IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	Directing group assisted alkane synthesis leading to liquid fuel formation	
Project Number	**IMURA0632**	
Monash Main Supervisor (Name, Email Id, Phone)	Prof. David W. Lupton david.lupton@monash.edu	*Full name, Email*
Monash Co-supervisor(s) (Name, Email Id, Phone)	N/A	
Monash Department:	Chemistry	
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IITB Co-supervisor(s) (Name, Email Id, Phone)	N/A	
IITB Department:	Chemistry	

Research Academy Themes:

Highlight which of the Academy's Theme(s) this project will address?
(*Feel free to nominate more than one. For more information, see www.iitbmonash.org)*

1. Advanced computational engineering, simulation and manufacture
2. Infrastructure Engineering
3. **Clean Energy**
4. Water
5. Nanotechnology
6. Biotechnology and Stem Cell Research
7. Humanities and Social Sciences

The research problem

The growing consumption of the non-renewable fossil fuels and their deteriorating natural reserves has threatened the sustainability of human civilization. Although significant effort has been invested over the last few decades to promote the usage of renewable energy stock, the idea is yet to meet the inflating economic demand. Hence it has become essential to come up with alternative resource supply. Among the few existing methods of fuel grade alkane synthesis Fischer-Tropsch catalysis is the most widely accepted and extensively used. However, generation of significant amount of unwanted lighter *n*-alkanes (C_3-C_8) deteriorates the grade of the fuel. Hence the desired larger *n*-alkanes of chain length C_9-C_{19}, known as

Fischer-Tropsch diesel, comes with a high cost. In this regard an alternative approach with enhanced efficiency and selectivity is highly desirable.

Project aims

In our upcoming venture we intend to a) develop a better replacement method of existing Fisher-Tropsch catalysis for the synthesis of fuel grade alkanes b) employ the concept of C–H activation in synthesis of long chain alkane with suitable metal and ligand combination c) optimize and diversify the metathesis catalyst which can open up a new horizon to mitigate the issue of energy crisis efficiently.

Expected outcomes

a) Method will be optimized and scope will be evaluated
b) Results will be published in peer-reviewed journals
c) Effective catalysts may be patented following the guidelines
d) Application of catalyst in industrial and academic settings
e) Further evaluation of existing methodology in the context of our findings

How will the project address the Goals of the above Themes?

Performing metal catalyzed olefin insertion in alkanes serves as an interesting step to begin with. This is lucrative owing to the abundance of widely abundant alkanes as a starting precursor. A prudent choice of a metal for the purpose would help in directing the incoming electrophile to the desired position. Functionalization could be achieved by transition metal catalyzed highly selective olefin insertion. Possibility for any bond isomerization will be mitigated to yield a single long chained alkane. This would mean synthesis of alkanes having chain lengths between C_9-C_{19} will be readily feasible.

Traditional metathesis reaction suffers from serious limitations of double bond ismerization and desired product yielding is retarded by the formation of branched product. Such a shortcoming can successfully be over ruled by employing this directing group assisted approach and synthesis of any higher homologue of branched chain alkanes seemed feasible by this methodology. We expect that an extensive investigation in this very aspect will be greatly facilitated by this proposal.

Capabilities and Degrees Required

B. Sc. (Chemistry)
M. Sc. (Chemistry)

Potential Collaborators

Prof. David W. Lupton

Please provide a few key words relating to this project to make it easier for the students to apply.

Alkane Metathesis; C–H Activation; Directing group assisted; Catalyst development; Long chain alkane; Fuel grade

Additional costs and equipment

Rs. 15,00,000/- [Fifteen Lakhs (INR)]

Detailed justification - Additional costs and equipment

Please justify why is this level funding is required?

This project is primarily designed for the development of new synthetic methodology and mechanistic understanding. Substrates, which are not commercially available, will involve multi-step preparations. Such experiments demand expensive fine chemicals, solvents and glasswares. Deuterated solvents are essential for NMR characterization. Furthermore, isotopically enriched compounds for mechanistic investigations would be even more expensive. Requested amount is bare minimum for smooth running of the proposed work.

Please note that palladium is unavoidable to carry out the proposed reaction. A large amount of various expensive palladium salts will be required for the project development. Not only metal, the lignds required for this project is of high price. Different types of expensive pincer ligands are immensely important to explore the entire work. Besides, designing the ligands, proper directing groups required a large number of chemicals. Preparation of a library of different directing group and ligands for thorough testing demands huge amount of consumable money.