



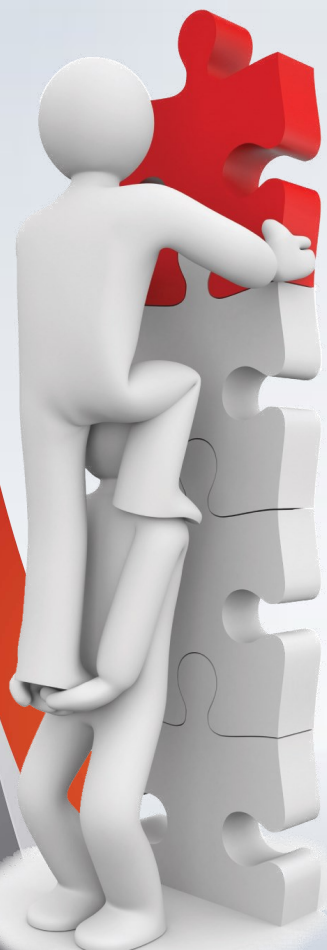
**KARYASHALA PROGRAM**

**(HIGH-END WORKSHOP): ACCELERATE VIGYAN SCHEME**

# **ONLINE WORKSHOP IN STRUCTURAL METHODS**

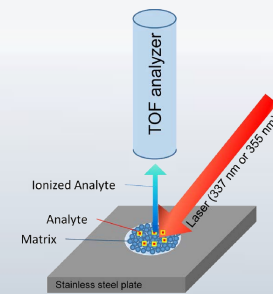
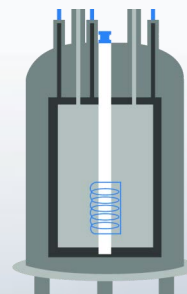
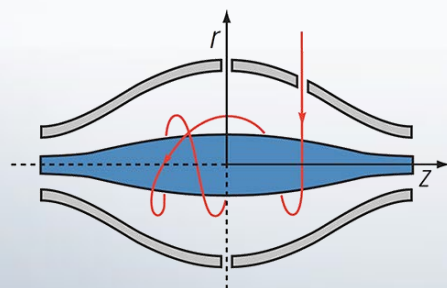
Jointly organised by

**Science and Engineering Research Board &  
IISER Thiruvananthapuram**



**September 27<sup>th</sup> - 1<sup>st</sup> October, 2021**

 [workshop.iisertvm.ac.in/karyashala/](http://workshop.iisertvm.ac.in/karyashala/)

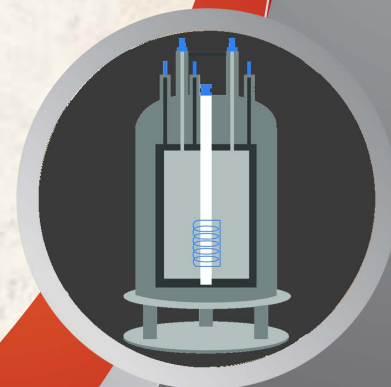


## ABOUT KARYASALA

The chemistry department of IISER Thiruvananthapuram is conducting the karyashala a high-end workshop training for scientific instruments such as Electron microscopes, NMR spectrometers, X-ray diffractometers and different mass instruments. The main objective of this workshop is 'to provide the students with a unique opportunity to work with most sophisticated instruments for structural characterization'.

There is a growing need for skilled personnel trained in sophisticated instrumentation. This workshop is focused on different techniques in Electron microscopy, NMR spectroscopy, X-ray diffraction, and Mass spectrometry. The intensive workshop will give the participants a valuable opportunity to gain a firm theoretical basis and obtain practical experience in the aforementioned high-end techniques, data processing, spectral analysis and interpretation. Due to Covid-19 all the sessions will be online guided by experienced members drawn from the IISER Thiruvananthapuram chemistry faculty

- ⇒ The program is designed for : PG students
- ⇒ Duration of the workshop : 5 days
- ⇒ Maximum number of participants : 100
- ⇒ Link to register for the workshop : [Click Here](#)





# PROGRAM

## Monday, September 27, 2021 - NMR - Day 1

09:00 - 09:30 **Inaugural Remarks:** Prof. J. N. Moorthy, Director, IISER Thiruvananthapuram

09:30 - 11:00 **Lecture** : Fundamentals of NMR, Signal generation, Description of pulse and Fourier transform NMR

14:00 - 15:30 **Video** : Sample preparation, understanding the parts of the NMR spectrometer and magnet.

**Video** : Steps required for measuring 1D spectra, Shimming, locking, description of acquisition parameter.

**Video** : Measurement of 1D NMR spectra ( $^1\text{H}$  and  $^{13}\text{C}$ ), Processing of NMR spectra, Integration, plotting, presentation of spectra, automation.

## Tuesday, September 28, 2021 - NMR - Day 2

09:30 - 11:00 **Lecture** : NMR spectral analysis of 1D and 2D NMR.

14:00 - 15:30 **Video** : Measuring different 2D NMR (COSY, HSQC), parameter set up, acquisition setup etc.

**Video** : Processing and Analysis of measured 2D spectra, plotting and printing.

**Lecture** : Principle & applications of essential techniques in Chemistry laboratory (TGA, DSC, FT-IR, CD, CV etc.)

**Video** : Acquisition and Analysis of these techniques .

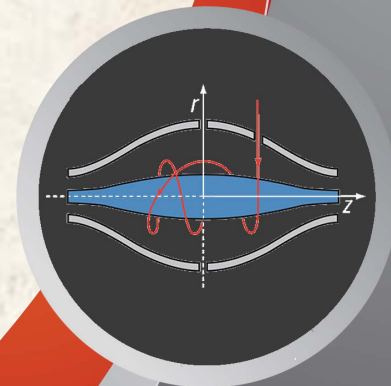
## Wednesday, September 29, 2021 - Electron Microscopes (TEM and SEM)

09:30 - 10:30 **Lecture** : Fundamentals of TEM.

11:00 - 12:30 **Video** : Sample preparation, sample loading, data acquiring and analysis.

14:00 - 15:00 **Lecture** : Fundamentals of SEM.

15:30 - 18:00 **Video** : Sample preparation, sample loading, data acquiring and analysis.



# PROGRAM

## Thursday, September 30, 2021 - X-Ray Diffraction

09:30 - 11:00 **Lecture** : Crystallographic symmetry and crystal systems, fundamentals of X-Ray diffraction.

11:30 - 13:00 **Video** : Understanding the parts of the X-ray diffractometer.

**Video** : Mounting the crystal, evaluation of quality of crystal, unit cell data collection, full data collection.

**Video** : Working up raw data for modelling.

14:00 - 15:00 **Lecture** : Modelling of crystal structure (without disorder) and CIF file preparation.

15:15 - 17:15 **Lecture** : Modelling of crystal structure (with disorder) and CIF file preparation.

## Friday, October 01, 2021 - Mass Spectrometry (HRMS-ESI, MALDI, LRMS, GC-MS)

09:30 - 11:30 **Lecture** : Principle and Type of Mass Spectrometry.

**Lecture** : Fragmentation and Spectral Analysis including EI and CI ionization.

**Video** : Components of GC-MS including column oven and mass analyzer.

**Video** : Sample preparation, creating methods, inject through GC column and direct injection to MS without using GC column.

12:00 - 13:00 **Lecture** : Principle of ESI and MALDI including APCI and APPI

14:00 - 18:00 **Video** : Components of MS including HR Q-Exactive Orbitrap, TOF, MALDI and Ion-Trap.

**Video** : Sample preparation, creating methods, understanding the auto sampler and Cleaning methods. Inject samples with and without column.

**Video** : Analysis of the spectra using the software.

18:00 - 18:15 **Closing Remarks** : Prof. Mahesh Hariharan, HoD, School of Chemistry, IISER TVM

