
TNp1	Water purification using green technology
TNp2	Development of Antibacterial agents
TNp3	Protection of the eye and optical devices from strong laser light
	Mrs J Sewry
JSp1	Service-Learning with Mobile Science Lab
JSp2	Practical skills in the wake of COVID-19
	Dr V Smith
VSp1	Co-crystal formation
	Prof GM Watkins
GWp1	Nanomaterials: supramolecular structure from metal coordination with 1, 2, 4, 5 benzenetetracarboxylic acid and pyridine:. A pyrolysis investigation

• DESCRIPTIONS OF RESEARCH PROJECTS 2021

Dr J Britton

JBp1 Creation of photonic crystals for optical limiting.

Due to the rise in laser-based attacks on civilian aircraft pilot's eyes, it has become increasingly necessary to develop effective optical limiters to protect said pilots. A lot of work has already gone into creating passive optical limiters from phthalocyanines and compounds similar to them, along with a few different types of nanomaterials either alone or linked to phthalocyanines.

The aim of this project is to examine another potential nanomaterial optical limiting candidate in the form of photonic crystals. These structures are similar to quantum dots in that they can have confinement in either one, two or three dimensions. Where the difference lies is that whilst quantum dots confine electrons, photonic crystals confine photons.

This would mean that it is possible to synthesize a photonic crystal which would specifically retard the propagation of a wavelength of light through it. In addition to this, if phthalocyanines were used along with the photonic crystals, the wavelength to be limited would be slowed down enough that the phthalocyanine may have increased interaction with the light instead of the majority just passing straight through.

JBp2 Synthesis of ZnO and TiO2 nanorod arrays for use in dye-sensitized solar cells in conjunction with phthalocyanines.

Nanowires (NW) are defined as metallic or semiconducting particles having a high aspect ratio, with cross-sectional diameters of about 1 μm, and lengths as long as tens of microns. Well-aligned one-dimensional nanowire arrays have been widely investigated as photoelectrodes for solar energy conversion because they provide direct electrical pathways ensuring the rapid collection of carriers generated throughout the device, as well as affording large junction areas and low reflectance owing to light scattering and trapping.

Solar energy conversion is a highly attractive process for clean and renewable power for the future. Excitonic solar cells (SCs), including organic and dye-sensitized solar cells (DSSC), appear to have significant potential as a low-cost alternative to conventional inorganic photovoltaic (PV) devices. The synthesis and application of nanostructures in solar cells have attracted much attention. Metal oxide nanowire (NW) arrays with large surface area and short diffusion length for minority carriers represent a new class of photoelectrode materials that hold great promise for photoelectrochemical (PEC) hydrogen generation applications. Up to now, various metal oxide nanostructures such as TiO2, ZnO, Fe2O3, ZrO2, Nb2O5, Al2O3 and CeO2 have been successfully employed as photoelectrodes in SCs. Among the above-mentioned metal oxide nanostructures, the study of TiO2 and ZnO is of particular interest due to the fact that they are the best candidates as photoelectrode used in SCs.

Phthalocyanines (Pcs) have also played a very important role in the development of DSSCs, as they are promising candidates for incorporation in these devices. Good efficiencies have been obtained by the use of Pcs as the light harvester, and, most importantly, a number of synthetic strategies have been developed for engineered dyes based on the Pc scaffold, due to the synthetic versatility and robustness of these macrocycles.

Return to RESEARCH PROJECT (SHORT TITLES) 2020

Dr T Geswindt

TGp1 The chemical origin of steam nano-bubbles

It has recently been reported that, when a low-concentration suspension of metal or carbon nano-particles dispersed in water is illuminated by sunlight, water vapour well above 100°C can be produced; with and overall energy efficiency of *ca* 24% and only a marginal heating of the bulk water.

This newly discovered direct conversion of sunlight into steam is sensational and has a tremendous potential as a game-changer for applications in process technology, solar fuels and various medical applications. However, the underlying physics and chemistry of this phenomenon is poorly understood – as it is expected that the emerging vapour would collapse and immediately condense upon contact with the surrounding colder liquid. Moreover, the dependency on the chemical composition of the aqueous solution certainly has an influence on the process efficacy, albeit hardly studied given the recent nature of this discovery.

In this research project, I would like to unravel the underlying chemistry and physics of this process by a combination of high-speed imaging, atomic force spectroscopy, Raman and related surface enhanced Raman spectroscopic methods (in collaboration with Stellenbosch University's Laser Physics group), ATR FT-IR spectroscopy, spectroscopic ellipsometry and theoretical modelling (DFT, TD-DFT, QM, MM). My working hypothesis is that the gas dissolved in the liquid plays an important role in the stabilization of the vapour bubble and the gas concentration will therefore be one of the crucial parameters to vary.

TGp2 Functionalization of polymeric supports with aliphatic (poly)amines in the use of PGM separation

It is known that (poly)amines illustrates selectivity toward the preferential separation of certain PGMs above others. The aim of this project is to functionalize silica (and subsequently polymeric supports) with selected amines in order to determine its efficacy in extraction of PGMs from industrial feed solutions.

Return to RESEARCH PROJECT (SHORT TITLES) 2021

Prof R Klein

RKp1 Exploring Multicomponent reactions – an application of green chemistry principles

Multicomponent reactions are the combination of three or more molecules to give a final product in a one pot reaction. These types of reactions have the obvious advantage of achieving a target quickly and efficiently with fewer work up and purification steps, and in addition often demonstrate excellent atom economy, the use of catalytic methods and the potential to reduce energy use.[1]

We would like to use the Hantsch dihydropyridine synthesis to develop a range of compounds with biological potential. The focus of this project will be to explore the possibilities of this reaction in producing differentially substituted dihydropyridines under mild conditions.

James E. Biggs-Houck, Ashkaan Younai, Jared T Shaw, Recent advances in multicomponent reactions for diversity-oriented synthesis, Current Opinion in Chemical Biology, Volume 14, Issue 3, 2010, Pages 371-382, ISSN 1367-5931, http://dx.doi.org/10.1016/j.cbpa.2010.03.003.

(http://www.sciencedirect.com/science/article/pii/S1367593110000268)

RKp2 Catalysis

A chiral catalyst has been developed in our labs that is capable of catalysing a range of reactions. This project will look at making complexes using the new ligand system and a range of first row transition metals and test them in the aldol reaction and reduction reactions. If possible we would like to grow crystals of one or more of these complexes.

RKp3 Green chemistry

We live in one of the most beautiful havens of biodiversity in the world! But we face the challenge of increasing our involvement in industrial chemistry in order to use our natural resources to promote jobs in order to grow our economy and support our population. We have the opportunity to do this in a sustainable way. This project will look at applying the principles of green chemistry to improving the synthesis a compound with known anti-HIV activity. There will be catalysis, aldol chemistry, use of benign solvents and the application of many standard laboratory procedures.

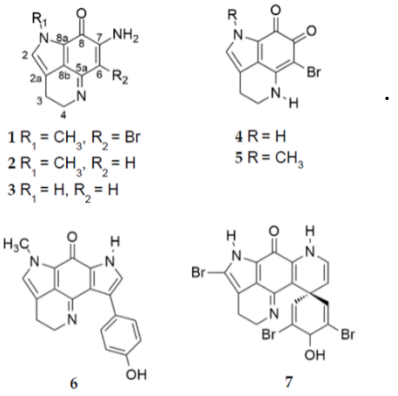
Return to [RESEARCH PROJECT (SHORT TITLES) 2021]

Prof RW Krause

RuiKp1 Synthesis and evaluation of derivatives of pyrrolo-marine alkaloids

Marine alkaloids represent a diverse group of molecules with at least one basic nitrogen atom, that have played a key role in developing therapies for a range of diseases from cancer to diabetes.
Many examples are extracted from marine organisms like sponges, and can have a huge diversity of structures.
Recently we have isolated some marine alkaloids from the Tsitsikamma region in South Africa with good anti-viral and anti-cancer activities. This project will look at the synthesis of some simple pyrroloimine derivatives as part of a fragment-based drug design programme.

A

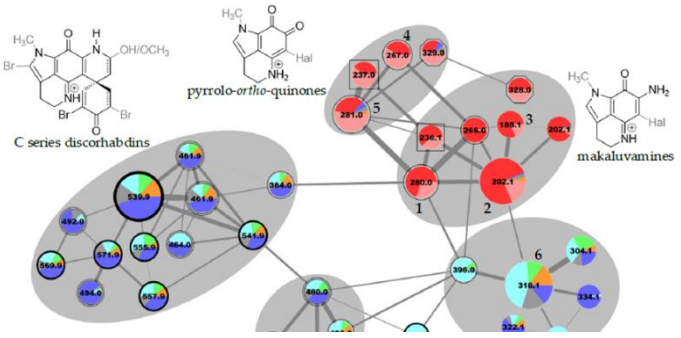


RuiKp2 Molecular Networking Mass Spectrometric tools for Stromatolite chemistry

Stromatolites are layered rocky structures containing communities of bacteria and sedimentary particles. A few years ago, modern stromatolites with interesting cyanobacteria were found in Algoa bay.

We recently started a project to look at the secondary metabolites produced by these creatures and how they could be useful in medicinal chemistry. To do this, we are using extensive mass-spectrometry and then machine learning to build networks of known and unknown fragments via the GNPS.

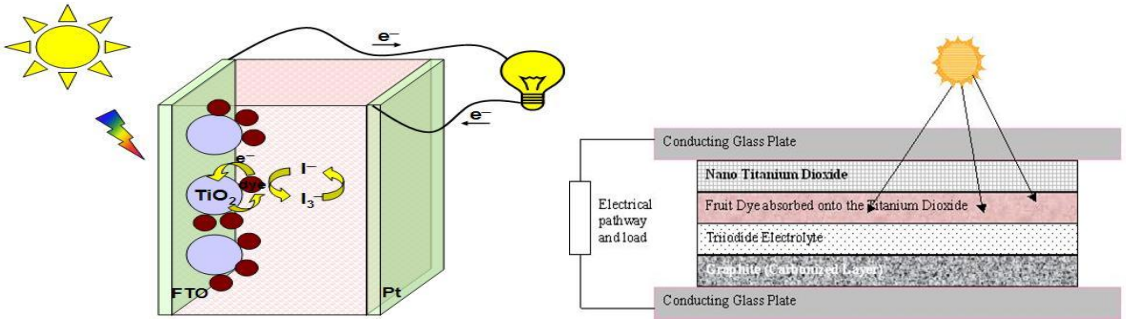
This project will look at some of these South African stromatolites and the compounds produced



RuiKp3 Stimuli-Responsive Liposomes

Mycobacterium Avium Complex (MAC) is a bacterial condition similar to TB that mostly affects people with cancer or HIV. The treatment of this condition requires careful delivery of a combination of drugs, and has to be managed with the drug regimen for the other condition (e.g. anti-retrovials for HIV). To achieve this a new class of material called stimuli-responsive liposomes are being developed. Liposomes are lipid-based nano-capsules that change shape or conformation when they encounter a stimulus such as pH change or light and therefore only release a drug under certain conditions.
This project will look at the synthesis and application of some stimuli-responsive liposomes from soy-bean lecithin and incorporate nanomaterials for stability and drug delivery.
Ref Stimuli-Responsive Nanocarriers for Drug Delivery, Mura, S.; Nicolas, J.; Couvreur, P.* Nat. Mater. 2013, DOI: 10.1038/nmat3776.

RuiKp4 A low-cost DSSC with carbon nanotube counter electrode and natural photosensitisers



This project will look at constructing a type of solar cell called a dye-sensitized solar cell (DSSC) made by combining nanomaterials for the anode and cathode and a natural pigment as a dye. In the process you will make and characterize the nanomaterials and examine the performance of the final solar cells.

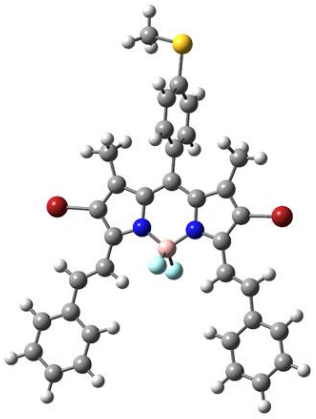
Part of the project will look at how this simple cell could be taken to schools or science shows to be used to teach science concepts, by getting school groups to also conduct research about which construction and natural pigment combinations work best etc.

K. H. Solangi, M. R. Islam, R. Saidui, N. A. Rahim and H. Fayez, Renewable and Sustainable Energy Reviews 15 (2011) 2149–2163.

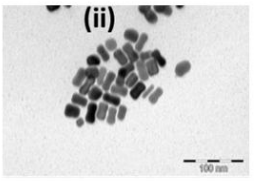
Return to RESEARCH PROJECT (SHORT TITLES) 2021

Prof J Mack

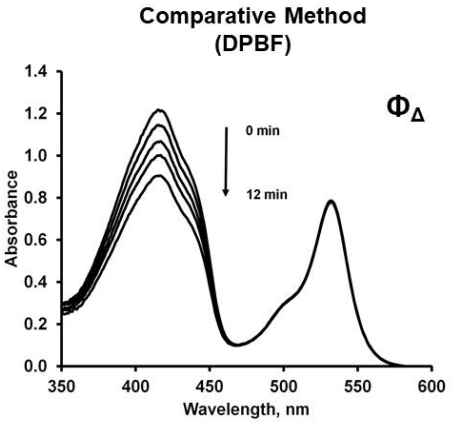
JMp1 **<u>BODIPY nanoparticle conjugates</u> for photodynamic therapy** (Co-supervisor: Prof. T. Nyokong)



BODIPY dye



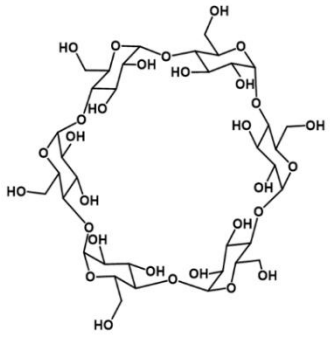
Au nanoparticles



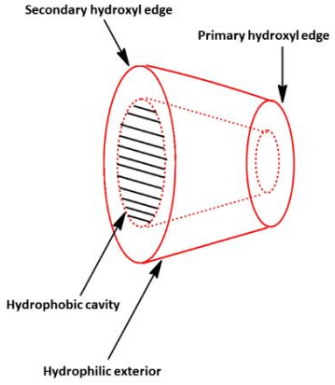
In recent years, there has been significant interest in the use of boron dipyrromethene (BODIPY) dyes as photosensitizer dyes in photodynamic therapy (PDT). Although BODIPYs normally have very low triplet state quantum yields and emit and absorb outside the optical window for tissue penetration, structural modification with heavy halogen atoms and substituents that extend the π-conjugation system addresses these issues. The goal will be to conjugate novel BODIPY dyes to gold nanoparticles for possible use as photosensitizers in photodynamic therapy (PDT) during the treatment of several different types of cancer. The project will involve the use of a laser flash photolysis system, the measurement of singlet oxygen quantum yields and PDT related studies with MCF-7 breast cancer cells to assess the suitability of the nanoparticle conjugates for use in biomedical applications.

Reference: G. Kubheka, I. Uddin, E. Amahuya, J. Mack, T. Nyokong, J. Porphyrins Phthalocyanines **2016**, 20, 1016-1024.

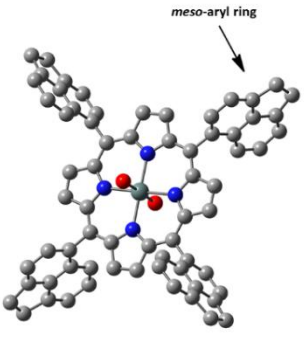
JMp2 **<u>Cyclodextrin inclusion complexes</u> for photodynamic therapy** (Co-supervisors: Prof. T. Nyokong)



β-cyclodextrin chemical structure



Schematic diagram of cyclodextrin cylinder

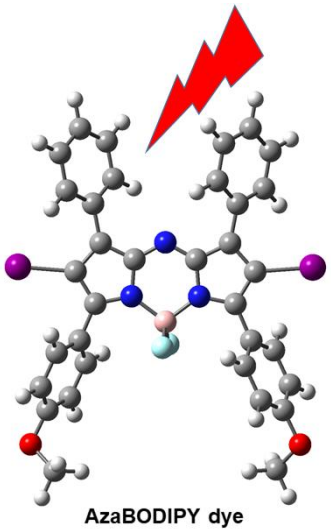


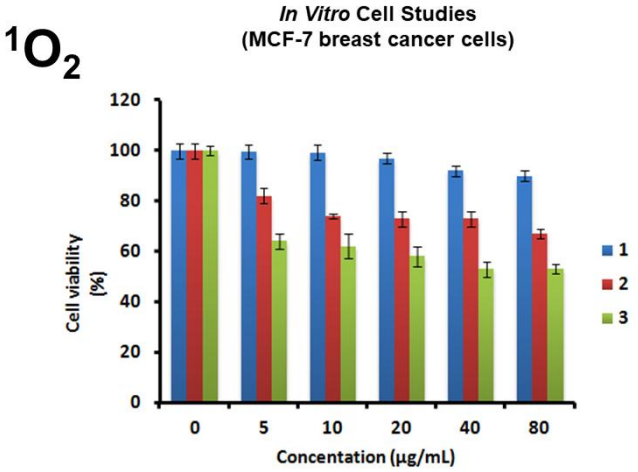
Porphyrin dye

In recent years there has been considerable interest in the preparation of readily-synthesized porphyrin analogues, such as corroles, that absorb at the red end of the visible region and have high singlet oxygen quantum yields, since these properties make them potentially suitable for biomedical applications such as bioimaging and photodynamic therapy (PDT). The project will involve the synthesis of a novel series of porphyrin analogues with bulky *meso*-aryl rings, so that water-soluble cyclodextrin inclusion complexes can be formed. After the characterization of the properties of the dyes and their inclusion complexes with a wide range of different spectroscopic techniques, the goal will be to test their photodynamic activity *in vitro* against MCF-7 breast cancer cells.

Reference: J. Mack, Chem. Rev. **2017**, 117, 3444-3478.

JMp3 **AzaBODIPY encapsulation micelles for photodynamic therapy** (Co-supervisor: Prof. T. Nyokong)

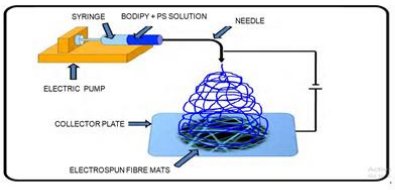


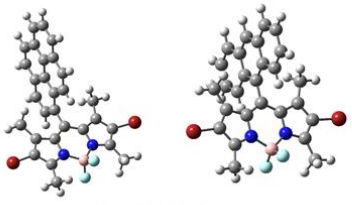


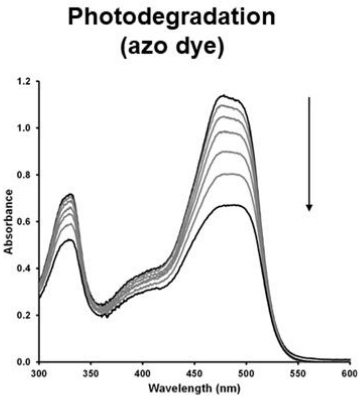
The goal of the project will be to synthesize and characterize a series of near-infrared absorbing AzaBODIPY dyes that absorb deep within the therapeutic window (650-1000 nm) that is useful for biomedical applications by extending the π-conjugation system of the AzaBODIPY chromophore. Heavy atoms will be incorporated to enhance the singlet oxygen yields and make the dyes suitable for use as photosensitizers in PDT. Once the photophysical properties of the dyes have been fully investigated, water-soluble encapsulation micelles will be formed with Pluronic® F-127 polymer. The photodynamic activity of the dyes and their encapsulation complexes will be tested *in vitro* against MCF-7 breast cancer cells.

Reference: H. Lu, J. Mack, Y. Yang, Z. Shen, Chem. Soc. Rev. **2014**, 43, 4778-4823.

JMp4 **Photodegradation of azo-dyes by BODIPY-embedded nanofibres** (Co-supervisor: Prof. T. Nyokong)







In recent years, BODIPY dyes have been brominated and iodinated so that their singlet oxygen quantum yields are significantly enhanced. The high photostability of these dyes makes them ideal candidates for use in singlet oxygen photodegradation applications such as industrial wastewater remediation. The goal of the project will be to prepare a series of brominated and iodinated BODIPYs that can be conjugated to magnetic nanoparticles and to use electrospray polymerization to embed the nanoparticle conjugates into polystyrene nanofibers. The photophysical properties of the BODIPY dyes and their nanoparticle conjugates will then be investigated, and the suitability of the BODIPY-embedded nanofibers for use in the photodegradation of azo-dyes, which are recalcitrant pollutants found in a wide range of wastewaters, will be assessed.

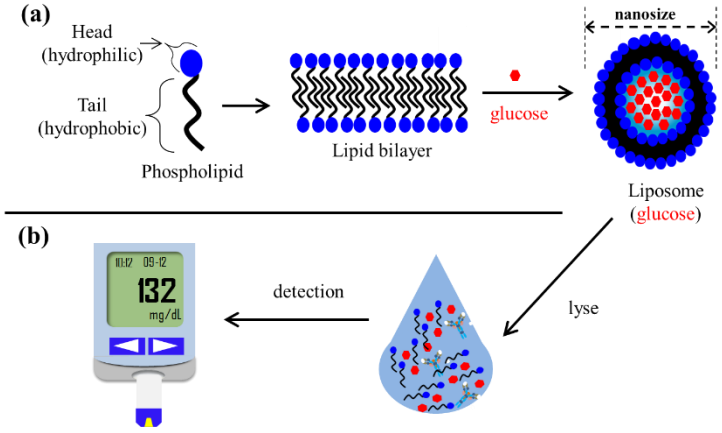
Reference: A. K. Lebechi, T. Nyokong, J. Mack, Macroheterocycles **2017**, 10, 460-46

Return to RESEARCH PROJECT (SHORT TITLES) 2021

Dr P Mashazi

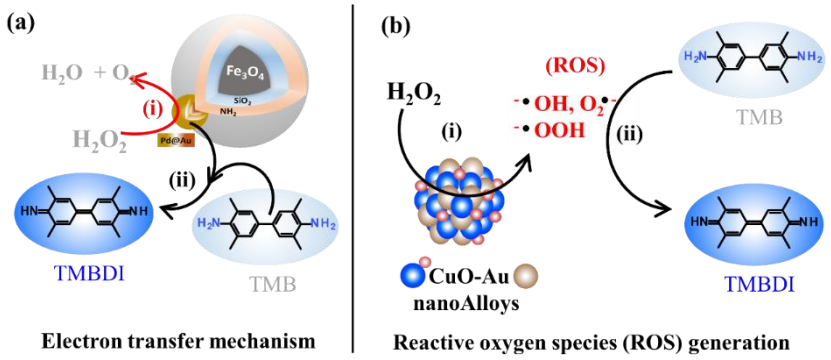
PNMp1 Preparation and characterization of pH-sensitive nanosize liposomes encapsulating D-glucose for electrochemical detection

The project will investigate methods for controlled preparation of pH-responsive liposomes loaded with D-glucose for electrochemical detection. The choice of the method for their preparation, the size control, optimum D-glucose encapsulation and the shelf-life (long-term stability) will be investigated. The research will also focus on the thorough characterization of these materials to obtain homogeneous sizes and determine the encapsulation efficiency. The formulation of these is off-importance in achieving the pH response for the release of encapsulated glucose molecules. Scheme below shows the schematic representation of the preparation of liposomes.



PNMp2 Preparation and evaluation of enzymatic properties of nanomaterials core-shell and alloys

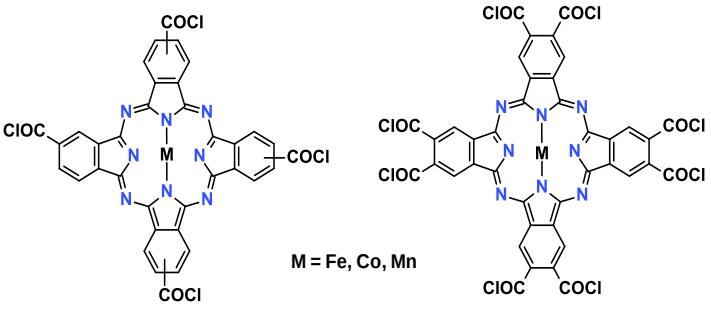
The research will investigate the preparation of size-controlled nanoparticles of bimetallic nanoparticles for their evaluation as nanozymes. The preparation method will determine whether the alloy or core-shell structure of nanomaterial formed. Studying the prepared nanomaterials as enzyme mimetic will involve determining their potential peroxidase or catalase-like properties. The preparation, characterization and evaluation of these materials is off-importance as they could be use as substitutes for peroxidase or catalase enzymes in biochemical analysis. The scheme below shows some of the materials that have been investigated in my research group and that enzymatic mechanism were observed to be via (a) electron transfer or (b) reactive oxygen species (ROS) generation. The effect of nanomaterial composition will further elucidate the preference of either of the mechanisms.



PNMp3 Synthesis and spectroscopic characterization of tetra and octa-carboxylic acid chloride metallophthalocyanines and their thin monolayer films onto gold surfaces

Phthalocyanines, Pcs, are N-4 macrocycles that have been shown to exhibit numerous applications; such as in medicine as photosensitive drugs for the treatment of cancer, chemical industry as catalysts for photodegradation of pollutants, electrocatalysts for detecting molecules of research interest. Their applications are affected by the central metal ion within the phthalocyanine ring structure and by the functional groups on the peripheral and non-peripheral positions. The metal ions and functional groups also affect their spectroscopic as well as electrocatalytic properties.

In this research, metallophthalocyanines (MPc) containing peripheral acid chloride groups and electroactive central metal ions will be synthesized. These complexes will be immobilized onto gold electrode surface to form pH sensitive electrochemical sensors. The research will involve the synthesis and characterization of MPcs shown in the Figure below. Their immobilization onto gold electrode surface as monolayer thin films will also be investigated for the detection of neurotransmitters.



tetra-carboxylic acid chloride metallophthalocyanine (tCOClMPc)

octa-carboxylic acid chloride metallophthalocyanine (oCOClMPc)

Return to RESEARCH PROJECT (SHORT TITLES) 2021

Professor T Nyokong

TNp1 Water purification using green technology (Co-supervised by Dr Britton– TWO projects).

The focus of this project is the use of nanotechnology combined with porphyrin-type dyes to develop materials that can provide solutions for water decontamination through advanced oxidation processes (AOPs). AOP uses molecular dioxygen and is an important strategy for pollution control, since it generally does not result in the formation of additional pollutants as by products [1]. AOP is considered as one of the most promising emerging green technologies for water treatment, due to the possibility of harnessing two readily available natural resources: dissolved oxygen and solar energy. Thus, the aim of the joint project is to link metallic and/or metal oxide nano/micro-particles to porphyrin-type complexes (Fig. 1) such as metallophthalocyanines (MPcs) and metalloporphyrins (MPs) to create new hybrid materials (Fig. 1, using ZnO as an example) for their intelligent use in environmental control.

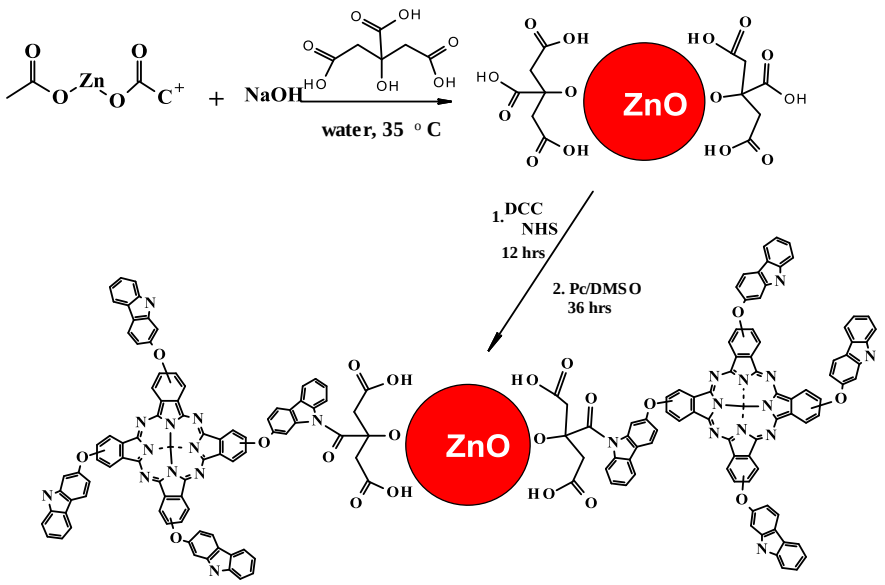
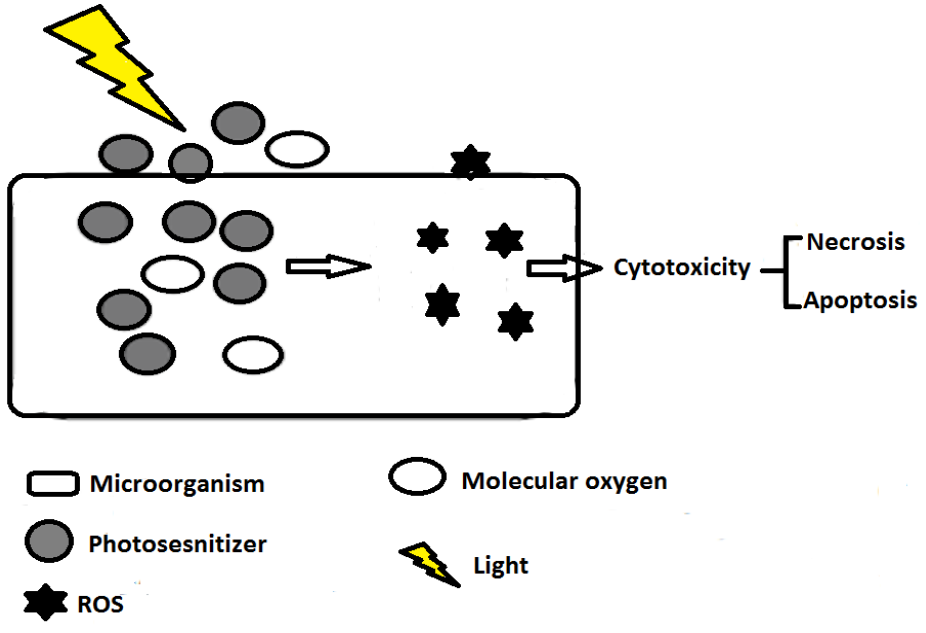


Fig. 1. Conjugation of nanoparticles to MPcs through an amide bond. DCC= dicyclohexylcarbodiimide, NHS = *N*-Hydroxysuccinimide, DMSO - dimethylsufoxide

TNp2 Development of Antibacterial agents (Co-supervised by Dr Britton, TWO projects).

Antibiotics provide a remedy for microbial infections. However, in the past few decades, an increased number of drug resistant pathogens have been identified. The photoinactivation of microorganisms has been suggested as a means to avoid this problem. Photodynamic antimicrobial chemotherapy (PACT) is an alternative method to deal with bacterial and fungal infections, which requires a photosensitizer that can be illuminated with light to cause the oxidative destruction of microbial pathogens. The design of novel porphyrin – type complexes that have high singlet oxygen quantum yields is of great importance [2]. Many nanoparticles (NPs) such as plasmonic gold and silver NPs also exhibit antimicrobial behaviour and can be combined with porphyrin-type to form functional materials that will not only further enhance the PACT activity but will enhance photosensitizer delivery.



Scheme 1: Schematic diagram illustrating the principle of PACT [3].

For both projects 1 and 2, the porphyrin-type molecules and conjugates will be embedded in electrospun fibers for recovery and re-use. Electrospun nonwoven mats have a high surface area, small pore size, and high porosity. In this project, ZnO and TiO_2 nanofibers will be fabricated by electrospinning the solution of titanium or zinc compounds in the presence of polyvinylpyrrolidone (PVP). The ZnO/TiO_2 nanofibers will be decorated with MPcs following calcination with the aim of yielding regeneratable and possibly reusable catalysts. Since no catalytic activity is associated with the polymer and it merely acts as a support, calcination of the fibers not only yields purely crystalline fibers but also eliminates the possible shielding of the activity of the embedded catalysts by the polymer. Other fibers such as polystyrene containing porphyrin – type complexes will also be developed. The synthesis of the materials will be developed in parallel with the testing of the materials in applications related to organic/inorganic pollutant photodegradation and PACT.

TNp3 Protection of the eye and optical devices from strong laser light (Co-supervised by Drs Britton and Mack, TWO projects).

In recent years, the number of cases of pilots being exposed to laser, the so called "lasered" whilst landing aeroplanes has increased dramatically. Non-linear optical (NLO) devices that limit high incident power light (Fig. 2) has been proposed as a potential solution to these problems. Optical limiting (OL) is a specific branch of nonlinear optics and it refers to decreased transmittance of a material with increased incident light intensity.

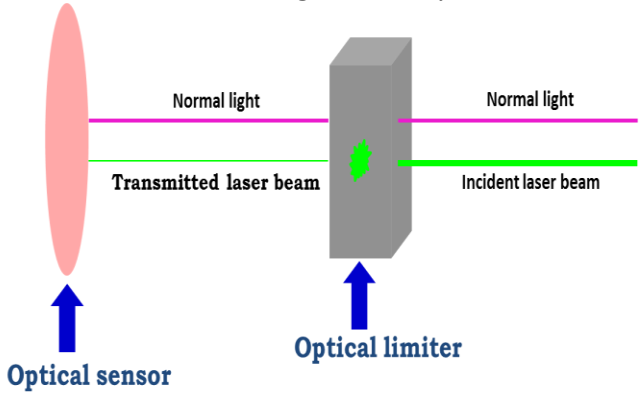


Fig. 2 Representation of optical limiting

There is a desperate and urgent need for materials which exhibit optical limiting capabilities and can prevent damage to the pilots' eyes and other optical devices. Phthalocyanines (Pcs) display nonlinear optical properties [3]. These molecules can thus be used for protection of optical elements (e.g. eyes) against damage by exposure to sudden high intensity light. OL is a nonlinear effect consisting of a decrease in the transmittance of NLO material (such as Pc) under high-intensity illumination. Phthalocyanines containing In and Ga as central metals exhibit good NLO properties and will be synthesized

1. P. Khoza, T. Nyokong, Visible light transformation of Rhodamine 6G using tetracarbazole zinc phthalocyanine when embedded in electrospun fibers and in the presence of ZnO and Ag particles, J Coord Chem 68(7) (2015) 1117-1131.

2. O. L Osifeko, I. Uddin, P. N. Mashazi, T. Nyokong, Physicochemical and Antimicrobial Photodynamic Therapy of unsymmetrical Indium phthalocyanines-Fe_3O_4-Silica core-shell conjugate, New J Chem 40 (2016) 2710 – 2721.
3. N. Nwaji, O. M. Bankole, J. Britton, T. Nyokong, Photophysical and Nonlinear Optical Study of Benzothiazole Substituted Phthalocyanine in Solution and Thin Film, J. Porphyrins Phthalocyanines 21 (2017) 263-272

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TNp5 Protection of the eye and optical devices from strong laser light (Co-supervised by Drs Britton and Mack, TWO projects).

In recent years, the number of cases of pilots being exposed to laser, the so called "lasered" whilst landing aeroplanes has increased dramatically. Non-linear optical (NLO) devices that limit high incident power light (Fig. 2) has been proposed as a potential solution to these problems. Optical limiting (OL) is a specific branch of nonlinear optics and it refers to decreased transmittance of a material with increased incident light intensity.

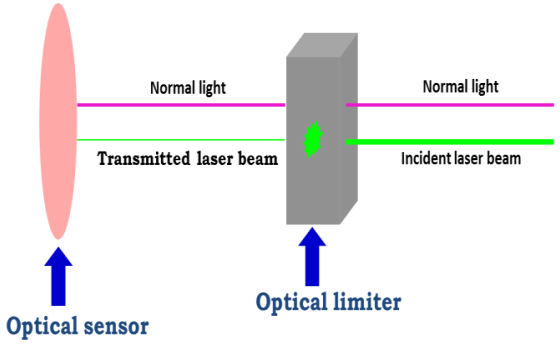


Fig. 2 Representation of optical limiting

There is a desperate and urgent need for materials which exhibit optical limiting capabilities and can prevent damage to the pilots' eyes and other optical devices. Phthalocyanines (Pcs)

display nonlinear optical properties [3]. These molecules can thus be used for protection of optical elements (e.g. eyes) against damage by exposure to sudden high intensity light. OL is a nonlinear effect consisting of a decrease in the transmittance of NLO material (such as Pc) under high-intensity illumination. Phthalocyanines containing In and Ga as central metals exhibit good NLO properties and will be synthesized

1. P. Khoza, T. Nyokong, Visible light transformation of Rhodamine 6G using tetracarbazole zinc phthalocyanine when embedded in electrospun fibers and in the presence of ZnO and Ag particles, J Coord Chem 68(7) (2015) 1117-1131.
2. O. L Osifeko, I. Uddin, P. N. Mashazi, T. Nyokong, Physicochemical and Antimicrobial Photodynamic Therapy of unsymmetrical Indium phthalocyanines-Fe_3O_4-Silica core-shell conjugate, New J Chem 40 (2016) 2710 – 2721.
3. N. Nwaji, O. M. Bankole, J. Britton, T. Nyokong, Photophysical and Nonlinear Optical Study of Benzothiazole Substituted Phthalocyanine in Solution and Thin Film, J. Porphyrins Phthalocyanines 21 (2017) 263-272

Return to RESEARCH PROJECT (SHORT TITLES) 2020

Mrs J Sewry

JSp1(1) Service-Learning: Working with the Mobile Science Laboratory

"Service-Learning is a method of teaching, learning and reflecting that combines academic classroom curriculum with meaningful service, frequently youth service, throughout the community"[http://en.wkikpedia.org/wiki/Service_learning]

The project entails assisting the Mobile Science Laboratory's team in designing curriculum-based practicals with pre and post lessons for Grade 10-12 learners. The researcher will take the pre and post lessons out to the schools two afternoons a term around the practical that the mobile science lab will run, and research the impact of the lessons and practicals. The practicals are aligned to the National Curriculum Statement and Assessment (CAPS). The researcher will also have to reflect on the work.

JSp2 Practical skills in the wake of COVID-19

Since students did not get the opportunity to do much in the laboratory during 2020, it would be good to assess their understanding and practical ability in the laboratory. This project will look at one practical and assess the students before, during and after the practical. Research ethics will be required for this project. The project could be based on the rubric proposed by Veale, Jeena and Sithebe, https://pubs.acs.org/doi/suppl/10.1021/acs.jchemed.9b00703/suppl_file/ed9b00703_si_001.pdf

Return to RESEARCH PROJECT (SHORT TITLES) 2021

Dr V Smith

VSp1 Co-crystal formation

The physicochemical modification of the properties of (new) drug molecules can be achieved by altering their solid state packing arrangements. In this project we will use cocrystal formation in order to induce physicochemical modification (co-supervised by Dr D. S. Khanye).

The bioavailability of drug molecules is intimately linked to both solubility and dissolution rate. Solubility and dissolution rate, in turn, influences the effectiveness of these molecules as suitable drug candidates while it may also lead to other adverse side effects. Physicochemical properties such as melting point, solubility and dissolution rate are dependent on the packing arrangement of molecules in the solid state, hydrogen bonding, van der Waal's and other electrostatic interactions. Moreover, since each drug

molecule has distinct physicochemical properties finding the optimal solid form is important for intellectual property, processing, enabling drug delivery and is key to obtaining regulatory approval.[1]

Cocrystals are solids that are crystalline single phase materials composed of two or more different molecular and/or ionic compounds generally in a stoichiometric ratio. Cocrystals are thus unique crystalline structures having unique properties.[1-3] Cocrystals are prepared by dissolving both the drug molecule and a co-former (a pharmaceutically acceptable molecule not necessarily a drug molecule) in a common solvent that is allowed to crystallize by slow evaporation.

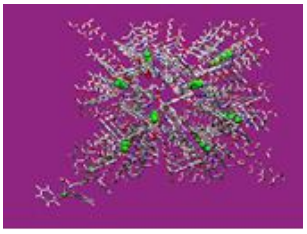
The putative drug molecules to be used in this investigation are chalcone-based drug molecules while the co-formers are selected amino acids.

M. J. Zaworotko *et al. Cryst. Growth Des.*, **2012**, 12, 2147-2152.
A. D. Bond *CrystEngComm*, **2007**, 9, 833-834.
G. P. Stahly, *Cryst. Growth Des.*, **2007**, 7, 1007-1026.
Return to [RESEARCH PROJECT (SHORT TITLES) 2021]

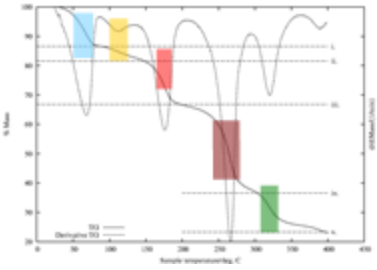
Prof GM Watkins

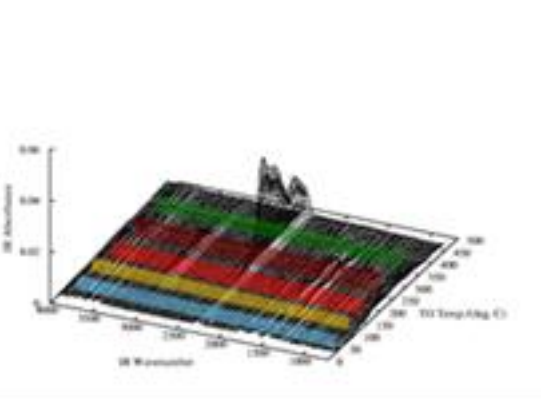
GWp1 Nanomaterials: supramolecular structure from metal coordination with 1, 2, 4, 5-benzenetetracarboxylic acid and pyridine:. A pyrolysis investigation.

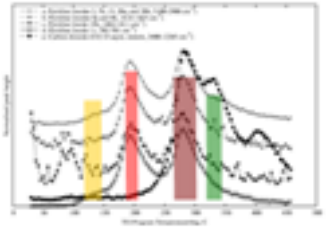
The MOF starting material is consists of a bridge benzenetetra carboxylate frame work, 2 pyridines and an axial H_2O bound to the copper. There is restricted channeling, containing 5 guest H_2O (z axis: cavity = 185 $Å^3$/unit cell).

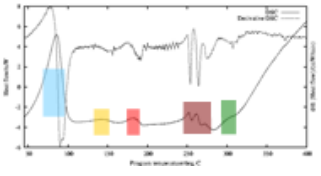


View down z axis









The starting material material undergoes loss of $6H_2O$ between 25 and 85 ºC (blue: DSC - endotherm; TG - single step), loss of ½ pyridine from 85 to 150 ºC (yellow: DSC - endotherm; TG - broad step, EGA profile), loss of a further 1½ pyridine from 150 to 197 ºC (red : DSC - endotherm; TG - single step, EGA profile). Further heating causes decomposition, with rapid loss of loss of 2 pyridine, $1½CO_2$ and $1H_2O$

between 197 to 303 ºC (brown: DSC – multistep endotherm; TG - broad step, EGA profile). Between 303 and 400 ºC final loss of ½CO2 and 3CO occurs (green : DSC - endotherm; TG - single step, EGA profile). The thermolysis is shown in the time resolved stack plot.

Inclusion behavioural study of the material is limited by the need for exact thermal control. Below 85 ºC inclusion of small solvent and gas molecules only is most likely possible ($[Cu_2(H_2C_{10}O_8)(C_5H_5N)_2]$). However the nature of the stable pyrolytic material formed between 150 and 197 ºC and its suitability to include guest molecules is to be investigated.

This project may make use of infrared and Raman spectroscopy, solid-state UV/VIS spectroscopy, TG-FTIR spectroscopy, thermal analysis, XRD, BET and XPS, amongst others.

Return to RESEARCH PROJECT (SHORT TITLES) 2021

PLEASE CHOOSE YOUR RESEARCH PROJECT AND ENTER YOUR CHOICES . at https://goo.gl/forms/UBY2QaKJCKlOwnEj2 ….

NOTE: PLEASE USE SHORT TITLES (PROVIDED AT THE BEGINNING OF THIS SECTION) WHEN FILLING OUT CHOICES.

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9. THE REVIEW ESSAY (C)

Introduction:

An essay on a subject which should not be directly related to the project, must be selected from the list supplied below. The Essay Supervisor must not be the same person as the Project Supervisor. The essay must be prepared in close consultation with the supervisor.

A first draft must be submitted by the middle of the second term. The supervisor must record the dates when the FIRST and FINAL drafts of the Essay were seen and approved. The First Draft and the Supervisor's comments must be handed in with the Final Draft to aid in the assessment of the candidate's contribution.

Students are required to submit their typed FINAL draft with their first draft by the end of the 2nd term. A Turnitin report must ccompnay the final report. The essay, which should extend to about twenty A4 pages (about 5000 words), is sent to the external examiner for marking. At the end of the second term, each student will present a short seminar on the essay topic.

SEMINAR ON "THE REVIEW ESSAY"

POINTS FOR DISCUSSION

Reading for the essay	making notes Quotations and plagiarism
References	Styles
Language and Grammar	Punctuation Paragraphs
Layout	(1½ to 2 x spacing)
Interaction with supervisor	Drafts
Final product	Ring binding Checking
Examining	

REVIEW ESSAY DATES:

Start	Beginning of 1st term
Hand in first draft	End of 1st Term
Seminars	Provisionally last week of lectures in 2nd Term
Hand in final version	Last day of lectures for 2nd Term

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• REVIEW ESSAY TOPICS 2021

Dr J Britton	
JBe1	Discuss how ultrasound can be used for treating cancer.
Dr T Geswindt	
TGe1	The quantitative determination of pesticide residues on fruit (e.g. avocado) by means of LC-MS/MS and GC-MS/MS
Prof R Klein	
RKe1	Teaching stereochemistry – methods and challenges
RKe2	Advantages and disadvantages of multicomponent reactions
Prof RW Krause	
RuiKe1	Stimuli-responsive materials in drug delivery
RuiK2	The role of natural products in modern drug discovery
RuiK3	Biological interactions of nanoparticles
Dr KA Lobb	
KALe1	Applications of Car-Parrinello molecular dynamics
Prof J Mack	
JMe1	The synthesis, properties and applications of boron azadipyrromethene (azaBODIPY) dyes
JMe2	Antibiotic resistance and photodynamic antimicrobial chemotherapy
JMe3	The biomedical applications of gold nanoparticles
JMe4	The research and development of quantum dot solar cells
JMe5	Theory and applications of MCD spectroscopy
Dr P Mashazi	
PNMe1	Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS): Principles, Data Acquisition and Analysis
PNMe2	X-ray photoelectron spectroscopy (XPS): Data evaluation towards universal and standardised data analysis
Mrs J Sewry	
JSe1	How did covid change the way we teach Chemistry?
JSe2	Practical skills in the wake of COVID-19
Dr VJ Smith	
VSe1	Metal-organic Frameworks (MOFs) as Materials for the Rehabilitation of the Environment

PLEASE CHOOSE YOUR ESSAY TOPIC AND ENTER YOUR CHOICES . at https://goo.gl/forms/UBY2QaKJCKlOwnEj2 ….

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10. APPENDIX I: COMMUNICATING CHEMISTRY
Writing a scientific report

As professional chemists, we (should!) record all of our experiments in lab books. But lab books are not very useful to other chemists who want to find out about our work. As a professional chemist, you will therefore need to write short reports summarising your work, and some fuller technical reports. The latter might take the form of:

- Honours project report
- MSc or PhD thesis
- Full research papers

Most full scientific reports cover these areas. The 1:2:3 guideline for length usually gives a well-balanced report, but is not always appropriate.

1. Introduction and background
2. Experimental details
3. Results and discussion
4. References
5. Summary or Abstract

[There may be additional brief sections]

• INTRODUCTION AND BACKGROUND

This is usually divided into three sub-sections:

- Brief summary of why the topic of the report is important/interesting
- Review of work in the area by others
- Statement of the specific aim(s) of the work

N.B. The introduction provides a general review of the topic - specific aspects of the work will require mini-reviews/references, as part of the 'Results & Discussion' section

• EXPERIMENTAL

This should report two things:

a) A clear, concise description of what you did, so others can repeat it

b) An accurate record of your data, so others can confirm your interpretation.

- You usually report only the final experimental procedures in detail (e.g. optimised reaction conditions, final design of apparatus, and successful collection of data). How you arrived at these procedures will be discussed in the 'Results and Discussion' section, and the 'Experimental' section may contain a brief description of these other experiments.
- You are strongly advised to follow the RSC format for presenting experimental details - see appropriate RSC journals.
- It is a good idea to start writing up your “Experimental” section in parallel with your lab research because:
  i) It is quite time-consuming and fiddly, and can be a daunting job if left to the end.
  ii) Writing up your 'Experimental' can help identify missing data or the need for extra experiments, and these can be dealt with immediately.
- Check and double check the "Experimental" section - these are your definitive results, so your scientific integrity is on show!

• RESULTS & DISCUSSION

- You need to be familiar with the work, and have worked out all of the key results.
- Schematically map out the story you will be telling, using headings/drawings/arrows.
- Use the scheme to produce headings and sub-headings for your report.

(Tip: These headings may remain in your final report (often very helpful to the reader, especially in long reports), or may simply provide guidance for the structure of your report (e.g. in a paper). In theses, the 'Results & Discussion' section may be divided into several chapters, to provide more clarity. Your story need not be chronological - look at all of your results, and decide how best to explain them to your reader).

- Write the story out in rough, referring extensively to tables, diagrams and schemes (yet to be drawn). The R&D section should summarise your experimental results, and provide brief confirmatory evidence that your interpretation is correct.
- Now draft out the graphics.
- Produce the final report in the correct format.

• SUMMARY

Important - most reports must have a summary or abstract. Other scientists will often use the summary to help to decide whether to read a report/paper/thesis, and summaries often generate keywords that are used to locate important work. There is sometimes a specific format and length for summaries, but here is some advice:

- Decide the key results you want to report
- Identify three or four headings (e.g. aims, methods, key results, conclusion), and one or two graphics
- Use the headings to write a mini-story - it should be possible for a non-expert to read it in 3-4 minutes, and understand why you did the work, the main method(s) you used, the key results you obtained, and your principal conclusions

• REFERENCES

It is important that these are:

- Complete (don't miss any key papers)
- Accurate (get the citation right)
- Presented in a standard (varies) format

• ADDITIONAL SECTIONS

- **Keywords** are often required in papers, for cross-referencing in Chemical Abstracts or other databases, so others can find your work
- **Other layouts** are sometimes specified for scientific reports - e.g.
  Separate 'Results' and 'Discussion' sections
  Experimental 'Methods' section preceding 'Discussion'
- **Glossary** may be needed (e.g. abbreviations in a thesis)
- **Appendices** often contain useful additional data (e.g. NMR spectra, X-ray data, computer programs, equipment specifications)
- **Acknowledgments** - don't forget to thank everyone who helped with the work

11. APPENDIX II COMMUNICATING CHEMISTRY

• GIVING AN ORAL PRESENTATION

You will almost certainly have to give many short talks during your career as a chemist. It may be just to a group of 5-6 colleagues at group meetings, or it may be to bigger audiences. However, you are the expert on your subject matter! You have done the experiments, or have read about your subject. So be confident, and don't go too fast or include too much detail. You must plan a talk that suits you (for style) and the audience (for clarity and interest) - just think about what are the good and bad points in lectures/talks you've attended. So here are some guidelines for a

20 minute chemistry talk, using PowerPoint presentation, there are also additional tips later in this section.

Planning

a) Divide your talk into 3 or 4 parts. Here is a common format, with approximate times suggested:

Introduction	3 min
Core (1 or 2 sections)	10 min
(Your results, or key points)	
Summary or conclusion	2 min
Questions	5 min

b) Jot down what you want to say using:

- Snappy headings
- Brief sentences
- Structures
- Schemes
- Small tables/graphs/charts ... visual aids

c) Plan out about 6-8 slides

- Keep slides **simple.**
- Each slide will need to be up for **>1 min.**
- Structure your slides to help **guide** and **inform** your audience
- (N.B. slides can contain **prompts** for you).

Preparation

a) Make up slides:

- Use **big** drawings/type.
- Use **colour** for emphasis.
- **Check** that they are easily read at a distance.

b) Try the talk:

- Just try **explaining** everything aloud, referring to your slides.
- If you're very nervous, write it all out **as a back-up, but do not read from your detailed notes.**
- Make **headings on a card** for reference.
- Possibly add something for **variety** (visual aid, anecdote).
- **Run through** the talk 3-4 times, ideally to a friend, until you're happy with content and length.

Giving your talk successfully

- Beforehand, check that you can work the projector/lighting etc.
- Try to stand relaxed, without fidgeting, and looking confident!
- Take it easy ... there's no rush ... refer to slides, but look at the audience as much as possible.

The end of the talk

- Try to finish on a high point (something successful).
- Make it clear you've finished - e.g.
  “Thank you for your attention” (not "That's it!")

After your talk

- Get some feedback - you need an honest friend to tell you the best things about your talk ... and also the features that were less successful.

Some additional tips:

Preparation

- Using composite slides (where you add or reveal information to gradually generate a complex slide) works well.
- Mixed media presentations (e.g. slides + demonstration + video projector) are great, but lots of quick changes between different media can bewilder an audience

Giving your talk

- If you are offered a microphone in a large room, use it
- Maybe write out your first sentence ... but make yourself use card headings thereafter
- Look at the audience ... although just over their heads has the same effect!
- Try not to block your audience's view of the screen - if you want to point to something on a slide, simply point a laser point at the appropriate bit of the slide.
- If you stumble over your words, or spot any mistakes on your slides, just carry on regardless ... like any other performer would!

At the end

- If questions are asked, take your time to answer, and admit if you don't know. One good tactic is to repeat the question in your own words, which:
- Ensures everyone can hear the question
- Means it is clear what question you'll answer and buys you a bit of time to think of an answer!

12. INITIAL CHOICE FORM

The form can be found on the NEXT page (page 38)
And can be used to jot down what you would like to do

<u>The FINAL CHOICE FORM</u>

Will be completed during the *FIRST WEEK* of the Honours Course via a Google form.

Details will be given during the first week of class.

CHOICE INDICATION

As a preliminary, though not binding, indication of your **probable** choice of Topics, please circle the ***FIFTEEN*** lecture topics likely to be chosen by you, fill in details of your essay (first, second, and third choices) and project (first, second, and third choices).

LECTURE TOPICS:

PAPER 1:	RuiK2	VS1	GW2	RK3			
PAPER 2:	PTK1	RuiK3	JM2	PNM2	JS1	RK1	GW3
PAPER 3:	PTK2	DSK1	RuiK4	TG1	KAL1	JM3	GW1
Conts. Assess.	VL1	RK2	KAL3	JS2	JM1	RuiK1	

PROJECT: (SHORT TITLE) **INITIALS**

1st Choice: **Supervisor:**

2nd Choice: **Supervisor:**

3rd Choice

ESSAY: (NUMBER) [make sure you choose a DIFFERENT supervisor here]

1st Choice: **Supervisor:**

2nd Choice: **Supervisor:**

3rd Choice