RHODES UNIVERSITY

Where leaders learn

DEPARTMENT OF CHEMISTRY

HONOURS

2019

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CHEMISTRY HONOURS – 2018
Head of the Department: Prof R Krause
Course Coordinator: Dr R Klein (r.klein@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.

1.1 DP REQUIREMENTS

1. Must participate in all chosen lectures, and must submit all assessments.
2. Must attend **all seminars** in the Chemistry Department.
3. Between 8 am and 5 pm every honours student is expected to be in lectures or working on their project (unless they are tutoring or demonstrating).
4. Failure to adhere to submission dates will result in loss of DP.
5. In order to achieve a passing grade a subminimum of 50% is required in both project and theory.
6. DP refusals 9 October

1.2 FINANCIAL ASPECTS

Each student is responsible for financing his or her studies. Financial aid questions should be directed to the post graduate funding office (email) (website)

Fees for Honours (2018):

Academic deposit:	Please see 2018 Fees booklet for appropriate options
Residence deposit:	Please see 2018 Fees booklet for appropriate options
Tuition fee:	Please refer to fees booklet at www.ru.ac.za/fees for information
Residence fee:	Please refer to fees booklet at www.ru.ac.za/fees for information

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2. PROGRAMME FOR ORIENTATION WEEK Tuesday 05/2/2018 - Friday 08/2/2018

Tuesday 5th February

9:00 General outline of the Honours Course (Prof Krause; Dr Klein)

10:00 **Introduction to the "Review Essay"**

See also the attached handout on Writing a Scientific Report, Appendix 2.

11:00 **Seminar on "Introduction to Research Projects"**

(Chaired by Dr Klein with discussion by Staff). Chemistry Tea Room (F29)

POINTS FOR DISCUSSION

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!

14:00 – 15:30 Meet with lecturers to discuss projects, essays and lecture choices

Wednesday 6th February **REGISTER at the Student Bureau**.

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

09:00 Service learning and Community Engagement (Mrs Sewry)

09:30 – 10:30 Meet with lecturers to discuss projects, essays and lecture choices

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

11:00 Computer facilities and registering to use Scifinder Scholar (Dr K Lobb). Chemistry computer lab (F15)

14:00 Tour of building and location of instruments. Visit to Stores and Workshop (Prof Watkins, Dr Smith) Meet in Chemistry Tea Room (F29)

Thursday 7th February

9:00 to 16:30 Social meeting of Chemistry staff and students. Details will be confirmed upon your arrival.

Friday 8th February

9:00 Complete RUConnected final choices of topics, projects and essays

TBC Tutor training (Dr Khene)

16:00 STAFF ONLY Meeting (Reading room S38: finalizing of Honours programme).

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

Monday 11th February

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.

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3. PROGRAMME FOR 2019

Date TBA for below (***provisionally 2nd week of 1st Term***)

14:15 **Presentations on project plan**

FORTHCOMING ATTRACTIONS!

Towards the end of the second term (***provisionally last week of lectures in 2nd Term***) students will be required to give talks (15 min) on the subject of their REVIEW ESSAYS.

In September/October (***provisionally*** last week of September/ 1st week of October) students will be required to give talks (20 min) on the subject of their RESEARCH PROJECTS (see handout).

Summary of submission and presentation dates (by Term):

First term:

- Presentation of project plan 2nd week of 1st term (***provisionally 2nd week of 1st Term***)

  (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.** Make sure that you run through this plan with your supervisor on or before Friday!

  (see the attached Appendix on "Giving an Oral Presentation")
- **A structured beginning to the research essay** (Library tour @ 2pm, and the use Scifinder Scholar and other electronic resources)
- Hand in 1st draft of essay (end of 1st Term)

Second term:

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

Third term:

- Collect June scripts

Fourth term:

- Hand 1st draft of project (1st day of 4th Term) and
- Hand in Final version of project (1st Friday of October) of project report
- Project seminar (***provisionally*** last week of September/ 1st week of October)

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4. DETAILS OF THE HONOURS COURSE

COURSE STRUCTURE

(A) 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. Each topic is allocated 10 x 1 hr lectures

The topics vary from year-to-year with the staff available and their interests, and depend on the number of students opting for 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 seminar with NMMU, WSU and 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 your first draft into consideration.

Joint Honours: Chemistry/X

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 for their Third year Chemistry.

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5. COURSE ASSESSMENT

(Total marks 800)

(A) Lecture topics

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. The relevant time per module will be deducted from the 3 hour examination time, where this option is taken up.

(B) Class Marks

The course class component mark (Total 350) is broken down as follows:

June Exam	**40**	**5%**
Project		
Seminar	50	
Written Report	150	
Total	**200**	**25%**
Essay		
Seminar	20	
Written Essay	90	
Total	**110**	**13.25%**

Theory Marks

The course theory component mark (Total 450) consists of marks for 12 modules evaluated either by continuous assessment or by examination.

Theory Marks	(12 x 37.5)	**56.25%**
Total	**450**	

Course total: 800

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6. 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 **THREE** groups (see below) and **FIVE** topics must be chosen from **EACH** group. 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. Complete the form at https://goo.gl/forms/UBY2QaKJCKlOwnEj2

Paper 1	PK1	Advanced NMR spectroscopy	
	SK1	Electrochemistry and Impedance Spectroscopy	
	RuiK1/3	Supramolecular Chemistry in Medicine (and/or option Ruik3)	
	VS1	Solid State properties of materials	
	PNM1	Intelligent nanomaterials and their applications	
	SA1*	Industrial Perspective Of Analytical Chemistry	
	GW2	Vibrational spectroscopy	
	RK3	Advanced retrosynthesis and Green Chemistry	
	KAL2	Molecular Modelling: Chemical Properties and Reactivity	
	JM1	Molecular Modelling: molecular symmetry and TD-DFT calculations	

Paper 2	PTK1	Asymmetric synthesis	
	RuiK2/4	Chemical Aspects of Biosynthesis (and/or option Ruik4)	
	KAL3*	Molecular Modelling: Interactions and Dynamics	
	JM2	Porphyrinoid chemistry	
	PNM2	Design and development of biosensors	
	JS1	Introduction to Chemometrics	
	GW3	Inorganic reaction mechanisms	

Paper 3	PTK2	Strategies in drug synthesis and design	
	DSK1	Physicochemical Properties in Drug Design	
	SK2*	Science origins and limitations	
	RK1	Catalysis in organic chemistry	
	KAL1	NMR spectroscopy	
	JM3	Optical spectroscopy	
	JS2*	Service-Learning in Chemistry	
	GW1	**Symmetry and group theory**	

- Topics with * are examined by various "in course" assessments.
- A minimum of two examinable topics are required per paper, and a minimum of three continuous assessed courses (*) are required.

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 the 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.

Theory component dates

Mid-year Exam:	June
Re-write failed June questions:	2nd Friday of 3rd term
Final Examination:	November

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6.1 DETAILED CONTENTS OF LECTURE TOPICS

RK2 INTRODUCTION TO RESEARCH METHODS (NOTE this is a REQUIRED topic for all students)

The aims of this course are to explore research skills which are not covered in undergraduate practical and theory courses as well as encourage students to develop critical skills in reading, synthetic experiment design, and in analysis of experimental outcomes. The course will combine theoretical principles with practical experimentation in the context of equipment and opportunities available within the department. There will be opportunities to consider the range of demands on students and how to manage your time and resources.

Paper 1

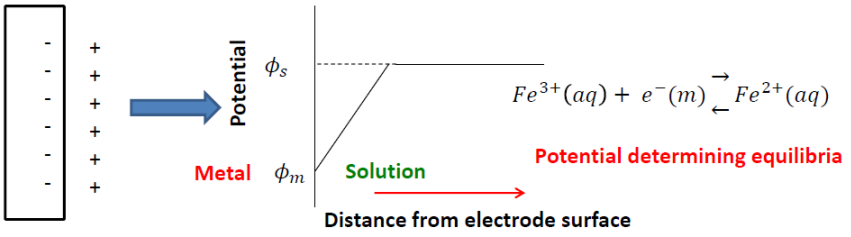
Dr P KEMPGENS (ROOM S42)

PK1 Advanced NMR spectroscopy (LECTURE TOPICS (A))

A 2D NMR experiment will be described from a mathematical approach. Two different mathematical approaches will be used, namely the density matrix formalism and the product operator treatment.

PROF S KHENE (ROOM S39)

SK1 Physical Electrochemistry and Impedance Spectroscopy (LECTURE TOPICS (A))



Electrochemistry offers a unique and powerful approach to examine electron transfer events. It provides key insights into fundamental factors which drive electron transfer processes. The aim of this course is to provide an introductory account of the science of electrochemistry. The aim is to explain the origins of electrode potentials, show their link with chemical thermodynamics and to indicate why their measurement is important in chemistry.

Impedance spectroscopy (IS) plays an important role in fundamental and applied electrochemistry and material science. Impedance Spectroscopy measures the impedance of a system over a range of frequencies, to reveal the frequency response of the system, including the energy storage and dissipation properties.

PROF R KRAUSE (ROOM F42)

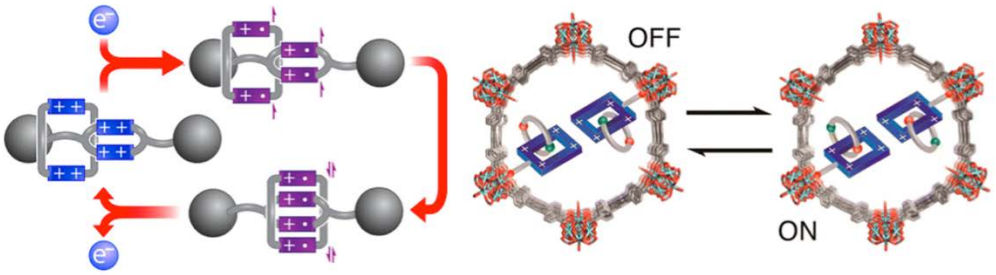
(**Note** ONLY two of RuiK1- RuiK4 will be presented, depending on numbers) **(LECTURE TOPICS (A))**

RuiK1 Supramolecular Chemistry in Medicine (presented with Dr Smith)

You're a chemical soup – so how do collections of chemicals and lots of water, stick together and interact with one another so that living things like us can exist?

When molecules are arranged in specific structures and interact by "non-covalent" bonds, you are dealing with supramolecular chemistry. This is chemistry beyond the molecule and the chemical bond. Supramolecules span the range of tiny to enormous, and have many applications from data-storage, sensors, and catalysis to nano-machines and on/off switches.

In this module Drs Smith and Krause will explore with you, some of the recent developments in supramolecular chemistry and where this fascinating field is headed.



RuiK3 Nanoparticles, Drug Delivery, and Biological Interactions

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 S36)

VS1 Solid State Properties of Materials (LECTURE TOPICS (A))

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 (LECTURE TOPICS (A))

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

VISITING LECTURER

VL1 Industrial Perspective of Analytical Chemistry (LECTURE TOPICS (A))

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 and introduces the various technologies and stakeholders encountered in the workplace. 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 project and presentation).

PROF G M WATKINS (ROOM S2)

GW2 Vibrational spectroscopy (LECTURE TOPICS (A))

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 S35)

RK3 Advanced retrosynthesis and green chemistry (LECTURE TOPICS (A))

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.

PROF KA LOBB (ROOM S40)

KAL2 Molecular Modelling: Chemical Properties and Reactivity (LECTURE TOPICS (A))

This course is a practical introduction to molecular modelling, which starts with construction of unimolecular (including conformational search) and periodic systems. There is a general background to molecular mechanics and ab initio methods, with focus on ab initio methods and the calculation of various properties of molecules. Finally, reactivity and the potential energy surface are presented with the calculation of stationary states including the location and characterization of minima and transition states.

Continuous assessment will involve the completion of a small project in lieu of an exam question.

Dr J MACK (NIC G28)

JM1 Molecular Modelling: molecular symmetry and TD-DFT calculations (LECTURE TOPICS (A))

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.

Paper 2

PROF PT KAYE (ROOM S41)

PTK1 Asymmetric synthesis (LECTURE TOPICS (A))

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)

(**Note** ONLY two of RuiK1- RuiK4 will be presented, depending on numbers) **(LECTURE TOPICS (A))**

RuiK2 Chemical Aspects of the Biosynthesis of Natural Products

In Natural Product Chemistry, every known organism from the smallest virus to the largest tree or mammal produces a vast array of compounds using a surprisingly small number of common processes. This course will explore some of these aspects from how an organism converts a DNA signal into a natural product. These syntheses are the building blocks of metabolism and finally, how can chemists exploit some of the interesting pathways to discover and build new medicines.

RuiK4 Potholes and Detours - (Advanced Synthetic Strategies)
Ever wonder why that publication came up with such a strange reagent or synthetic route? Often it's because they came to a synthetic pothole and had to find a detour.

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 in Organic Chemistry" and "Asymmetric Synthesis" taught in other modules, and will draw on literature examples.

PROF KA LOBB (ROOM S40)

KAL3 Molecular Modelling: Interactions and Dynamics (LECTURE TOPICS (A))

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.

Dr J MACK (NIC G28)

JM2 Porphyrinoid chemistry (LECTURE TOPICS (A))

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 (LECTURE TOPICS (A))

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 F38)

JS1 Introduction to chemometrics (LECTURE TOPICS (A))

"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 S2)

GW3 Inorganic reaction mechanisms (LECTURE TOPICS (A))

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

Paper 3

PROF PT KAYE (ROOM S41)

PTK2 Strategies in drug synthesis and design (LECTURE TOPICS (A))

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 (F43)

DSK1 Physicochemical Properties in Drug Design (LECTURE TOPICS (A))

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 MUST ALSO TAKE **PTK1.**

PROF S KHENE (ROOM S39)

SK2 Science Origins and Limitations (LECTURE TOPICS (A))

Science is a recent product of human culture and the drive to understand our natural world is a distinctive feature of human nature. Science is a socially constructed enterprise for obtaining knowledge of the natural world. This course aims to trace the historical development of science and to define what scientific knowledge means. This course will demand substantial amount of reading, discussion, and writing. Assessment will be in the form of an exam based on an essay and course readings.

PROF R KLEIN (ROOM S35)

RK1 Catalysis in organic chemistry (LECTURE TOPICS (A))

Catalysis is one of the most economically important areas of chemical practice and research. This course will include an overview of homogenous and heterogeneous catalysts used in organic chemistry. An emphasis will be placed on processes which are used industrially, and those which yield asymmetric products. Selected mechanisms will also be considered.

PROF KA LOBB (ROOM S40)

KAL1 NMR spectroscopy (LECTURE TOPICS (A))

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.

Dr J MACK (NIC G28)

JM3 Optical spectroscopy of aromatic π-systems and transition metal complexes (LECTURE TOPICS (A))

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.

MRS JD SEWRY (ROOM F38)

JS2 Service-Learning in Chemistry (LECTURE TOPICS (A))

This course will entail one lecture on an Introduction to Service Learning. Thereafter, the students will have to work in groups and do the following: at each of 2 schools: contact and make arrangements with the school, do a lecture demonstration of a "Pollutant's Tale" and do two hands-on workshops with the learners. The workshop and a reflection on the task will be handed in to be examined. Assessment will be by continuous assessment.

PROF G M WATKINS (ROOM S2)

GW1 Symmetry and Group Theory (NOTE: this is a required topic for all students.) (LECTURE TOPICS (A))

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)

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

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7. 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 Report should be concise and care should be taken with both grammar and spelling.. The report should be typed and bound with a plastic spiral binding (contact the Chemistry Store). 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 marking etc., should be done in the evenings. The Seminar will be assessed by staff and will count for 50 of the 200 marks.

RESEARCH PROJECT DATES:

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

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7.1 RESEARCH PROJECT (SHORT TITLES) 2019

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

	Dr J Britton
(1)	Photonic crystals
(2)	"Janus" nanoparticles
	Professor P T Kaye
(1)	Synthesis and Biological Screening
	Dr P Kempgens
(1)	NMR investigations
(2)	Selective deuteration
	Prof S Khene
(1)	Electrochemical sensors
(2)	Spectroscopy and Electrochemical properties
	Prof R Klein (no project will be offered in 2019)
(1)	Multicomponent reactions
(2)	Catalysis
(3)	Green chemistry
	Prof RW Krause
(1)	Pyrrolo- marine alkaloids
(2)	Mass Spectrometric tools for Stromatolite chemistry
(3)	Stimuli-Responsive Liposomes.
(4)	A low-cost DSSC
	Prof KA Lobb
(1)	Carbocations
(2)	HIV treatments
	Dr J Mack
(1)	BODIPY nanoparticle conjegates
(2)	Water soluble porphyrins
(3)	Optical limiting AzaBODIPYs
(4)	BODIPY-embedded nanofibres
	Dr P Mashazi
(1)	Transducer sensor surfaces
(2)	Hybrid nanostructured materials
(3)	metal-metal oxide nanoparticles
	Professor T Nyokong
(1)	Sonodynamic therapy
(2)	Chemophototherapy
(3)	Covalent organic frameworks
(4)	Nano-cages, -worms, -rod
(5)	Cultural heritage
	Mrs J Sewry
(1)	Service-Learning
(2)	Labskills
	Dr V Smith
(1)	Co-crystal formation
	Prof GM Watkins
(1)	Benzenecarboxylates
(2)	Benzenetetracarboxylic acid
(3)	Tetracarboxyphthalocyanine

7.2 DESCRIPTIONS OF RESEARCH PROJECTS 2019

Dr J Britton

(1) 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.

(2) The synthesis of "Janus" nanoparticles for use in nonlinear optics

A "Janus" nanoparticle is essentially one which has at least two hemispheres of different materials. Such an arrangement, as opposed to one where the nanoparticle is only made of one material, can result in some interesting interactions, though it is dependent on what materials the nanoparticle is made from.

The idea for this project is to create a "Janus" nanoparticle out of two different polymers, each of which may or may not contain different nonlinear compounds, which will hopefully have some degree of transparency to them. This will result in a compound that will interfere with the transmission of light through it, hopefully only at high light intensities.

Figure 1 indicates the general setup for making a polymeric "Janus" nanoparticle. What occurs is that the two polymeric mixtures are introduced into another flowing solvent at the same time and point. Due to the fast flow of the other solvent, and the fact that said solvent will usually not be able to dissolve the polymers being used, beads of blended polymer mixture are removed from where the two polymer solutions are meeting the flowing solvent.

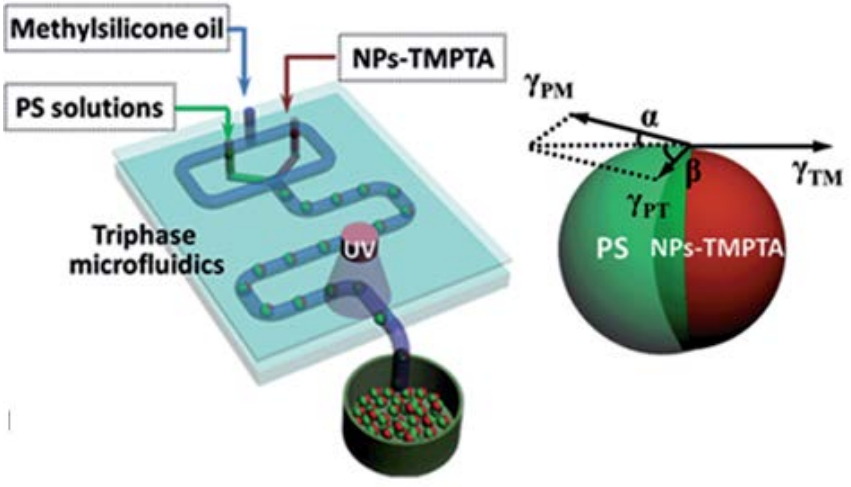


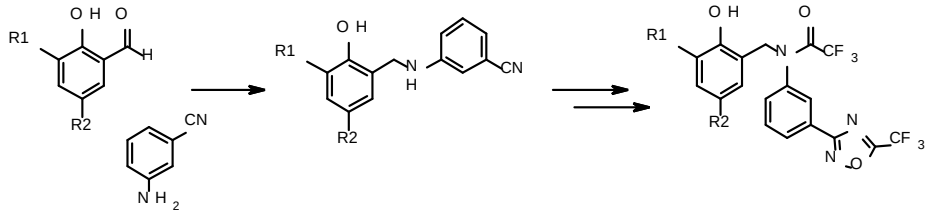
Figure 1: General microfluidics setup for "Janus" nanoparticle synthesis.

Return to RESEARCH PROJECT (SHORT TITLES) 2019

Professor P T Kaye

(1) <u>Synthesis and Biological Screening</u> of 5-Trifluoromethyl-1,2,4-oxadiazoles (Co-supervisor: Dr R. Klein)

Novel 3-substituted 5-trifluoromethyl-1,2,4-oxadiazoles **1**, prepared in our group exhibit significant anti-malarial activity at very low micromolar concentrations, while one of these compounds exhibits sub-micromolar inhibition of *Trypanosoma brucei* (responsible for sleeping sickness). Some of these compounds also exhibit promising selective anticancer potential (IC_{50} < 20µM against HeLa and MDA-MB-231 cancer cells). This project will involve the preparation of additional 5-trifluoromethyl-1,2,4-oxadiazoles, using an established method, to permit finalization of the study for publication.



Return to RESEARCH PROJECT (SHORT TITLES) 2019

Dr P Kempgens

(1) <u>NMR investigations</u> of organolithium compounds (in collaboration with Dr Klein)

Organometallic compounds are used widely in organic synthesis even though their structure and behavior are often poorly understood. With the power of nuclear magnetic resonance spectroscopy we are able to analyse and understand complexes in solution and even make predictions about their reactivity. In this project we will prepare two or three organolithium compounds using diverse techniques including catalysis. Some of these compounds will contain more than one lithium nucleus. We will then study them by NMR to show the nature and arrangement of the lithium nuclei.

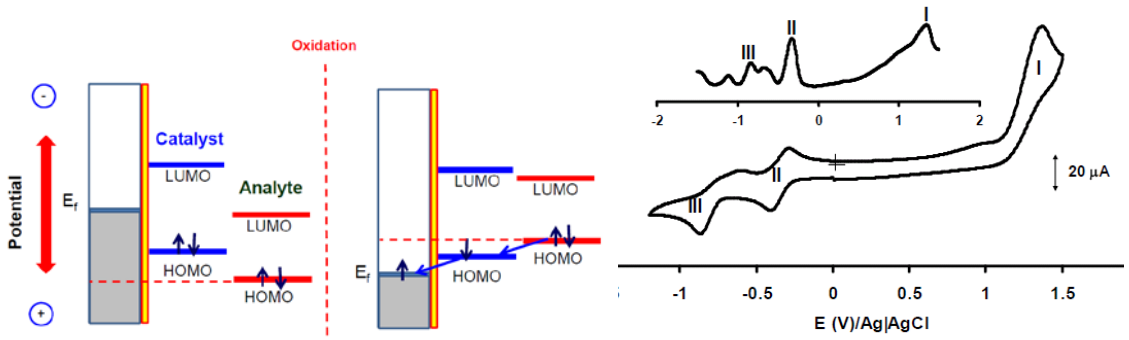
(2) <u>Selective deuteration</u> of some simple organic molecules and applications to NMR.

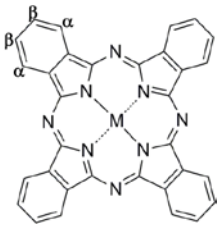
Some simple organic molecules will have to be selectively deuterated according to published procedures. The 1H NMR spectra exhibit triplets due to the coupling to deuterium which are asymmetric. It is believed that the asymmetry of the lineshapes is due to the interference term between quadrupolar and chemical shift anisotropy relaxations of deuterium. The NMR part of the project involves acquisition of 1H NMR spectra at different magnetic field strengths and measurement of the 2H relaxation time T1. For molecules containing more than a single deuterium, 2H COSY-type NMR experiments will be performed to reveal the ^{n}J(2H-2H) coupling.

Return to RESEARCH PROJECT (SHORT TITLES) 2019

Prof S Khene

(1) Development of Electrochemical sensors



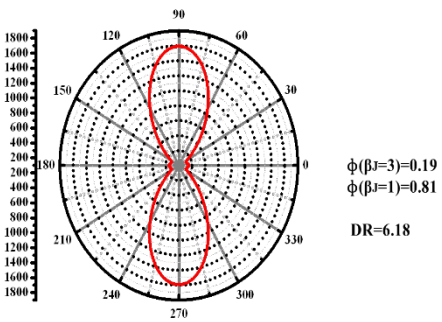


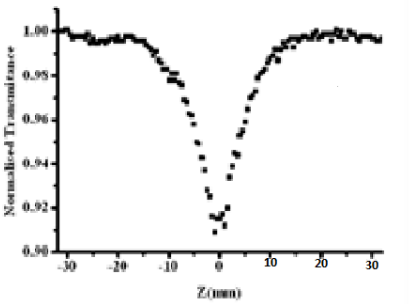
Over the years a considerable number of different metallophthalocyanines (MPcs) have been produced and found their application in various fields such as, synthesis of carbon nanotubes, nonlinear optics and solar cells. Metallophthalocyanines are also well known electrocatalysts for the oxidation of a variety of analytes including chlorophenols. The electronic structures of MPcs are known to have a strong effect on their electrocatalytic activity.Theoretical interpretation of MPcs electronic spectra has been a subject of great interest for a long time. In the past calculations which made use of semi-empirical methods, with questionable accuracy, were used.

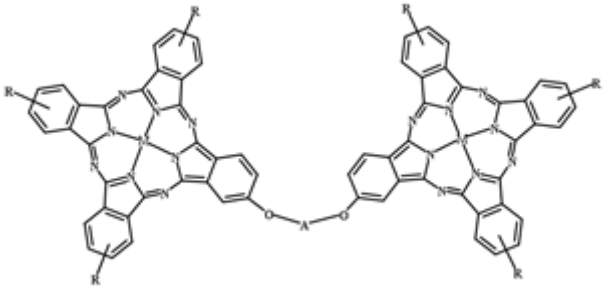
Recently more accurate high level density functional theory (DFT) calculations are in use. DFT calculations will help with the prediction of global and local reactivity of MPc complexes involved in electrocatalytic processes, thus making it possible to predict regions or atoms which are involved in electro catalysis.

The aim of the research is to (i) synthesise novel binuclear metallo phthalocyanine molecules for electrocatalyis, (ii) study of their thermodynamic properties and (iii) electrochemical properties. DFT calculations will be carried out to explain the spectroscopic and electrocatalytic properties of these complexes. The project will involve making use of these complexes for fabrication of electrochemical sensors for detection of various analytes and pollutants.

(2) Spectroscopy and Electrochemical properties of Metallophthalocyanines and Binuclear metallophthalocyanines for possible application in photovoltaic and nonlinear optical systems.







Organic materials with second-order nonlinear optical (NLO) material properties are useful in applications such as optical data processing and storage devices and can be easily processed and integrated into optical devices. Phthalocyanines exhibit large and rapid nonlinearities to incident pulsed laser light, which can be fine-tuned by rational modification of the molecular structure. Phthalocyanine molecules are known to have large third-order optical nonlinearities which arise from the highly delocalised two dimensional heteroaromatic 18-π electron system, and hence have been intensively investigated for their NLO properties.

The Z-scan technique is employed to determine the second order NLO properties of binuclear phthalocyanines and monomeric phthalocyanines. Their spectroscopic and photophysical properties are determined using a range of different spectroscopic techniques, including magnetic circular dichroism (MCD), time correlated single photon counting spectroscopy (TCSPC), and UV-visible absorption spectroscopy. A combined analysis of the optical spectral data and the results of density functional theory (DFT) calculations is used to characterise the physical properties of these compounds.

Return to RESEARCH PROJECT (SHORT TITLES) 2019

Prof R Klein (not offered in 2019)

(1) 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)

(2) 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.

(3) 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.

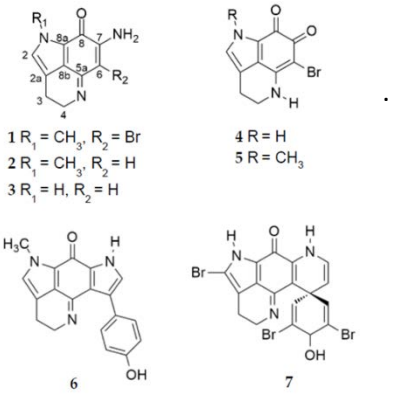
Return to RESEARCH PROJECT (SHORT TITLES) 2019

Prof RW Krause

(1) 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

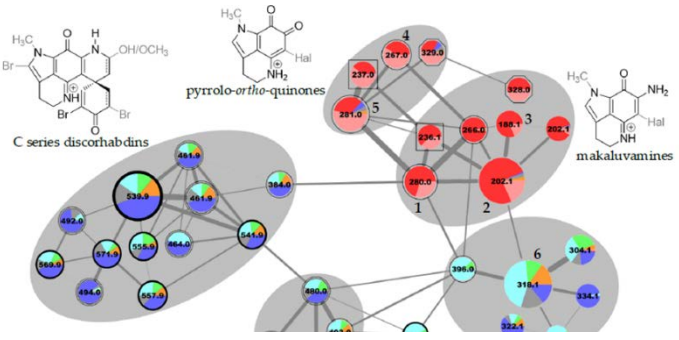


(2) Molecular Networking Mass Spectrometric tools for Stromatolite chemistry

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

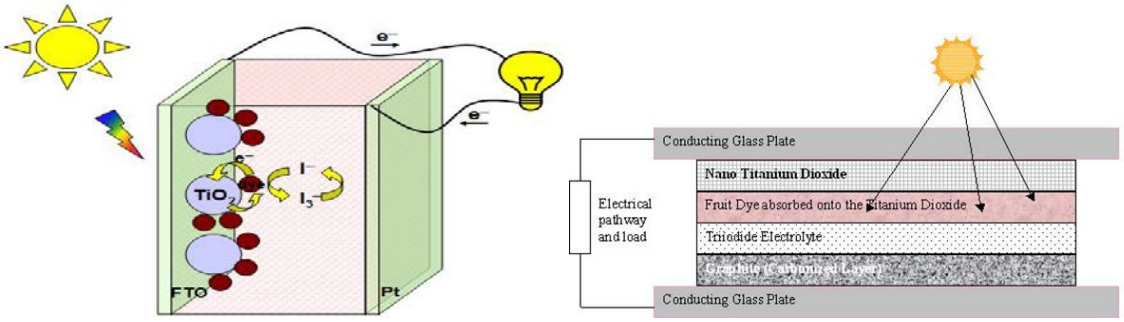


(3) Stimuli-Responsive Liposomes

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.

(4) 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) 2019

Prof KA Lobb

(1) Carbocations and carbocation rearrangements

Substituted bicyclo[2.2.1]heptane structures are of particular interest in this research group due to their tendency to undergo rearrangement involving carbocation intermediates in acidic environments. This project will involve the preparation of substituted bicyclo[2.2.1]heptyl carboxylic acids using an asymmetric Diels-Alder reaction. Following appropriate functionalization, these can become precursors for the study of carbocationic rearrangements. NMR and modelling are some of the tools that can be used to follow these rearrangements.

(2) Chemical Libraries and High-Throughput Virtual Screening in the search for new HIV treatments

This is a computational chemistry project. Using natural products with known activity against HIV (including Polycitone A, Betulinic Acid and Calanolide A) this study will involve construction of models that will be evaluated against several HIV-1 subtype C targets using computational techniques. This will include generation of chemical libraries, docking and high-throughput virtual screening, evaluation of physico-chemical properties of the ligands within the chemical libraries and molecular dynamics of protein-ligand complexes for promising cases.

Return to RESEARCH PROJECT (SHORT TITLES) 2019

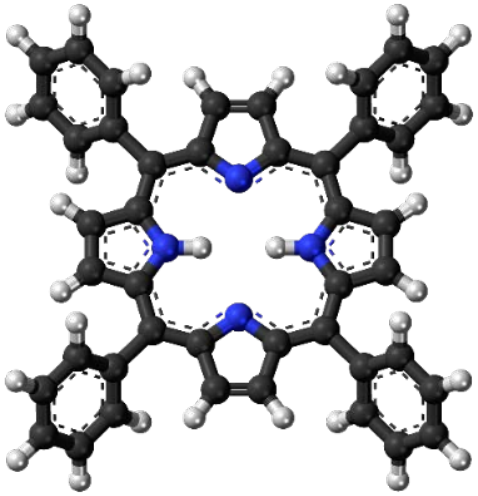
Dr J Mack

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

In recent years, there has been significant interest in the use of boron dipyrromethene (BODIPY) dyes as photosensitizers 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) and photodynamic antimicrobial chemotherapy (PACT). The project will involve the use of a laser flash photolysis system, the measurement of singlet oxygen quantum yields and PACT related studies with bacteria to assess their suitability for use in biomedical applications.

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

(2) **<u>Water soluble porphyrins</u> for biomedical applications** (Co-supervisors: Prof. T. Nyokong and Dr. B. Babu)



In recent years there has been considerable interest in the preparation of water soluble porphyrins and porphyrin analogues that absorb and emit light at the red end of the visible region and have high singlet oxygen quantum yields, since this makes them suitable for biomedical applications such as bioimaging, photodynamic therapy (PDT) and photodynamic antimicrobial chemotherapy (PACT). The project will involve the synthesis of water soluble porphyrins and the use of a laser flash photolysis system, the measurement of singlet oxygen quantum yields and PACT related studies with bacteria to assess their suitability for use in biomedical applications.

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

(3) **<u>Optical limiting AzaBODIPYs</u>** (Co-supervisor: Prof. T. Nyokong)

In recent years there has been a growing problem in aviation safety with the irresponsible use of laser pointers during the runway approach of aircraft and this has created a need for the development of optical limiting materials that can limit the transmission of high intensity laser pulses while remaining largely transparent under normal light conditions. The goal of the project will be to prepare a series of near infrared absorbing AzaBODIPY dyes by extending the π-conjugation system and the preparation of AzaBODIPY-embedded polymer thin films. Photophysical and non-linear optical measurements will be carried out to assess the suitability of the novel AzaBODIPY compounds that are prepared for optical limiting applications.

Reference: G. Kubheka, O. Achadu, J. Mack, T. Nyokong, New Journal of Chemistry **2017**, 41, 12319-12325.

(4) 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 photodegradation applications. The goal of the project will be to prepare a series of brominated BODIPYs that can be conjugated to magnetic nanoparticles and to use electrospray polymerization to embed the nanoparticle conjugates into nanofibers. The photophysical properties of the BODIPY dyes and their nanoparticle conjugates will then be investigated and the suitability of the BODIPY-embedded nanofibers to carry out the photodegradation of azo-dyes will be assessed.

Reference: A. K. Lebechi, T. Nyokong, J. Mack, Macroheterocycles **2017**, 10, 460-466.

Return to RESEARCH PROJECT (SHORT TITLES) 2019

Dr P Mashazi

(1) Orientation of biomolecules and their immobilization on the transducer sensor surfaces

Biosensors have found various applications in the early detection and monitoring of disease and virus infections. They also have been used extensively in the point-of-care testing for monitoring of chronic diseases so that timeous administering of medication is effective to sick people. Glucose monitoring and pregnancy test systems are the two examples that form the state-of-the-art and are the benchmark on biosensor research. Several other systems exists however these are laboratory based techniques with the benchmark being the enzyme-linked immunosobent assay (ELISA). Nowadays, there is a drive away from the laboratory based techniques towards point-of-care/home-care monitoring and testing. This is an area where biosensors are pioneering. Biomolecules for specific analyte detection will be integrated onto an electroactive surface and studied their potential in detecting the analyte of interest selectively and specifically. Several electroactive materials will be chosen with the aim of enhancing the attachment and orientation of the biomolecules onto the conducting or semi- conducting surfaces. For increasing sensitivity of the biosensor, electroactive nano/materials will be incorporated to enhance/amplify the electrical signal so that very low analytes concentrations may be detected.

(2) Enhanced electrochemical signal through the use of hybrid nanostructured materials

Nano-size and nano-structured materials have found various applications in sensors technologies as they have been shown to amplify the electrochemical signal of the analytes at very low concentrations. In this research project, the design of nanostructured materials and their integration with other catalytic materials will be investigated. The project will look into incorporating conducting polymeric materials, electro-active organometallic compounds together with nano-sized and -structured materials. The aim will be to exploiting intrinsic properties from both materials for the synergistic electron transfer properties to and fro the transducer surface. Several systems will be investigated and tested using electrochemical, spectroscopic and microscopic methods. The best performing systems will find various application in monitoring and detection of (i) environmental analytes such as pollutants such hazardous gases, (ii) biomedical analytes such as neurotransmitters as indication of Parkinson diseases, (iii) industrial analytes such as pathogens in water and metal contaminants from industrial waste, etc. The systems will mimic those currently used for online monitoring of industrial waste and gas sensors industries.

(3) Synthesis and properties of metal-metal oxide nanoparticles of different sizes and shapes as sensing materials

Metal nanomaterials have received research attention and this is because of their tic properties as nanostructured making these systems good for biomolecule separation. When capped with metallic core-shells of platinum group metals, such as platinu,(Pt), gold (Au), silver (Ag), ruthenium (Ru) and rhodium (Rh), the iron oxide nanoparticles exhibit different properties which are provided by the metallc shells. The properties such as anti-microbial, catalytic and biocompatibility are aimed to be introduced by the metallic shells. This project will therefore be an investigation of the preparation of iron oxide nanoparticles of different sizes and shapes and capping these with metallic or biometallic shells of platinum group metals and

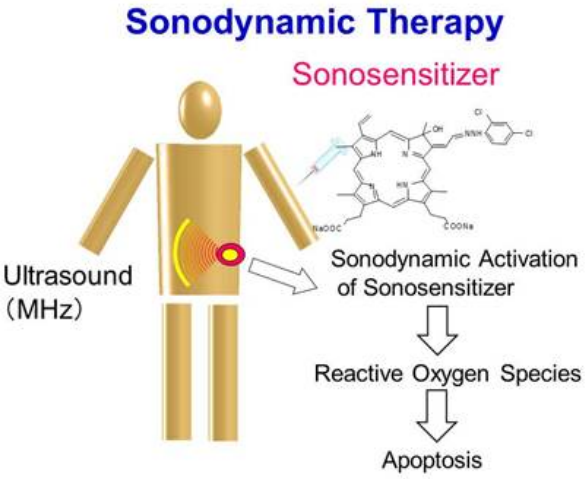
studying the electocatalytic properties of the prepared core-shell nanomaterials. Different shapes and sizes of these systems are envisaged to yield even more interesting properties and these will be investigated.

Return to [RESEARCH PROJECT (SHORT TITLES) 2019]

Professor T Nyokong

(1) **Sonodynamic therapy-- New Directions in cancer treatment** (co-supervised by Dr Jonathan Britton and Dr John Mack)

Over the past two decades, photodynamic therapy (PDT) has emerged as a minimally invasive cancer treatment. However, despite the great achievements of PDT in clinical applications, it has limitations including limited penetrability of visible light into deep tumor tissues, and thus PDT is less effective for large tumours. Sonodynamic therapy (SDT) has been established and developed as a novel promising non-invasive approach on the basis of PDT. With similar principles to PDT, SDT is an ultrasound-based approach that involves utilization of low-intensity ultrasound and a chemical (a sonosensitizer) that can be activated by sonication. Unlike visible light, ultrasound is a type of mechanical wave that can penetrate a cancer target buried deep within human tissue. Therefore, SDT overcomes the major limitation of PDT. The project will involve the study of new sonosensitizers including porphyrins and phthalocyanines (Pcs). The drugs will be used in cancer cells. The mechanism of sonodynamic therapy will be evaluated.



(http://america.pink/sonodynamic-therapy_4097346.html)

References. 1. Drug Discovery Today _ Volume 19, Number 4 _ April 2014. 2. ANTICANCER RESEARCH *31*: 2425-2430 (2011)

(2) **Chemophototherapy-- New Directions in cancer treatment** (co-supervised by Dr Jonathan Britton and Dr John Mack)

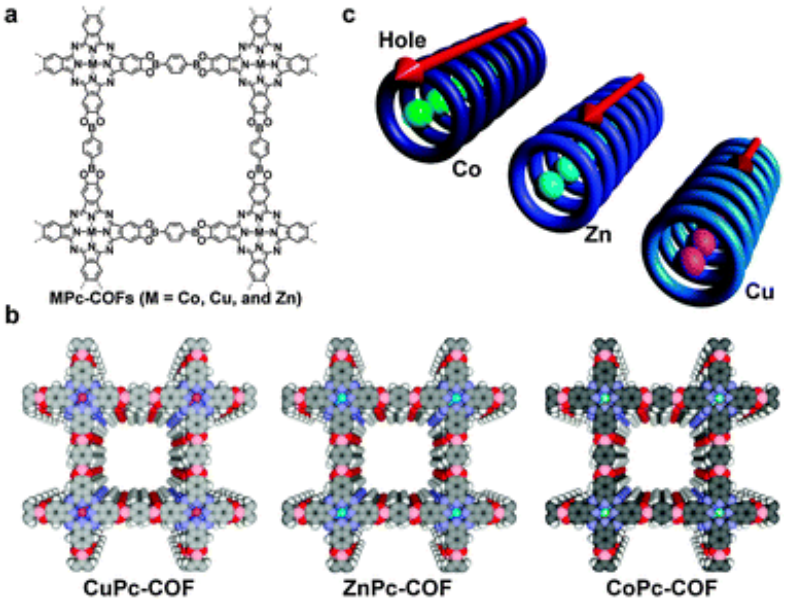
As stated in (A), PDT can cure early tumors and small lesions. For advanced cancers, PDT alone cannot achieve cure and recurrence is often seen. The use of PDT in combination with chemotherapy (chemophototherapy, CPT) is an interesting concept which can provide a more potent treatment than using either treatment alone. The project will combine PDT agents such as porphyrins and phthalocyanines with chemotherapy drugs in the markets such as cis-platinum and others. The combination drugs will be used in cancer cells.

References: 1. Dyes and Pigments 95 (2012) 572-579, 2. *Adv. Sci.* 2016, 1600106

(3) **Covalent organic frameworks (COF) for gas sensing** (co-supervised by Dr Jonathan Britton and Dr John Mack)

Covalent organic frameworks (COFs) are structurally precise, crystalline materials that have attracted significant attention due to their potential applications in efficient gas adsorption and sensing. They can easily

be synthesized under solvothermal conditions. In this project, phthalocyanine COFs (see figure below) will be synthesized and used for sensing of pollutant gases in air.

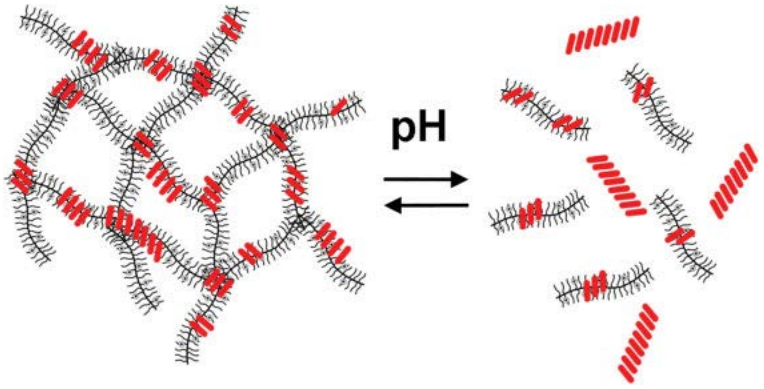


Chem. Commun., 2012, **48**, 8952–8954

References: 1. Acc. Chem. Res. 2015, 48, 900−910. 2. Cryst Eng Comm, 2013, 15, 7157–7160

(4) Formation of porphyrin/phthalocyanine <u>nano-cages, -worms, -rod</u> etc (co-supervised by Dr Jonathan Britton and Dr John Mack)

The spontaneous formation of non-covalently assembled structures holds high promise for nanotechnology, e.g., in building smart drug carriers, sensors or materials with extraordinary property combinations. Aggregates of porphyrin/phthalocyanines can adopt orderly arrays which are essential for technological and commercial purposes. The orderly COFs may exhibit interesting non-linear optical responses, electroluminescence, photoluminescence and conductive properties which are enhanced by the extended π-conjugated macrocyclic rings and extensive overlap of the π-molecular orbitals. The project will involve the synthesis of ordered porphyrin/phthalocyanine arrays for nonlinear optical and other applications



Cage **worm**

References: 1. Macromol. Rapid Commun. 2011, 32, 706–711, 2. *J. Porphyrins Phthalocyanines* 2015; **19**: 1147–1158

(5) Development of nanoparticles for restoration of <u>cultural heritage</u> (In collaboration with Prof Rodica Ion, Romania, co-supervised by Dr Jonathan Britton and Dr John Mack)

The conservation of the Cultural Heritage is fundamental for future generations. Research on the conservation of cultural heritage is growing rapidly. The use of nanotechnology in conservation has also grown considerably. Treating wood (paper) with nanotechnology based products is expected to result in

wood (paper) that it is resistance to fire, UV light, moisture and pests. In addition, Ag and Pt nanoparticles in particular have antimicrobial activities. The method is based on penetration of the nanoparticles on the paper and wood fibers, adhering to them

The aim of the project is to preserve wood and paper using nanoparticles. This will involve the placement of nanoparticles within the wood/paper microstructure. The penetration and retention of nanoparticles within the wood/paper as well as the amounts of nanoparticles per unit size of paper or wood will be examined. The size and shape of the nanoparticles will have an effect on the preservation of wood and paper. Thus we plan to synthesize different types and sizes of metal nanoparticles. The work will concentrate on Au, Ag, Pd and Pt nanoparticles. Cultural ceramics, books, etc can be restored using the nanoparticles (see example below).

Before After restoration

Nature Nanotechnology **10**, 287–290 (2015)

References:

1. A. Blee and J.G. Matisons, Nanoparticles and the conservation of cultural heritage Mater. Forum 32 (2008) 121-128.
2. R. M. Ion, S. M. Doncea, M.L. Ion, V. RÇŽdit, V. AmÇŽriut, Surface investigations of old book paper treated with hydroxyapatite nanoparticles, Appl. Surf. Scie.285P (2013) 27-32.

Return to RESEARCH PROJECT (SHORT TITLES) 2019

Mrs J Sewry

(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.

(2) Evaluation of students' use of Labskills.

"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.wikipedia.org/wiki/Service_learning]

The project entails doing research into chemical education. The student will evaluate the use of Labskills during practicals.

Return to RESEARCH PROJECT (SHORT TITLES) 2019

Dr V Smith

(1) 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 (cosupervised by Dr D. S. Khanye).

The bioavailability of putative 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.

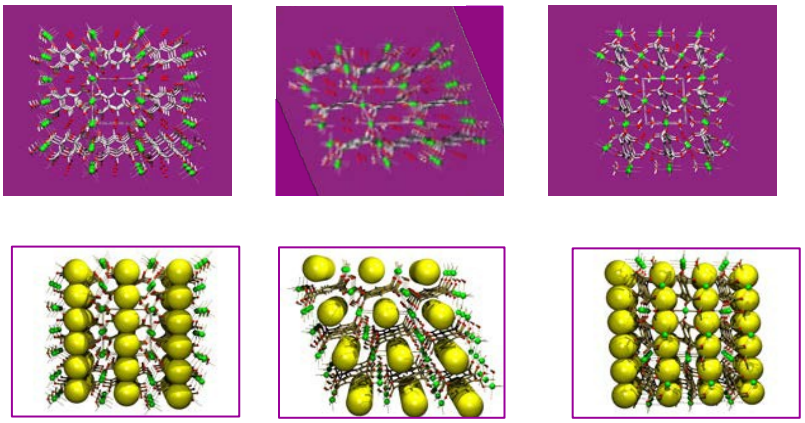
A. D. Bond *CrystEngComm*, **2007**, 9, 833-834.

G. P. Stahly, *Cryst. Growth Des.*, **2007**, 7, 1007-1026.

Return to RESEARCH PROJECT (SHORT TITLES) 2019

Prof GM Watkins

(1) Nanomaterials: supramolecular structures from metal coordination with benzenecarboxylates:
Tectons are molecules that, due to covalent and van der Waal's forces induce the assembly of 2D or 3D supramolecular networks. These materials offer unique properties that have industrial applications such as allowing for selective adsorption, acting as molecular sieves, as potential hydrogen storage materials, allowing for selective partial oxidation (*eg.* of *p*-xylene), *etc*. Hydrothermal, gel and ambient reactions of M(II) salts (M= Co, Ni, Cu, Zn) with 1, 2, 4, 5-benzenetetracarboxylic acid produces materials that potentially have such properties.



Nickel (green) Oxygen (red) Carbon (black)

Figure 1: Crystal structure of {[Ni2(B4C)(H2O)4].2H2O}n And the *in silico* virtual pore on solvent loss.

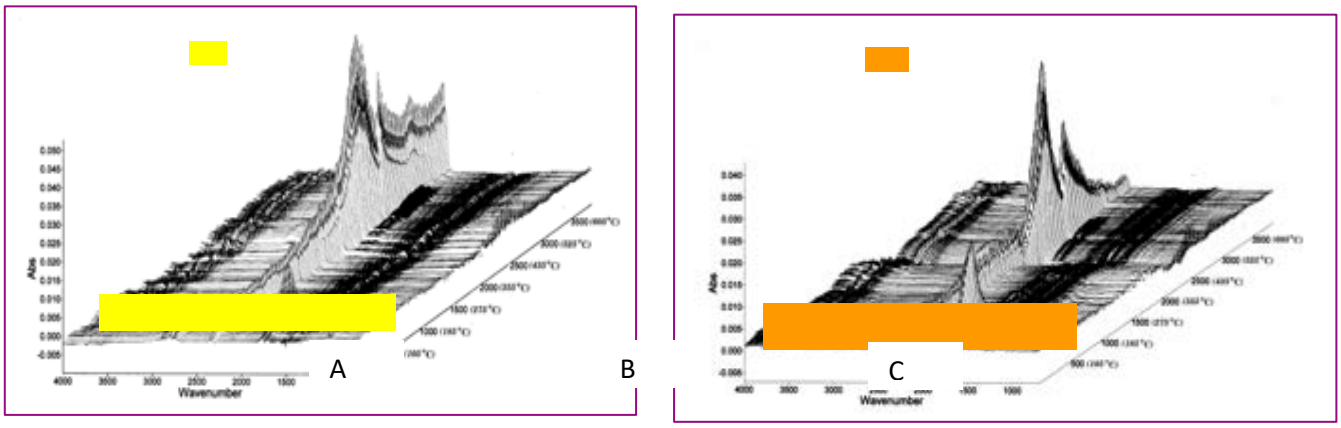


Figure 2: Evolved gas analysis of one of our MOFs after resolvation with formaldehyde and acetaldehyde.

Several projects in this area are available; for example:

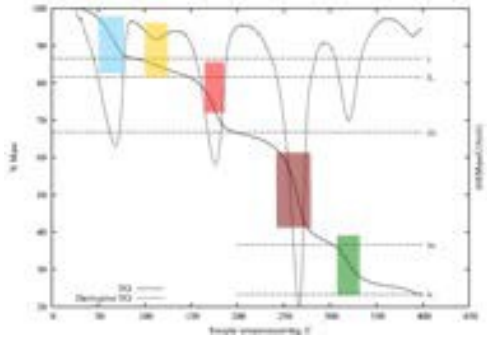
Mn(II) and Mn(III) materials with 1, 2, 4, 5-benzenetetracarboxylic acid are to be studied.

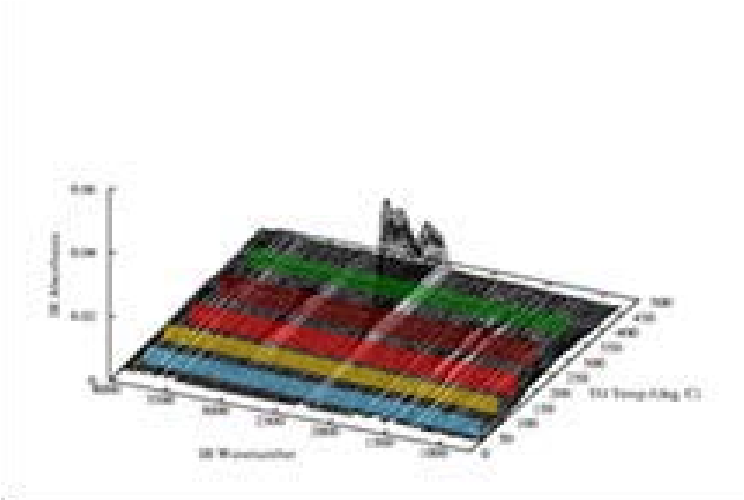
Projects involving metal binding, and mixed MOF with 4,4' bipyridine and their N-oxides are also of interest as these molecules are also expected to show strong fluorescence, and potential as sensors. Other benzenepolycarboxylic acid metal complexes are also to be investigated for their MOF characteristics.

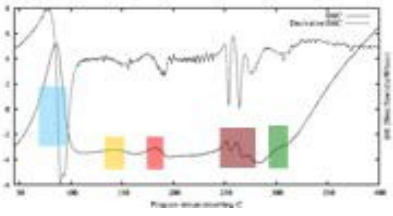
This project may make use of infrared and Raman spectroscopy, solid-state UV/VIS spectroscopy, TG-FTIR spectroscopy, thermal analysis, XRD, BET and XPS, amongst others.

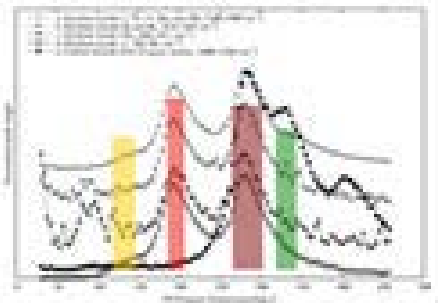
(2) Nanomaterials: supramolecular structure from metal coordination with 1, 2, 4, 5-benzenetetracarboxylic acid and pyridine:.

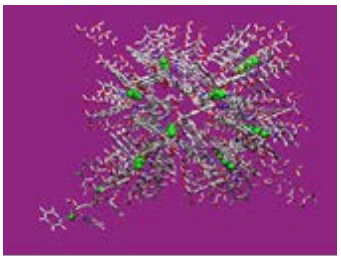
This is is a material with a bridge benzenetetracarboxylate frame work, 2 pyridines and and axial H2O bound to the copper. There is restricted channeling, containing 5 guest H2O (z axis: cavity = 185 Å3/unit cell).











View down z axis

The material undergoes loss of 6H2O 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, 1½CO2 and 1H2O 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 possible. The nature of the stable material formed between 150 and 197 ºC ([Cu2 (H2C10O8)(C5H5N)2]) 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.

(3) Nanomaterials: A MOF utilising a tetracarboxyphthalocyanine. (Dr Britton supervisor please see his project)

Return to RESEARCH PROJECT (SHORT TITLES) 2019

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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8. 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. 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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8.1 REVIEW ESSAY TOPICS 2019

Dr J Britton

(1) Describe the different operation modes and applications of an Atomic Force Microscope (AFM)

Dr DS Khanye

(2) Treatment of Schistosomiasis

(3) Structure-based Drug Design in Anti-Infective Agents

(4) Medicinal Applications of Oxaboroles

Dr S Khene

(5) Modeling of nonlinear optical properties of phthalocyanines

(6) Light conversion process in photosynthesis

(7) A brief account: Evolution of photosynthesis

Dr R Klein

(8) Teaching stereochemistry – methods and challenges

(9) Advantages and disadvantages of multicomponent reactions

Prof RW Krause

(10) Stimuli-responsive materials in drug delivery

(11) The role of natural products in modern drug discovery

(12) Biological interactions of nanoparticles

Dr KA Lobb

(13) Atomic structure and bonding – core concepts in the teaching of chemistry.

(14) Nuclear chemistry and nuclear energy in the South African context.

(15) Applications of Car-Parrinello molecular dynamics.

Dr J Mack

(16) The synthesis, properties and applications of boron aza-dipyrromethene (aza-BODIPY) dyes

(17) The biomedical applications of gold nanoparticles

(18) Magnetic circular dichroism (MCD) spectroscopy

(19) The research and development of quantum dot solar cells

Dr P Mashazi

(20) Design and development of microfluidic biosensors for multiplexed detection

Mrs J Sewry

(21) Stoichiometry: misconceptions and difficulties

(22) Using Principal Component Analysis in analytical Chemistry

(23) Ethics in practising Science

Dr VJ Smith

(24) Metal-organic Frameworks (MOFs) as Materials for the Rehabilitation of the Environment

Prof GM Watkins

(25) Examples of equilibria reactions in every-day scenarios

(26) Modulated Differential Scanning Calorimetry

(27) The challenge of conducting chemical experiments on Mars

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

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9. 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]

9.1 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

9.2 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!

9.3 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.

9.4 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

9.5 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

9.6 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

10. APPENDIX II COMMUNICATING CHEMISTRY

10.1 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!

11. INITIAL CHOICE FORM

The form can be found on the NEXT page (page 38)
and
MUST be filled in BEFORE arrival at Rhodes

Please tear out, fill in the reverse side (page 38) and return this page (page 37 and 38) as soon as possible.

BUT NO LATER THAN 30th JANUARY 2018

You may also email it to Chemistry Dept: b.tarr@ru.ac.za

The FINAL CHOICE FORM

Will be completed during the *FIRST WEEK* of the Honours Course on RUConnected.

Details will be given during the first week of class.

Start Date: Tuesday 13th February 2018

Please complete and return this page as soon as possible, ***BUT NO LATER THAN 30th JANUARY 2018***

To: Dr R Klein, Room F39, Chemistry Department, RHODES UNIVERSITY, GRAHAMSTOWN 6140 (fax 046 622 5109).
E-mail: b.tarr@ru.ac.za (Office Administrator)

NAMES IN FULL (please print): _____

STUDENT NO.: _____

EMAIL ADDRESS: _____

TELEPHONE NO.: _____

CELL NO.:_____

SIGNED: _____ DATE:_____

CHOICE INDICATION

As a preliminary, though not binding, indication of your **probable** choice of Topics, please circle the ***FIFTEEN*** lecture topics (***FIVE FROM EACH GROUP***) likely to be chosen by you (Remember the 2 compulsory topics in Paper 2 and 3), fill in details of your essay (first and second choices) and project (first and second choices).

LECTURE TOPICS:

PAPER 1:	PK1	SK1	Ruik1	VS1	PNM1	SA1*	GW2	RK3	KAL2
PAPER 2:	PTK1	RK2*	RuiK2	KAL3*	JM1	PNM2	JS1	GW3	
PAPER 3:	PTK2	DSK1	SK2*	RK1	KAL1	JM2	JS2*	GW1	

PROJECT: (SHORT TITLE) _____ **INITIALS** _____

1st Choice: **Supervisor:**

2nd Choice: **Supervisor:**

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

1st Choice: **Supervisor:**

2nd Choice: **Supervisor:**