INDIAN INSTITUTE OF TECHNOLOGY DHARWAD

॥ सा विद्या या विमुक्तये ॥

भारतीय प्रौद्योगिकी संस्थान धारवाड

Indian Institute of Technology Dharwad

Department of Chemistry

Information Brochure

Ph.D. Admissions

Autumn Semester (2019-20)

A. SCHEDULE OF Ph.D. ADMISSION

S. No.	Particulars	Dates
1	Availability of online application forms	
2	Last date for submission of completed application forms	Friday, 17/05/2019
3	Listing of shortlisted candidates for the Selection Process[1]	Friday, 31/05/2019
4	Date for the Selection / Examination Process	Thursday, 04/07/2019
5	Declaration of the Result of the Written Test	Thursday, 04/07/2019
6	Date for the Interview Process	Thursday, 04/07/2019
7	Display of the final result[2]	Monday, 08/07/2019
8	Last date for the Fee Payment	Friday, 19/07/2019
9	Date of Joining	Monday, 29/07/2019

B. ELIGIBILITY FOR ADMISSION

1. M.Sc. or equivalent degree in Chemistry/Biochemistry/Chemical Biology.
2. M. Phil or equivalent degree in Chemistry/Biochemistry/Chemical Biology.
3. M. Tech or equivalent degree in Chemical Sciences / Biological Sciences.
4. For General/OBC category candidates and/or for candidates where no concession in academic performance is called for, the eligibility criteria in the qualifying degree is **First Class,** as specified by the candidate's Institution/University. If the Institution/University does not specify the division/class, then one of the following will be considered as the eligibility criteria:
    - a minimum of 60% marks (without round off) in aggregate. (OR)
    - a minimum Cumulative Grade Point Average (CGPA) or Cumulative Performance Index (CPI) of 6.0 on the scale of 0-10; with corresponding proportional requirements when the scales are other than on 0-10, (for example, 4.8 on a scale of 0-8).
5. For SC/ST/PwD category candidates, a relaxation of 5% in the qualifying degree (55% and/or CGPA of 5.5 on the scale of 10) is applicable.
6. If a candidate **does not have M. Phil or M. Tech./M.E. or equivalent degree**, the candidate **must fulfill ONE** of the following additional requirements:
    - Valid GATE Score.
    - Junior Research Fellowship (JRF) of CSIR/UGC/DBT/DST INSPIRE or any other funding agencies.

[1 & 2] Will be announced on the institute webpage

C. APPLICATION CATEGORIES AND FINANCIAL SUPPORT

The Department of Chemistry admits Ph.D. candidates under the full time research scholarship - Teaching Assistantship (TA) and Fellowship Award (FA).

C.1. Fellowship Awardees

Students with valid fellowship from CSIR, UGC, DBT, ICMR, etc. can apply in this category.

C.2. Teaching Assistantship (TA)

Funded by MHRD, the TAs are expected to assist in the academic/administrative work for smooth functioning of the Institute. Students under this category are entitled to financial support as per MHRD norms.

For students with MSc./M.Tech./M.E./M.Phil. or equivalent degree as the qualifying degree, the assistantship is payable for a maximum duration of 5 years or up to the thesis submission, whichever is earlier. At present, the monthly rate of assistantship is 25,000 for the first 2 years and enhanced rate of 28,000/- for the remaining period.

For students with B.Tech./B.E. or equivalent degree and students with M.Sc. or equivalent as the qualifying degree and having valid GATE score or having Junior Research fellowship (JRF) of UGC/CSIR or DST INSPIRE fellowship, the assistantship is payable for a maximum duration of 5 years or up to the thesis submission, whichever is earlier. At present, the monthly rate of assistantship is ₹25,000/- for the first two years and enhanced rate of ₹28,000/- for the remaining period.

To get Teaching Assistantship, the students concerned must assist in teaching, research and/or administrative work as assigned by the respective Academic Unit to the extent of 8 hours of work per week.

The continuation of the assistantship will be subject to satisfactory performance of the duties assigned by the Departments as well as satisfactory academic performance.

Employees on the rolls (with or without pay) of any organization are not eligible for admission under this category.

As per MHRD directives, the employees of any organizations with or without pay are not eligible for admission under TA category. Candidates selected in this category have to resign from the current job and submit a relieving letter from their employer before joining the programme. Students getting assistantships from the Institute may join projects sponsored by external agencies and obtain corresponding fellowships in lieu of TA ship.

D. GUIDELINES FOR THE SHORTLISTED APPLICANTS

The following are the important guidelines of the institute to be followed by the shortlisted applicants on the day(s) of the selection process.

1. Shortlisted applicants should report to the institute on 4th of July, 2019 at 8.00 am.
2. No accommodation will be provided for the candidates during the selection process or interview.
3. Applicants should bring:

a. Photo ID card (any one from these: PAN/AADHAR/Driving Licence/Voter ID/Passport/Govt. issued ID/Educational Institute ID)
b. Printed copy of the application
c. Thesis/dissertation/report of M.Tech./M.E./MSc-Engineering or equivalent degree
d. Copy of certificates and mark-sheets
e. Two recent passport size photographs
f. Non Programmable Scientific calculator

D.1. DO NOT's

a. Mobile phones are not allowed in the examination hall or in the interview room
b. Department's decision is the final decision regarding any matter pertaining to this selection process.
c. Institute doesn't take any responsibility of your luggage/items that you leave before entering the examination hall.

E. MODALITY OF THE SELECTION PROCESS

The selection process consists of Multiple Choice Questions (MCQ) type screening test followed by interview.

Document Verification: Only for candidates short-listed for interview. Certificate required are like Date of Birth certificate, Degree certificate along with marks cards, aggregate percentage, JRF offer letter from UGC/CSIR and INSPIRE fellowship, GATE Score, Cast certificate, Income certificate, Photo Identity, etc.

F. RESEARCH TOPICS

Problem statements with brief description

There are four topics floated in the department for the PhD program in this semester. Applicant has to choose one of these topics and fill in the application form.

1. Organic chemistry of the enzyme catalysed reactions in antibiotic compounds:

Enzymes are nature's organic chemists that carry out remarkable chemical reactions, particularly in the synthesis of antibiotics and other important compounds. To study the enzyme reaction mechanisms, one requires sound knowledge of chemistry and biochemistry**.** One particular area of interest is the ribosomally synthesized and post-translationally modified (RiPP) peptide natural products which show unique antibiotic properties. In today's world, the emergence of antibiotic resistance in bacteria is proving to be a serious and increasing threat to human health. Therefore, discovery of new structural motifs with novel antibacterial targets exhibiting activity against multi-drug resistant pathogens is of utmost importance. RiPP natural products, produced by bacteria, are an emerging class of peptide derived compounds with diverse structural features exhibiting wide array of bioactivities ranging from antibacterial to anticancer properties. RiPP precursor peptides are direct ribosomal gene products that undergo various post-translational modifications (PTMs) by enzymes to synthesize the mature, structurally complex antibiotics. We would like to study the chemistry of the enzyme mechanisms (such as C-H activation, C-C bond formation, molecular rearrangement, amide bond activation etc.) involved in synthesizing these natural products. One class of enzymes involved is called radical S-Adenosylmethionine (rSAM) enzymes that contain [4Fe-4S] clusters and carry out fascinating transformations using organic radical medicated chemistry. Recently, they were shown to catalyze reactions via an organometallic (Fe-C) intermediate as well. We would employ interdisciplinary techniques from chemistry, biochemistry/chemical biology, and molecular biology/microbiology during these studies and suitable collaborations (such as for protein crystallography, EPR techniques, and synthetic biology etc.) will be initiated to gain insights into the molecular details of these mechanisms. In addition, analog generation for medicinal chemistry, enzyme inhibitor development and structure-function elucidation of new compounds will also be undertaken in the future.

2. **Tryptophan derived bioactive natural products: Biosynthesis, structure and function**

Tryptophan, the most chemically complex and the least abundant of the 20 common proteinogenic amino acids, is a biosynthetic precursor to many complex microbial natural products (such as antibiotic pyrrolnitirin), which are promising scaffolds for drug discovery and development. The chemical features of tryptophan, including its ability to undergo chemistry at almost every atom makes it a unique biological precursor for the generation of chemical complexity. Recently it was discovered that tryptophan leads to the formation of a few novel anticancer compounds of highly functionalized alkaloid family which were shown to induce DNA single and double strand breaks and metal dependent DNA complex formation. Moreover, they also cause several chromosomal aberrations, and blocks the synthesis of DNA and RNA by inhibiting topoisomerase II. Our goal would be to study the biosynthesis (synthesis by enzymes in a biological set up) of such natural products *in-vitro*, understand the fundamental principles of the complex organic/inorganic chemistry (they also involve metalloenzymes) and characterize the molecular details of these proteins using various techniques from chemistry (synthetic chemistry, bioorganic/bioinorganic and biophysical chemistry) and biology (protein biochemistry, molecular and cell biology). This investigation

will also enable us to create variants of these compounds as potential anticancer agents by using chemo-enzymatic methods for future structure-activity relationship studies.

3. π-Conjugated two-dimensional crystalline/amorphous organic porous polymers

Two-dimensional (2D) materials have received wide attention since the demonstration of high charge mobility in graphene, that is often named a discovery of the century in solid state physics. Despite its many remarkable properties, graphene is a zero-band gap polymer which makes its application in semiconducting devices difficult if not impossible and further any chemical modifications of graphene introduce sp3 defects which break π-conjugation and thereby destroy the special electronic properties of the material. Therefore, the 2D conjugated polymers constructed of organic building blocks are envisaged to be potential alternative candidates to graphene in terms of introducing bandgap and ease of altering electronic topology. To date, several 2D π-conjugated polymers have been synthesized as crystalline covalent organic frameworks (COFs) or amorphous porous organic polymers. One general problem of all approaches is a lack of versatile building blocks (monomers) capable of maintaining direct π-conjugations in several directions, and, as a result, very limited electron delocalization in the currently accessible 2D polymers. Thus, we would like to design and synthesize 2D-organic polymers which will have efficient two-dimensional electronic delocalization and evaluate the electronic properties of these materials.

4. C-H activation derived novel π-conjugated organic electronic compounds for sensing and optoelectronic applications

Semiconducting π-conjugated organic molecules (oligomers, polymers) are of paramount importance owing to their applications in a wide variety of organic electronic devices such as sensors, organic light emitting diodes, organic field effect transistors, solar cells and photovoltaics etc. The successful development of organic electronic materials relies on the cheap, efficient and environmental benign synthetic methods. Of a particular interest, in recent times, C-H activation-functionalization has emerged as powerful synthetic tool for development of π-conjugated compounds owing to its potential to construct the materials without need of pre-activating bonds. Moreover, the method is also pivotal in functionalizing inactive C-H bonds which are traditionally considered as inert. The technique may enable the design and synthesis of novel material that are not possible with conventional synthetic methods. Therefore, we propose to apply the C-H activation strategy for the functionalization of chemically inert positions of the fundamentally important building blocks (anthracene, pyrene, perylene, indigo etc.) which are otherwise highly challenging for traditional synthetic methods. These intriguing precursors opens up a door for the realization of various NIR-absorbing, photo-luminescent and optoelectronic materials. The method will be further extended to develop novel one-dimensional and two-dimensional organic polymers. The optical and electronic properties of the synthesized materials will be studied and also explored their potentiality in photo-catalysis, sensing and optoelectronic applications.

G. SYLLABUS FOR SCREENING TEST AND INTERVIEWS

Common topics:

- Fundamental principles of chemistry
  Recommended text books: J. Clayden, L. G. Wade, J. D. Lee and P. Atkins

- Coordination chemistry: Various types of complexes, Crystal field splitting, magnetism
  Recommended text books: J. D. Lee and J. E. Huheey
- Organometallic chemistry: Metals aryls and alkyls, p-bound ligands etc, oxidative addition-reductive elimination, applications to organic chemistry
  Recommended text books: R.H. Crabtree and A. J. Elias
- Spectroscopy: Rotational, vibrational and electronic spectroscopy, NMR and mass spectrometry
  Recommended text books: C. N. Banwell, D. L. Pavia and H. Gunther
- Organic name reactions: Reactions and their mechanisms
  Recommended text books: W. Carruthers, J. Clayden

Additional syllabus for the candidates choosing research topics 1 and 2 (see the research topics)

- Basic Bioorganic chemistry and Biochemistry: Biomolecules (proteins, carbohydrates, nucleic acids and fatty acids) and their chemistry, biomimetic chemistry, metabolic pathways, biosynthesis of common biomolecules, enzymes and mechanisms, metalloenzymes, central dogma of life, basic concepts of medicinal chemistry

  Recommended text books: Voet and Voet, Lehninger, Hermann Dugas

Additional syllabus for the candidates choosing research topics 3 and 4 (see for the research topics)

- Basic Photochemistry: Jablonski diagram, UV-Vis and Fluorescence, phosphorescence and photochemistry of organic compounds, p-conjugation.
  Recommended text books: J. D. Coyle