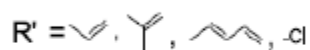
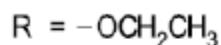
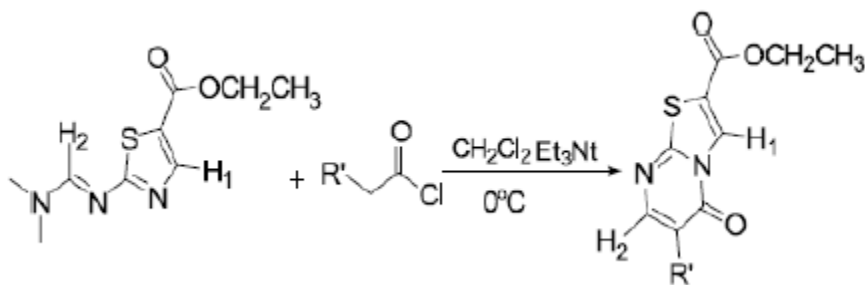


1A – Dr P Singh

Synthesis of thiazole-pyrimidines using hetero Diels-Alder methodology

ABSTRACT

Pyrimidines has gained considerable attention because of their role in biological systems, particularly in nucleic acids, which contain pyrimidines and purines as the main nucleobases. It has been noticed that introduction of an additional ring to the pyrimidines core tends to exert profound influence in conferring novel biological activities in these molecules. Consequently, in recent years, various thiazole incorporated pyrimidines have emerged as broad spectrum drugs in the field of chemotherapy and selective antitumour, antiviral, antitubercular and antifungal activities. Keeping in view the biological significance of these organic scaffolds, we propose to synthesize new functionalized thiazolo-pyrimidine derivatives using hetero Diels-Alder reaction as a synthetic methodology. Specifically, the [4+2] cycloaddition reaction of thiazolic azadiene will be performed with both mono-substituted and conjugated ketenes (Scheme below).

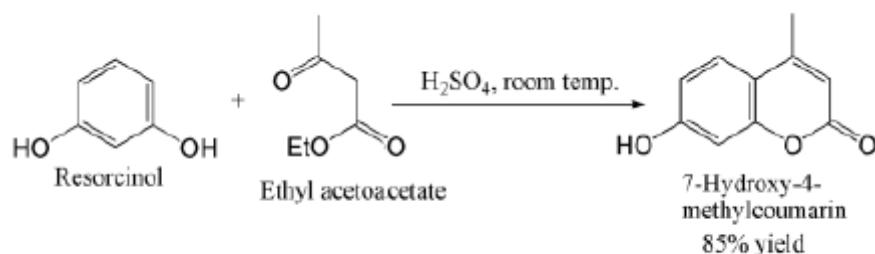


1B – Dr P Singh

Synthesis of different coumarin analogues of biological relevance

ABSTRACT

Coumarins with different activities are known to occur naturally for example Calanolide A and B which is isolated from the twigs and leaves of a Malaysian rainforest tree called *Calophyllum lanigerum* var. *austrororiaceum* and was found to possess anti-HIV activity. Other coumarins have been synthesized using different synthetic methods, which includes the Perkin reaction, Claisen rearrangement, Pechmann reaction, Wittig reaction and the Knoevenagel condensation. An example of a coumarin that has been synthesized using one of these methods, namely the Pechmann reaction is 7-hydroxycoumarin. 7-hydroxycoumarin inhibits the release of cyclin D1 which is present in large amounts in many types of cancers. Moreover, several other coumarin derivatives have been reported to exhibit a variety of biological activities including anti-tumor, anti-inflammatory, anti-diabetes, anti-ulcer, anti-bacterial etc. In view of the great biological significance of coumarins, we propose to synthesize substituted coumarins. The Pechmann reaction will be first used to synthesize the 4-phenylcoumarins because it is one of the most common procedures used in the preparation of coumarin and its derivatives. The Pechmann reaction involves the condensation of phenols with β -ketoesters in the presence of condensing agents (see scheme below).



2A – Dr R Moodley and Dr Karin Pruessner

Plant-mediated synthesis of nanoparticles using the crude MeOH extract and biologically active compounds from *Carpobrotus dimidiatus* (Natal sour fig)

ABSTRACT

There is growing interest in nanotechnology in a variety of disciplines ranging from material science to biomedical research. This is due to their unique properties that make them suitable for specific applications as a result of their nano-scale size and shape-dependent properties. There is a growing need for clean, non-toxic methods for synthesizing nanomaterials especially those targeted for biological applications. One such method is the use of extracellular plant-mediated synthesis which is a cost effective and eco-friendly technique. Moreover, it offers additional organic molecule end-capping of the nanoparticles. The use of plant extracts and pure phytochemicals is a relatively unexplored and underexploited nanoparticle synthesis methodology. There is much scope for improvement in bio-based methods of metal nanoparticle synthesis. Therefore, the use of plant material in the deliberate and controlled synthesis of nanoparticles is an area of research with considerable potential for development. In this project, the plant-mediated synthesis of nanoparticles using extracts and active compounds isolated from *Carpobrotus dimidiatus*, will be investigated. The synthesised nanoparticles will be characterised using a variety of characterisation techniques and their biological activity will also be determined.

Conceptual Framework

- Extraction, isolation and structure elucidation of active compounds from *C. dimidiatus* using spectroscopic techniques (NMR, GC-MS and IR).
- Synthesis of nanoparticles using extracts and pure phytochemicals.
- Characterisation of nanoparticles using SEM, TEM, XRD, FTIR, UV-Vis.
- Antioxidant activity (FRAP, DPPH and hydrogen peroxide) of pure phytochemicals and nanoparticles (freestanding and end-capped).

2B – Dr R Moodley and Prof SB Jonnalagadda

Soil Nutrient Content on Elemental Uptake and Distribution in Natal sour figs

(Carpobrotus dimidiatus)

ABSTRACT

Carpobrotus dimidiatus (Natal sour fig), of the plant family Mesembryanthemaceae, is a trailing succulent with edible fruits found on sand dunes along the coast from the Eastern Cape northwards through KwaZulu-Natal to Mozambique. In South Africa, the fruit are eaten raw, preserved, dried or prepared as a jam; the plant is also used medicinally to treat a variety of ailments. Plants are an important link in the transfer of metal contaminants from soil to humans. Exposure to high levels of these metal contaminants could lead to detrimental effects to human health. Studies on the elemental composition of medicinal plants are important to monitor heavy metal contamination and to identify potential routes of exposure. Awareness with regards to the safety of consuming wild plants needs to be generated since more and more industries are violating legislation and polluting the water body and soil on which these plants grow. This study on the elemental composition of medicinal plants as a function of soil quality will be done in an effort to create such awareness. The levels of the elements in the fruits will also be determined to evaluate their contribution to the diet.

Conceptual Framework

- To determine the elemental content of figs and leaves collected from ten different sites along the east coast of KwaZulu-Natal and to assess the fruits for nutritional value by comparing to recommended dietary allowances (RDAs).
- To evaluate the impact of soil quality on the chemical composition of leaves and fruits and to assess for heavy metal contamination by comparing to threshold values.
- To determine the proximate chemical composition of the fruits.

3 - Dr Karin Pruessner

Synthesis and Chemical Delithiation of Na(Co,Ni,Mn)O₂ Cathode Materials for Sodium-Ion Batteries

ABSTRACT

Rechargeable batteries basically consist of a cathode, an anode and an electrolyte. During the charge/discharge cycle, a charge carrying ion is shuttled between the cathode and the anode where it is accommodated in the crystal structures. Rechargeable batteries on Li-ion basis are currently the energy storage device of choice for portable electronic devices and power tools. As the demand for rechargeable batteries for large-scale applications such as electric vehicles and grid-scale energy-storage increases, the relative scarcity of lithium resources and therefore the price becomes a problem though. As a more cost-effective and environmentally friendly alternative, sodium-ion batteries have been suggested. In a sodium-ion battery, the Li-ion is replaced by the Na-ion as the charge carrier. Cathode, anode and electrolyte materials must be adapted to allow for diffusion of the larger Na ion and accommodation in the lattice. Layered NaCoO₂ is a candidate cathode material for these batteries. Solid-solutions of Ni and Mn in these structures are expected to improve electrochemical performance. We will synthesize cathode materials in the system Na(Co,Ni,Mn)O₂ in different compositions and chemically delithiate them using K₂S₂O₈ and/or sulfuric acid to simulate the electrochemical delithiation in the battery. Compositions of Na_{1-x}(Co,Ni,Mn)O₂ with x<1 will be established. X-Ray Diffraction (XRD), Raman Spectroscopy and Scanning (SEM) and Transmission Electron Microscopy (TEM) will be used to characterize the reaction products. Experimental results will be compared to simulations based on known structures in the system Na-Co-O from the literature.

4A – Dr M. Shozi and Mr P. Mpungose

Solution combustion synthesis of magnetically recoverable catalysts and their application in styrene oxidation

ABSTRACT

Styrene has been labelled as a carcinogen and a neurotoxicant, and therefore the conversion of styrene to a less toxic and valuable product has been the main focus for many academics and industries [1]. Conversion of styrene to benzaldehyde has received much interest. Benzaldehyde, a very valuable fine chemical which acts as an intermediate with a number of applications such as in resin additives, medicine, production of perfumes and dyes, is the major product in the styrene oxidation [2].

This project involves the solution combustion synthesis of various magnetically recoverable M-Fe₂O₄ (M = Cr, Mn, Co, Ni and Cu) catalysts. To gain insight into the physicochemical properties of these M-Fe₂O₄ catalysts, we need to investigate the electronic structure, local environment, and possible substitution of the metal ions in Fe₂O₄ by X-ray diffraction, TEM, SEM/EDX, Raman spectroscopy and BET surface area. The synthesized M-Fe₂O₄ catalysts will then be tested on styrene oxidation to benzaldehyde and/or styrene oxide.

References

1. I. Linhart, J. Mráz, L. Dabrowská, M. Mališ, J. Krouželka and M. Kořínek, *Toxicology Letters*, 2012, 213, 260-265.
2. L.-X. Zhang, Z.-L. Hua, X.-P. Dong, L. Li, H.-R. Chen and J.-L. Shi, *Journal of Molecular Catalysis A: Chemical*, 2007, 268, 155-162.

4B – Dr M. Shozi

Synthesis of biodiesel from vegetable oil using sulfated-zirconia catalysts

ABSTRACT

Biodiesel, a methyl ester, is an alternative to diesel that is made from a triglyceride (like vegetable oil) and either ethanol or methanol. The oil used in the process can come from many sources including soybeans, corn, canola, and used frying oil. Because it comes from renewable resource, it is referred to as a biofuel. The process involves taking the oil, a triglyceride, combining it with an alcohol, to form biodiesel, which is either an ethyl ester or a methyl ester. The process uses a base, either potassium hydroxide or sodium hydroxide, as a catalyst to help in the process and forms glycerol as a byproduct [1]. Catalysts will be synthesized and characterized via XRD, SEM-EDX, TEM, BET, ICP and IR. The catalysts will be used in the synthesis of biodiesel and compared to standard catalysts for this process such as NaOH and H₂SO₄.

References

1. K. Wilson and A.F. Lee, *Catalysis Science and Technology*, 2012, 2, 884-897.

5A – Dr PB Khoza

Synthesis of silica coated ZnSe and ZnS nanoparticles and their use in heavy metals detection

ABSTRACT

Quantum dots are semiconducting nanoparticles with a diameter range of 1-20 nm; due to their reduced size, they exhibit interesting photophysical and photochemical properties when compared to the corresponding bulk material [1]. Quantum dots with interesting properties comprise mainly of Cd which is a highly toxic heavy metal [2]. In this study, water soluble ZnSe/SiO₂ and ZnS/SiO₂ nanoparticles are synthesized and their photophysical behavior is studied. Nanoparticles synthesized will be characterized by TEM, XRD, IR, UV-Vis and PL. The nanoparticles will then be used in sensing heavy metals in water.

REFERENCES:

1. A. Mostafa, E.L Sayde Acc Chem Res. 237 2004 326-333.
2. N. Chen, Y. He, Y. Su, X. Li, Q. Huang, H. Wang, X. Zhang, R. Tai, C. Fan, Biomaterial 33 2012 1238-1244.

5B – Dr PB Khoza and Dr B O Owaga

Photocatalysis of CdS nanoparticles supported on chitosan microbeads

ABSTRACT

Single source molecular precursor method is well known for producing nanoparticles with remarkable photophysical and photochemical properties [1]. The method entails decomposing a precursor at very high temperatures so as to produce monodispersed nanoparticles. In this study, a novel precursor will be synthesized and the effect of various synthesis conditions, such as temperature, time and concentration, will be studied. Successful synthesis of the precursor will be confirmed with IR, ¹H NMR and XRD, and the formation of CdS nanoparticles will be confirmed by TEM, IR, XRD, UV-Vis and PL. The prepared nanoparticles will then be used as photocatalysts in the removal of organic dyes. For ease of recovery and recyclability, nanoparticles will be supported on chitosan microbeads. Chitosan microbeads will be characterized by IR, SEM-EDX and BET.

REFERENCES:

1. M.A Malik, N. Revaprasadu, P. O'Brien, Chem Mater. 13 2001 913-920.

6A – Prof B S Martincigh
Phototoxicity of cosmetic products

ABSTRACT

The use of cosmetics has been practised since the ancient Egyptian and Greek civilisations. They include a wide variety of products such as creams, lotions, lipsticks, powders, perfumes, oils, etc. Since these products are used on the skin, which is exposed to solar radiation, the possibility exists of phototoxic reactions and reaction with skin biomolecules.

This project will involve testing various cosmetic products for their ability to generate reactive oxygen species (ROS) on exposure to sunlight. ROS include singlet oxygen, superoxide anion, hydroxyl radicals, etc.

The laboratory work will involve irradiation of samples and the use of various analytical techniques to test for the presence of these ROS.

6B – Prof BS Martincigh

Metal complexes from hydroxydiphenylphosphine oxide

ABSTRACT

The alarming worldwide increase in the incidence of skin cancer has increased the use of photoprotective measures. One of these is the use of sunscreen products. The active ingredients in sunscreens include physical and chemical absorbers.

Chemical absorbers are typically conjugated organic molecules that absorb over the ultraviolet region of the electromagnetic spectrum. Some of these molecules photodegrade upon exposure to UV radiation and therefore do not afford the necessary protection. Some also generate toxic species such as reactive oxygen species.

This project will involve testing a selection of sunscreen absorbers for their ability to generate reactive oxygen species (ROS) on exposure to sunlight. ROS include singlet oxygen, superoxide anion, hydroxyl radicals, etc.

The laboratory work will involve irradiation of samples and the use of various analytical techniques to test for the presence of these ROS.

7 – Dr N Nombona

Enhancing electrochemical detection using phthalocyanine-graphene hybrids

ABSTRACT

Metallophthalocyanines (MPc) are remarkably versatile compounds with outstanding physicochemical and electronic properties. MPcs are commonly used as electrocatalysts and mediators for various electrochemical applications. However, physically adsorbed MPcs on electrode surfaces are not stable and as a result MPcs require suitable support to prepare stable electrodes and deliver excellent electrochemical applications. The introduction of MPc electrocatalytic centres to graphene based electrodes offers unique electrocatalytic properties as the graphene material acts as a support for the linking of the inorganic catalyst and facilitates electron transfer between the electroactive species and the electrode surface. This project aims to exploit the electrocatalytic properties of both materials for improved electron transfer on the electrode surface. Several conjugation strategies will be investigated and tested using electrochemical and spectroscopic methods. The best performing hybrid system will be used to examine improvement on the electrochemical detection of selected environmental pollutants.

8A – Prof VO Nyamori

Synthesis and characterization of ionic liquids and their application as an in-solvent

ABSTRACT

The name graphene (G) is derived from the graphite and alkene. G is a form of graphite with less than ten layers of six membered carbon species in a honeycombed network. Traditionally, G is regarded as the mother of conjugated carbon nanomaterials and is the thinnest known material. It resembles polycyclic aromatic hydrocarbons and benzene. G is made up of sp² carbon atoms and its π -electrons are delocalised throughout the 2D network. Types of G include monolayer, plane sheet, mesh and ribbons and there are two generations of G, i.e. first (2D) and second (3D). The various types and generations of G have different physicochemical properties. Applications of G range from flexible electronics to functional nano-devices (fig. 1), and G is so far the best carbon nanostructured material-based electrode for electrochemical capacitors. Understanding their physicochemical properties is often a key step in tailoring graphene-based composites towards various applications. For instance, carbon materials can be tailored to be pseudocapacitive by the introduction of heteroatom. Introduction of electro-active metallic particles in nanostructured carbon materials can positively modify physicochemical properties such as the pore size distribution, charge storage capabilities and electronic conductivity, amongst others.

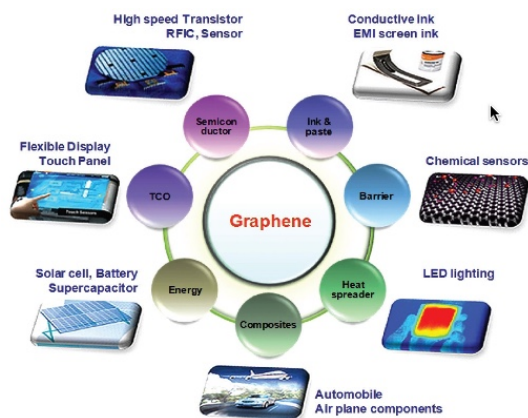


Fig 1: Applications of graphene

8B – Prof VO Nyamori and Dr BO Owaga

Synthesis of silver(I)-, copper(I)- and copper(II)-pyridinyl Schiff base complexes

ABSTRACT

There is an ever growing interest in synthesis and characterization of novel transition metal complexes. While precise reasons for these interests vary, the ultimate utility of the compounds is a major driving force. Due to the emerging challenges in management of diseases, there is a great need to develop new compounds with high pharmacological activity such as antitumor, antibacterial and antifungal properties. Silver(I) and copper(II) complexes have great potential in addressing some of the challenges hindering disease management [1, 2]. Silver(I), copper(I) and copper(II) complexes are potential candidates for use as a medicinal agents due to their low toxicity in the body.

Aim

This research project involves the synthesis of pyridinyl Schiff bases. These will in turn be applied in synthesis of silver(I), copper(I) and copper(II) complexes. The complexes thus obtained will be investigated for antimicrobial and antitumor potency.

Specifically, the project entails:

1. Syntheses and characterisation of pyridinyl Schiff base ligands via mechanochemistry technique.
2. Syntheses and characterisation of coordination complexes of silver(I), copper(I) and copper(II) using the ligands prepared in (1) above.
3. Investigate the chemical, physical, structural and in vitro biological (antimicrobial and antitumor) properties of the complexes.

REFERENCES

- [1] M.A. Abu-Youssef, R. Dey, Y. Gohar, A.a.A. Massoud, L. Öhrström, V. Langer, *Inorganic chemistry*, 46 (2007) 5893-5903.
- [2] F. Tisato, C. Marzano, M. Porchia, M. Pellei, C. Santini, *Medicinal research reviews*, 30 (2010) 708-749.

9A – Dr S Singh, Dr AS Mahomed and Prof HB Friedrich

Total oxidation of CO to CO₂ using metal oxides as catalysts

ABSTRACT

It is an absolutely necessary to convert emission gases such as carbon oxides and nitrogen oxides which are detrimental to the environment to less harmful gases. This study will focus on the total oxidation of CO using metal oxides as catalysts. Metal oxides have been reported to have high catalytic activity for the CO oxidation reaction [1,2]. A series of catalysts will be prepared for testing and these catalysts will be characterized by XRD, BET surface area, temperature studies and microscopy [3,4].

References

- [1] Y. Hasegawa, K. Fukumoto, T. Ishima, H. Yamamoto, M. Sano, T. Miyake, *Appl. Catal. B: Environ.*, 89 (3–4) (2009) 420.
- [2] H. Rongrong, L. Xie, S. Ding, J. Hou, Y. Cheng, D. Wang, *Catal. Today* 131 (2008) 513.
- [3] S. Sugiyama, T. Osaka, Y. Hirata, K. Sotowa, *Appl. Catal. A* 312 (2006) 52.
- [4] Venkata D.B.C. Dasireddy, Sooboo Singh, Holger B. Friedrich *Appl. Catal. A: General*, 421–422, 2012, 58.

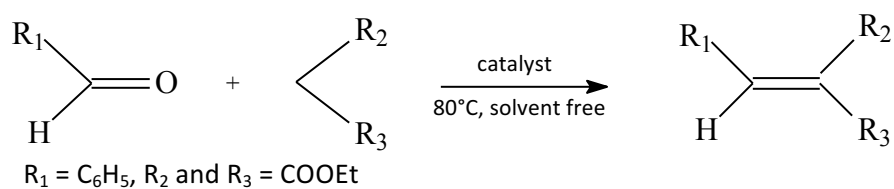
9B – Dr S Singh, Dr AS Mahomed and Prof HB Friedrich

Solvent-free Knoevenagel condensation over substituted hydroxyapatite catalysts

ABSTRACT

Knoevenagel condensation is an important reaction for the formation of olefins which are widely used in the pharmaceutical, perfume and polymer industries [1]. This reaction is usually carried out under homogenous conditions with an organic solvent and catalysed with bases such as ammonia, primary and secondary amines and materials containing acid-base sites [2-4]. The need to avoid the use of solvents in these reactions, have resulted in solvent free heterogenous catalysts receiving attention.

This project involves the synthesis and characterization of substituted hydroxyapatite catalysts which will be used in the condensation of aldehydes and esters to olefins in a solvent-free environment (Scheme 1).



Scheme 1 Knoevenagel solvent free condensation reaction

References

- [1] S. Saravanamurugan, M. Palanichamy, M. Hartman, V. Murugesan, *Appl. Catal. A* 298 (2006) 8.
- [2] S. Wang, Z. Ren, W. Cao, H. Tong, *Synth. Commun.* 31 (2001) 673.
- [3] T.S. Jin, X. Wang, L.B. Liu, T.S. Li, *J. Chem. Res.* 6 (2006) 346.
- [4] P. Sshanhan Rao, R.V. Venkatratnam, *Tetrahedron Lett.* 32 (1991) 5821.

10A – Prof HB Friedrich, Dr S Singh and SA Mahomed

Selective hydrogenation of aldehydes over mixed metal catalysts supported on alumina

ABSTRACT

Catalytic hydrogenation is an industrially important reaction for the conversion of low cost materials to valuable products using a supported metal catalyst [1]. Bimetallic and trimetallic heterogeneous catalysts are often more effective than monometallic catalysts, as they offer low temperature activity, higher selectivity and resistance to poisoning [2-5]. Catalysts used for hydrogenation reactions usually consist of supported metal particles. The metal is able to adsorb hydrogen and enables the hydrogenation reaction to occur. Based on previous studies, copper has shown to be effective in the preferential hydrogenation of aldehydes in the presence of alkenes. Mixed metal oxide catalysts are significantly different from the monometallic counterparts due to the combined effect of more metals producing a synergistic effect.

In this study, mixed metal oxide catalysts will be prepared by wet-impregnation method and co-precipitation method by using cobalt, nickel and silver metals on alumina support with the different metal loadings. These catalysts will be characterized using powder and in situ XRD, TPR, SEM-EDX, TEM, BET, ICP and IR to identify their physical and chemical properties for hydrogenation applications. A high pressure continuous flow-fixed bed reactor will be used to evaluate the catalytic performance under hydrogenation. Catalytic activity under hydrogenation for the octene-octanal mixture will be investigated with different intermetallic loadings, reaction temperatures, and pressure as well as at various LHSV. In selective hydrogenation of alkene-aldehyde system, the desired product is the alcohol from aldehyde.

References

- [1] S. Nishimura; *Platinum Metals Rev.* 46 (2002) 2, 73.
- [2] G.A. Somorjai, C.J. Klier, *React. Kinet. Catal. Lett.* 96 (2009) 191.
- [3] G. Lafaye, T. Ekou, C. Micheaud-Especel, C. Montassier, P. Marecot, *Applied Catalysis A: General* 257 (2004) 107.
- [4] Blaise Bridier, Javier Perez-Ramirez, Axel Knop-Gericke, Robert Schlögl, Detre Teschner, *Chemical Science* 2 (2011) 1379.
- [5] Alberto J. Marchi, Diego A. Gordo, Andrés F. Trasarti, Carlos R. Apesteguía, *Applied Catalysis A*: 249 (2003) 53.

10B – Prof HB Friedrich, Dr S Singh and SA Mahomed

Preferential oxidation of carbon monoxide in a fuel cell feed-stream

ABSTRACT

Preferential oxidation of CO at low temperatures in a reformat gas stream is important the fuel cell industry as it seeks to improve the quality of hydrogen used for this application. Hydrogen used in fuel cell which is produced by steam reforming contains about 1% CO [1]. CO adsorbs on the surface of the platinum electro-catalysts located inside the fuel cell, commonly the proton exchange membrane fuel cells (PEMFC), thereby causing it to rapidly lose its performance [2].

This investigation will involve the oxidization of CO present in hydrogen rich streams using metal oxide catalysts. The catalysts will be prepared by the wet-impregnation and co-precipitation method and will be characterized by various physical and chemical methods such as PXRD, TPR, SEM-EDX, TEM, BET, ICP and IR. Catalytic testing will be performed on a custom built test unit containing a fixed continuous flow reactor interfaced with a three channel Varian 490 Micro GC containing a molecular sieve 5A PLOT (10 m) and CP-Sil 5 CB (10 m) columns. Data evaluated using Galaxie Software.

References

- [1] T. Shodiya, O. Schmidt, W. Peng, N. Hotz, J. Catal. 300 (2013) 63-69.
- [2] P. Landon, J. Ferguson, B. E. Solsano, T. Garcia, A. F. Carley, A. A. Herzing, C.J. Kiely, S. E. Golunski, G. J. Hutchings, Chem. Comm., 2005, 3385-3387.

11A – Dr SA Mahomed, Dr S Singh and Prof HB Friedrich

Glycerol to propylene - tandem environmental catalysis

ABSTRACT

The use of glycerol as a green substrate can be highlighted in its transformation to propylene via propanol. The propylene itself is primarily used in the manufacture of plastics. The aim of this project would be to produce propanol via hydrogenolysis of glycerol and subsequently dehydrate the alcohol to the corresponding olefin.

11B – Dr SA Mahomed, Dr S Singh and Prof HB Friedrich

Understanding how vanadium interacts with MgO - a materials study

ABSTRACT

Incorporation of vanadium into MgO produces a material that contains several phases of metallic oxides. The speciation is dependent on the level of vanadium incorporated. The study will involve synthesizing several mixed oxide systems containing V and Mg and thereafter probing the structure using IR, XRD and solid-state NMR.

12A – Prof SB Jonnalagadda

Photocatalysed degradation of polychlorinated dibenzofurans and pollutants using modified titanium dioxide

ABSTRACT

PCDFs are known teratogens, mutagens, and suspected human carcinogens. PCDFs tend to co-occur with polychlorinated dibenzodioxins (PCDDs). PCDFs can be formed by pyrolysis or incineration at temperatures below 1200 °C of chlorine containing products, such as PVC, PCBs, and other organochlorides, or of non-chlorine containing products in the presence of chlorine donors. This project involves the studies on dechlorination of PCDFs by catalyzed oxidation using ozone in aqueous solutions using heterogeneous catalyst materials.

Emphasis will be on

- (i) Optimising the chemical parameters that effect degradation in presence of light irradiation and ozone aeration.
- (ii) Investigation of efficiencies of modified oxides loaded on TiO₂ supports as catalysts
- (iii) Comparison of the yields and conversions as function of light irradiation or ozonation time.

Upon successful completion of the project, a research publication is envisaged.

12B – Prof SB Jonnalagadda

Microwave assisted synthesis of novel pyridine derivatives

ABSTRACT

In the recent years, microwave (MW) irradiation has received significant attention as one of the promising green chemistry approaches in synthesis. The ability of MW-assisted organic synthesis is of significant benefit and the technique provides scope to vary the reaction conditions such as temperature, pressure, solvent and catalyst to improve the selectivity and yields.

The scope to design new multicomponent reactions (MCRs) has fascinated the researchers working in several areas like bioactive medicinal, combinatorial, pharmaceutical and heterocyclic synthesis. Advantages of MCRs are wide, including simple protocols, inexpensive reactants and green principles. Therefore, such efficient, environmentally benign protocols are befitting and well desired.

The proposed project involves the microwave assisted one-pot synthesis of series of substituted pyridine derivatives using a multi-component reaction involving reaction of malononitrile, substituted aldehydes, dimethyl acetylenedicarboxylate and substituted anilines in presence of a reusable heterogeneous catalyst and their characterization using various spectroscopic techniques.

Upon successful completion of the project, a research publication is envisaged.

13A – Dr B Moodley

An Investigation of Pharmaceutical Metabolites in Rivers

Rivers are an important source of water for many communities including informal settlements. However much waste including pharmaceutical waste has also been dumped into rivers leading to mass contamination, which affects the quality of water available for both human, agricultural and livestock use. Pharmaceutical waste not only contains the parent compound but as it passes through the body it is degraded into its metabolites which are just as contaminating as the parent compound. These organic contaminants can lead to bioaccumulation in aquatic life and humans leading to various health problems and also can lead to bacteria building up resistance to some drugs such as antibiotics found in the environment. It is therefore important for studies to be carried out on the organic contamination of rivers before suitable clean-up methods can be devised.

This project will involve sampling water and soil samples of a known river at various locations. The samples will be subjected to suitable extraction methods to separate the organic matrix from the rest of the sample as well as concentration methods. The extracts will be analyzed using various analytical chromatographic techniques with the aim of identifying and quantifying the organic components in the water samples.

13B – Dr B Moodley

Coring studies of major organic contaminants found in sediment at a wastewater treatment plant and along the Umgeni River

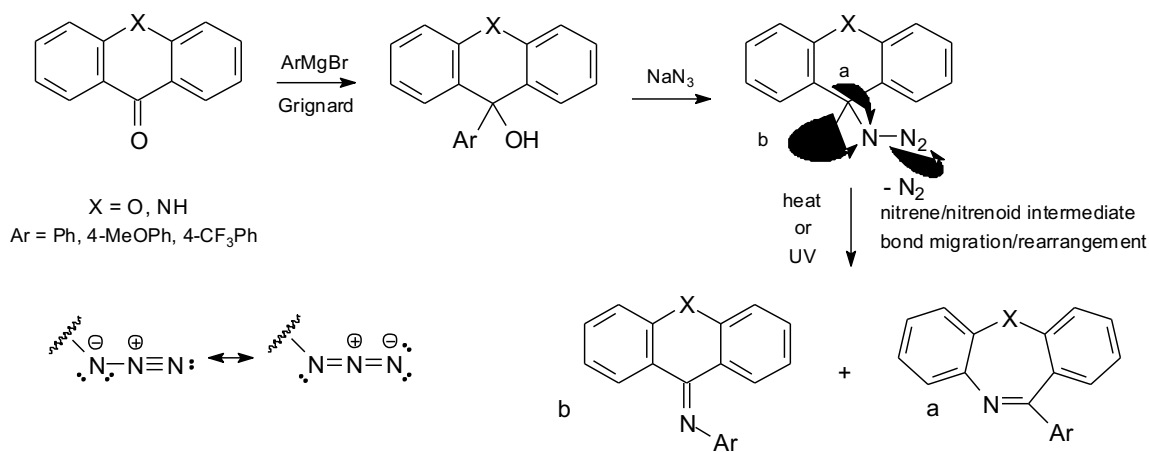
Rivers are an important source of water for many communities including informal settlements. However, much waste has also been dumped into rivers leading to mass contamination, which affects the quality of water available for both human, agricultural and livestock use. Organic contaminants in particular can lead to bioaccumulation in aquatic life and humans leading to various health problems. Water analysis is often difficult because the pollutants are found in such low concentrations. Analysis of the sediment has shown it to have much higher concentrations of the contaminants and can give a better idea of the presence and quantity of pollutants. In addition these pollutants tend to accumulate in the sediment over time and provide a good source of information on the past use/presence of these organic contaminants. Coring studies therefore allow for depth profiling of sediment to confirm that sediment does indeed serve as a “sink” for organic pollutants over time.

This project will involve obtaining cores of sediment samples from a wastewater treatment plant holding site as well as two or more locations along the Umgeni River. The sediment cores will be removed, sectioned and analysed. Each section is treated as an individual sample, extracted, pre-treated and analysed using conventional techniques such as GC-MS or LC-MS and a profile of the organic pollutants at different depths is determined.

14A – Dr Coombes

Ring Expansion, by Thermolysis and/or Photolysis of 9-azidoxanthene/acridines

Syntheses of 11-*p*-aryldibenz[b,f][1,4]oxazepines / dibenzo[b,f][1,4]diazepines



The project involves the syntheses, from xanthone / acridone, of various 9-azidoxanthenes / acridines, which rearrange smoothly on heating or UV photolysis to give mixtures of 9-*p*-arylxantheneimines / acridineimines and 11-*p*-aryldibenz[b,f][1,4]oxazepines/[dibenzo[b,f][1,4]diazepines. Previous studies have resulted in product ratios which suggest that the reaction intermediate is not a formal SN₁-type two step reaction involving a full-blown nitrene intermediate, but rather an SN₂-ish semi-simultaneous reaction involving an electron deficient nitrenoid.

15A – Prof MD Bala

Applications of green chemistry: Transition metal-free catalysts for transfer hydrogenation of ketones

N-heterocyclic carbenes (NHC) have become well established as alternative ligands to phosphines in many transition metal catalysed processes. In recent times, salt precursors to the ligands have also been utilised as organic catalysts in transition metal-free transformations including transfer hydrogenation. This process is considered green as it eliminates the need for transition metals in the process.

Catalytic hydrogenation is a very simple but versatile process en route to many pharmaceutical and fine chemicals. Transfer hydrogenation (TH) of ketones to alcohols is generally considered an environmentally benign and mild method of hydrogenation through the elimination of molecular hydrogen gas as source of hydrogen.

In this project, well established protocols will be utilized to synthesize imidazolium based ionic salts, fully characterise them and then use the salts as metal free catalysts for the conversion of acetophenone and other ketones to alcohols via TH.

References

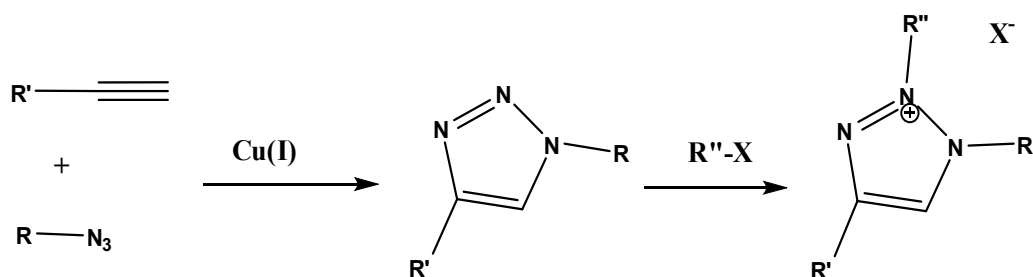
1. Serra, D.; Cao, P.; Cabrera, J.; Padilla, R.; Rominger, F.; Limbach, M. *Organometallics* 2011, 30 (7), 1885-1895.
 2. Simons, R. S.; Custer, P.; Tessier, C. A.; Youngs, W. J. *Organometallics* 2003, 22 (9), 1979-1982.
- Stephan, S.; Albrecht, M.; Loch, J. A.; Faller, J. W. ; Crabtree, R. H. *Organometallics* 2001, 20, 5485-5488.

15B – Prof MD Bala

Applications of green chemistry2: ‘click’ chemistry for the synthesis and characterisation of triazolium based ionic salts

Ionic salts and ionic liquids have found application as alternative solvents, ligand precursors and additives in many chemical transformations and especially in catalysis.

In this project, the green chemistry principle of ‘click’ chemistry will be utilized to assemble a set of well documented ionic salts based on the triazole entity. The salts will be fully characterized and some of their more important properties investigated.



R, R', R'' and X are all variables to be decided.

References

1. V. V. Rostovtsev, L. G. Green, V. V. Fokin and K. B. Sharpless (2002), *Angew. Chem. Int. Ed.* 41, 2596.
2. W. Herman (2002), *Angew. Chem. Int. Ed.* 41, 1290.
3. J.E. Hein and V.V. Fokin (2010) *Chem. Soc. Rev.* 39, 1302.

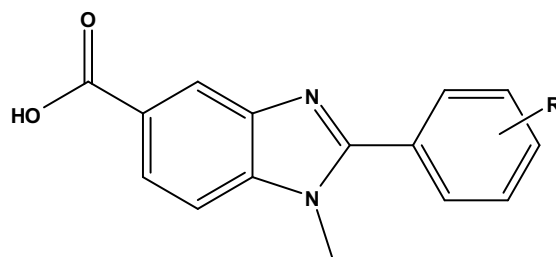
16A – Prof NA Koorbanally and Mr S Shintre

Synthesis and characterisation of fluorinated benzimidazole

Fluorine, a small and highly electronegative atom, plays a remarkable role in medicinal chemistry and hence its selective installation into a therapeutic or diagnostic candidate can enhance a number of properties like pharmacokinetic, physicochemical, metabolic stability and membrane permeability. Amongst nitrogen containing heterocycles, benzimidazoles are found to be a trendy moiety employed for drug discovery due to the unique structural features and a wide range of biological activities. Furthermore, these pendants are found in several drugs in the market and in clinically approved “drug-like” candidates.

Benzimidazoles have a five membered nitrogen based heterocyclic ring, again with the nitrogen atom bonded directly to the benzene ring adjacent to the heterocyclic ring. These compounds are known to contain antidiabetic, anticancer, anti-tubucular, antibacterial, antifungal, antimalarial and anti-inflammatory activity.

This project involves the synthesis and characterisation of three fluorinated benzimidazole derivatives (1-3) (Figure 1), by using three different fluorinated benzaldehydes. The molecules 1-3 can be achieved in a five step reaction procedure. Once synthesised, the molecules can be tested for their bioactivity and the different structures compared to see which of the different substitution patterns are best suited for a particular bioactivity.



- 1 R= 4-F
- 2 R= 4-CF₃
- 3 R= 3,4-diF

Figure 1. Benzimidazole compounds to be synthesized

16B – Prof NA Koorbanally and S Alapour

The Synthesis of dihydrobenzo[1,4]oxazines

Dihydrobenzo[1,4]oxazines are highly important for their interesting biological properties. They are used as neuroprotectants and inhibitors of nitric oxide synthases. They are also applied for the synthesis of fungicides and herbicides. In addition, they have been utilized for construction of different bioactive natural products. Chiral dihydrobenzo[1,4]oxazine compounds are also employed as catalysts for the asymmetric transfer-hydrogenation of α,β -unsaturated aldehydes. Consequently, several methods have been developed for the synthesis of these heterocyclic chemical.

We aim to synthesize dihydrobenzo[1,4]oxazines using the IUC (Intramolecular Ullman Coupling) reaction after four steps. In the first step we plan to protect commercially available alaninol **1** under standard conditions to **2**, which will then be converted to cyclic sulfamidate **3** by a catalytic oxidation reaction. Reaction of **3** with the sodium anion of phenol **4** (prepared by bromination of commercially available 2,3-difluorophenol) can afford the intermediate N-sulfate **5** to which we can apply the IUC reaction for the synthesis of Boc-protected [1,4]benzoxazin (**6**) (Figure 1).

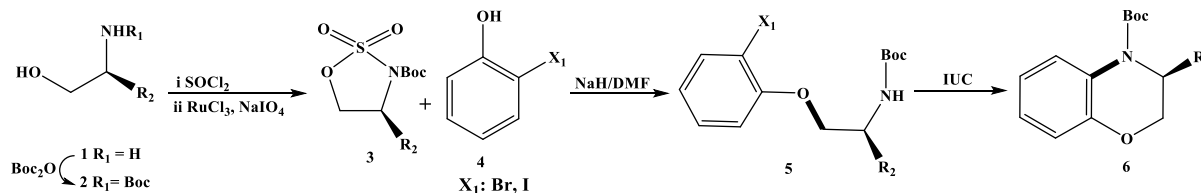


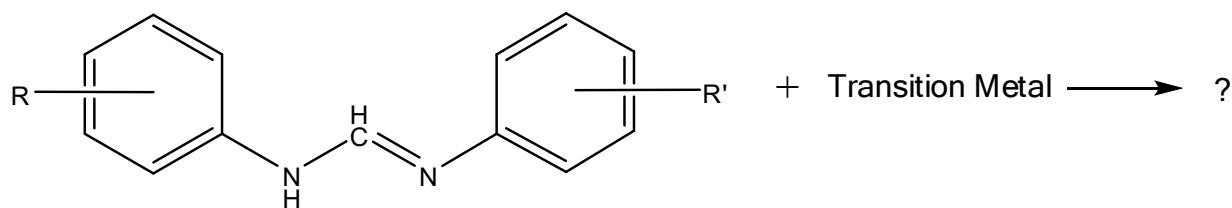
Figure 1. Synthetic scheme for the synthesis of Boc protected [1,4]benzoxacin

17 – Dr B Owaga

Transition metal cocomplexes of *N,N'*-dipyridinylamidine for ROP

N,N'-diarylformimidamides, ArNHC(H)NAr , are easy to make ligands and can form a variety of molecular arrangements when coordinated to transition metals. They are also easy to functionalize enabling one to control the electronic and steric properties of the ligand and in turn the metal complex. Our interest is in the electronic properties of transition metal complexes (mainly from group 11) of these ligands.

The project aims at developing *N,N'*-diphenylformimidamides with different donor atoms on substituents on the aryl ring and thereafter using the ligands to synthesizing hetero transition metal complexes. Thermal and electronic properties of the resulting complexes are of interest. All the prepared ligands and complexes will be fully characterized by spectroscopic and analytical techniques and by single crystal X-ray diffraction studies



R = -OMe, -COOH