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## **VISION**

To create, disseminate and translate knowledge in science, engineering and allied disciplines that will best serve the society.



# About IIT Kanpur

MOINT OF TECHNOLOGY

- Motto : तमसो मा ज्योतिर्गमय
- Public engineering institution in Kanpur, Uttar Pradesh, Established in 1959
- Institute of National Importance by GOI
- During the first ten years of its existence, a consortium of nine US universities helped set up IIT Kanpur's research laboratories and academic programmes under the Kanpur Indo-American Programme (KIAP)
- The campus is designed by Achyut Kavinde in a modernist style

# About the Department

- One of the premier departments at IITK
- Contributes to research and industry
- Address problems of societal importance
- The Department started its journey in early 1960's under the headship of Prof. C.N.R. Rao
- The faculty propelled the department forward with excellence in modern chemistry teaching and research.
- To name a few present faculty members with distinguished awards;
   Prof. Vinod K Singh –Synthetic Organic Chemistry –Padma Shri
   Prof. Amalendu Chandra –Statistical mechanics and molecular simulations Shanti Swaroop Bhatnagar
  - Prof. J. N. Moorthy Physical Organic Chemistry-Shanti Swaroop Bhatnagar
  - **Prof. V. Chandrasekhar** Bioinorganic and Supramolecular Chemistry–Shanti Swaroop Bhatnagar
  - **Prof. Sandeep Verma** Chemical Biology–Shanti Swaroop Bhatnagar

### From the HODs Desk

The Department of Chemistry at IIT Kanpur reiterates its commitment to excellence in contemporary research and teaching. Some courses initiated by my former and present colleagues in this department have become beacons for chemical education in India. We also have one of the strongest Industry-Academia connections. As its newly appointed head, I invite you to explore our department and witness the impactful research and educational initiatives that define us: together, let us embark on a journey of discovery, innovation, and excellence in the fascinating world of Chemistry - a fundamental science of all things in and around us.



**Professor Gurunath Ramanathan** 

# Labs in the department

Main group, Coordination, Organometallic Lab	Theoretical Chemistry Group	
Inorganic Synthesis And Bioinspired Catalysis	Molecular Functional Materials Research	
Organometallic Synthesis and Catalysis	Quantum Thermodynamics Group	
Multifunctional Molecular Nanofilms	Femto Lab	
Bioinorganic Laboratory	Computational Chemistry lab	
Total synthesis of biologically active natural products.	Plasmonic Chemistry Research Group	
Energetic Materials Lab	Bio-Nanoparticle Lab	
Organic Photochemistry	Theoretical Chemistry Research Group	
Organic Synthesis and Bioorganic lab	Ultrafast Spectroscopy Laboratory	
Synthetic organic chemistry	Supramolecular Lab	

## Recent Notable Achievements

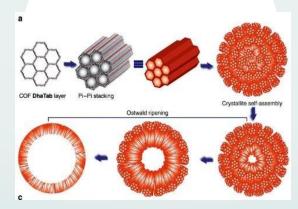


Synthesis of Chiral Hexahydropyrroloindoles



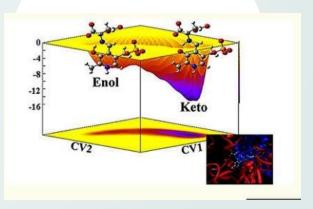


#### Hollow Frameworks





#### Multiscale Modelling



## Major Degree Programs

#### Master of Science (M.Sc)

Post bachelors degree in chemistry Admission via Joint Admission Test to M.Sc. (JAM) Combination of compulsory and elective courses Are required to carry out research

#### Dual- majors (BS-MS)

Bachelors–Masters Integrated program 5 years



### Bachelor of Science (BS.)

4-year

Admission via Joint Entrance Examination (JEE)

Basic courses Electives in chemistry and open electives Research projects (UGP)

#### **Minors**

Done along with Bachelor's degree Offered in Organic, Inorganic and Physical Chemistry

#### PhD

Doctorate in Philosophy
5 years
Admission by either of the
two nation-wide
examinations post M.Sc
Rigorous Interview

### INORGANIC CHEMISTRY

The research interests of inorganic section span diverse areas that include

- Coordination chemistry
- Bioinorganic chemistry
- Organometallic chemistry
- Catalysis
- Supramolecular chemistry

#### Some of them are

- The study of inorganic entities in biological systems is major topic of interest
- Studies on heme centers in heme protein
- Topics related to medicinal inorganic chemistry
- The creation of new chemical entities with interesting structures
- Magnetic and electrochemical properties for applications in catalysis and material chemistry





## **ORGANIC CHEMISTRY**

Research areas in organic chemistry– Includes an eclectic mix of Traditional and Contemporary fields such as

- Bioorganic chemistry,
- New reaction development,
- Natural product synthesis,
- Photochemistry,
- Chemical biology,
- Organic materials
- Catalysis.

In addition to studying the chemistry of small molecules,

- The synthesis and application of carbohydrate and peptide based architectures
- Metal-organic frameworks for applications in medicine and material science

are also being performed in a number of laboratories.

### PHYSICAL CHEMISTRY

Research areas in the domain of physical chemistry encompass

- Computational and Theoretical chemistry
- Reaction dynamics
- Spectroscopy
- Materials chemistry

#### Specific areas include

- Fundamental gas phase molecular dynamics
- Statistical mechanics

#### Application of modern techniques like

- Ultrafast pulse-shaping
- Molecular beams
- Single molecule spectroscopy and imaging
- Fluorescence correlation and up-conversion

Both experimental and theoretical research components are strongly represented.



# Basic Chemistry Lab

Permanganometric Titrations	Viscosities of Solutions		
Acid – Base Titration	Chemical Kinetics		
Iodometric Titrations	Heterogeneous Equilibrium		
Complexometric Titrations	Photochemical Oxidation – Reduction		
Preparation and Analysis of a Metal Complex	Conductometric titration of HCI Vs NaOH		
olynuclear Metal Complexes with  Multidentate Bridging  Ligands	Synthesis of antioxidants used as food preservative		
Chromatography of Natural Pigments	The Detection of Changes in the Conformation		
Preparation of Polymer Films	Determination of pl of Glycine		
Isolation of Caffeine from tea	Preparation of Fluorescein Dye		

# Organic qualitative and quantitative analysis

#### 1. Experimental Techniques

(A) Purification of Organic Compounds

- Recrystallisation
- Sublimation
- Steam distillation
- Distillation
- Bulb-to-bulb distillation

(B) Chromatography

- Thin layer chromatography (TLC)
- Column Chromatography
- Preparative TLC

(C) Physical Constants

- Melting Points and Boiling Points
- Optical rotation and molecular rotation

(D) Spectroscopic Methods

- Preparation of ester (Confirmation by IR, NMR)
- Structure elucidation (by spectral data)

2. Investigation and Characterization of Organic Compounds

- Detection of elements present in a given organic compound.
- Identification of functional groups in a given organic compound. Identification of unknown organic compounds.
- Separation of organic mixture by chemical methods, preparation of derivatives, and identification of the material

## Inorganic Chemistry Laboratory

Estimation of iron in minute quantities by **UV-vis spectrophotometry**Principles of **colorimetric analysis**: determination of iron content of an unknown sample.
Preparation of hexamminenickel(II)chloride: estimation of ammonia and nickel by **titrimetric** and **gravimetric** methods

Preparation of diamagnetic and paramagnetic main-group and transition-metal acetylacetonates

Synthesis, isolation and spectroscopic characterization of the complexes Synthesis and characterization of ferrocene and acetylferrocene Synthesis of the complex and their purification using chromatography Acid-base and redox titration of tablets containing Vitamin-C Estimation of ascorbic acid in Vitamin-C tablets

Paper chromatographic separation of Cu2+,Fe3+ and Ni2+
Utilization of paper chromatographic techniques to separate the metal salts

Spectrophotometric determination of phosphate: estimation of phosphate in cola drinks

Determination of concentration of phosphates applying Beer-Lambert law Potassium tris-oxalatoferrate(III): synthesis, analysis and photochemistry Synthesis of the complex and its utilization in **blue-printing experiment** 

## Physical Chemistry Laboratory

Calibration of volumetric apparatus Analysis of the rotational-vibrational spectra Determination of partial molal volume **Isotherm** for a three component system Kinetics of fast reactions by stopped-flow technique Spectrophotometric determination of acid dissociation constant The measurement of electrical conductance for the determination of the equivalent conductance at infinite dilution Rate of the hydrolysis of sucrose using **polarimeter** Determination of pKa of poly-basic acid with the pH meter Determination of critical micelle concentration Determination of transport number by moving boundary method **Polarizability** from refractive index measurements Formula and **stability constant** of a complex by spectrophotometry Fluorescence quantum yield determination of an unknown molecule. Fluorescence spectrum and stern-volmer quenching constant IR and Raman spectroscopy of solvent mixtures Computing Potential Energy Surface of molecules using Quantum Mechanics Introduction to Scanning Probe Microscopy

# Inorganic Chemistry Laboratory-II

Invisible ink Utilization of coordination chemistry
Ligand-exchange concept
Crystal-field splitting parameters of 3d metal ions.
Acidic and basic salts Hydrolysis of salts and its consequences.
Various spectroscopic techniques
Synthesis, isolation and characterization of complex
Geometrical isomers: synthesis, identification using spectroscopic techniques.
Investigation of acid hydrolysis of the complex
Resolution into optical antipodes Optical isomers
Titrimetric and gravimetric methods
Synthesis of an air-sensitive organometallic complex
Ferrocene, acetylferrocene Synthesis, chromatography, characterization

## Organic Preparations Lab

Benzil - Benzilic Acid Rearrangement

Fisher: Indole Synthesis:
Diazotization
Reductive Coupling Prep

Molecular Rearrangement Pinacol – Pinacolone – rearrangement

Reimer-Tiemann Reaction

Perkin Reaction

Aldol condensation and epoxidation





# Department Facilities

The Department of Chemistry has excellent facilities including a wide range of sophisticated instruments offering technical support to the research activities.

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High Field Nuclear Magnetic Resonance	Cyclic Voltammetry
Resonance Raman Spectrometer	Elemental Analyzer PE
Spectrophotometer	UV-VIS Spectrophotometer
Surface Plasmon Resonance	Micro-Analytical Facility
Mossbauer spectrometer	REACT IR (Metler Toledo)









## Department Facilities

### NMR Spectroscopy

The department operates three high field NMR (both 400 and 500 MHz) spectrometers for recording high resolution spectra from solution phase samples. NMR spectrometers are run and maintained by dedicated operators who also routinely train and assist students in recordingsimple 1-Dspectra as well as multidimensional hetero-nuclear experiments.

### Mass Spectrometry

This facility allows for collection of routine and high resolution mass spectra under a variety of ionization conditions om the state-of-the art. Waters Q-TOF Premier HAB213 and Waters GC Premier mass spectrometers.

# X-Ray Crystallography Determination of molecular structures of

Determination of molecular structures of organic, organometallic and coordination compounds are performed by single crystal Xray diffraction measurement using two state of-the-art single crystal X-ray diffractometers. (Bruker Apex-II and D8 Quest Single Crystal Microfocus X Ray Diffractometer) equipped with a low temperature device.

### Femtosecond Transient Absorption

### Spectrometer

Early time structural and excited-state dynamics of molecules and materials in the condensed phase can be studied using this facility. The time resolution of setup is 120 fs.

## Department Facilities

#### Resonance Raman Spectrometer

A tunable laser source (Argon ion) coupled to a high resolution Raman spectrometer enables us to record resonant Raman spectra of molecules and materials. This technique can be used to probe subtle changes in the structure of a complex molecular system.

### Other Department facilities

Include FT-IR spectrometer, UV-vis-NIR spectrophotometer, elemental (CHN)) analyzer, Mossbauer spectrometer, circular dichroism spectrometer, Pico second Time-Resolved Fluorimeter,

Atomic Force Microscope, powder Diffractometer, Thermo
Gravimetric/Differential Thermal
Analyzer,polarimeter,etc

### **EPR Spectroscopy**

Electron Paramagnetic Resonance spectroscopic measurements are done using Bruker EMX300 EPR spectrometer installed in the department. Our facility routinely records EPR spectra of solid, liquid and frozen samples under variable temperature condition.

#### Nano Science Center

Nano science center at the institute caters the state of the art facility and resources for carrying out research, development activities in the areas of soft nano fabrication. Some of the major equipments at the center are NSOM/RAMAN/Confocal/AFM, Scanning Electron Microscope with electron beam lithography, small angle and wide angle XRD.

### Past Recruiters





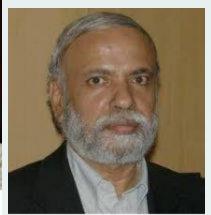
# Distinguished Alumni



P. Balaram



Swaminathan Sivaram - ...





Dr Sourav Pal



P. V. Ramachandran - P...



Prof. Pushpito K. Ghosh



Uday Maitra | The Depa...



Arun K. Ghosh | MCMP



Amitabha Chattopadhy.



## Thank You

#### **Ashok Kumar Das**

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