A report on

One-week hands-on training workshop on

ANALYTICAL ADVANCES IN STUDYING MOLECULES

Under the aegis of

DST-Synergistic Training Program Utilizing the Scientific and Technological Infrastructure (STUTI)

In association with

Sophisticated Analytical Instrument Facility (SAIF), Panjab University, Chandigarh (PMU)

Organized by

Department of Chemistry
BITS Pilani, Pilani Campus

15-21 October 2022

BITS Pilani
Pilani Campus

Panjab University

सत्यमेव जयते
विज्ञान एवं प्रौद्योगिकी विभाग
DEPARTMENT OF
SCIENCE & TECHNOLOGY

Contents

Information Brochure

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Pilani Campus

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About BITS Pilani:

Birla Institute of Technology & Science, Pilani (BITS Pilani) has been consistently ranked high, by both governmental and private ranking agencies for its innovative processes and capabilities that have enabled it to impart quality education and emerge as the best private science and engineering institute in India. As per various reports by business magazines, the student acceptance rate to BITS Pilani is one of the most stringent in the world. BITS Pilani continuously strives to cater to the expectations of its brilliant student cohort by excelling both in teaching and research. In recognition of the high standard that BITS Pilani strives to uphold, University Grant Commission, in 2018, has declared it as an "Institute of Eminence" (IoE).

Department of Chemistry, BITS Pilani, Pilani Campus:

Established in 1944, we are one of the oldest departments on the campus. The department has grown with strong research interests in the Physical Chemistry, Synthetic Organic Chemistry, Inorganic Chemistry, Bioorganic Chemistry, Medicinal Chemistry, Theoretical and Computational Chemistry, etc. Equipped with state-of-the-art instrumentation facilities and research laboratories, we are counted amongst the best departments for education in Chemistry across the country.

STUTI Program:

STUTI Program of the Department of Science & Technology (DST), Government of India, is intended to build human resource and its knowledge through open access to S&T Infrastructure across the country. This is achieved by organizing short term courses/workshops on the awareness, use and application of various instruments and analytical techniques. The Scheme provides grants for organizing training programs including boarding and lodging for participants, honorarium for resource persons, and training materials. The registration is free of cost. Reimbursements for train fare (AC three tier or non-AC) to the participating candidates from outstations are provided.

Topics for Discussion and Hands-on-Training:

Nuclear Magnetic Resonance Spectroscopy, Chromatography, Mass Spectrometry, Ultraviolet-Visible Spectroscopy, Fluorescence Spectroscopy, Infrared Spectroscopy, Raman Spectroscopy, Scanning Electron Microscopy, and Transmission Electron Microscopy.

Panjab University

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DEPARTMENT OF SCIENCE & TECHNOLOGY

Azadi Ka Amrit Mahotsav

Resource Persons:

- **Prof. Diwan S. Rawat**, Delhi University
- **Prof. Jyotishman Dasgupta**, Tata Institute of Fundamental Research, Mumbai
- **Prof. N. Suryaprakash**, Indian Institute of Science, Bangalore
- **Prof. P. K. Madhu**, Tata Institute of Fundamental Research, Hyderabad
- **Prof. Sobhan Sen**, Jawaharlal Nehru University, New Delhi
- **Prof. R. Ravi Krishna**, Indian Institute of Technology Madras
- **Prof. Soumen Kanti Manna**, Saha Institute of Nuclear Physics, Kolkata
- **Prof. SVK Kumar**, Tata Institute of Fundamental Research, Mumbai
- **Prof. Anindya Datta**, Indian Institute of Technology Bombay
- **Prof. Parasuraman Jaisankar**, Indian Institute of Chemical Biology, Kolkata
- **Dr. Indranath Chakraborty**, Indian Institute of Technology Kharagpur
- **Dr. B. M. Krishna Mariserla**, Indian Institute of Technology Jodhpur
- **Prof. Ramesh Ramapanicker**, Indian Institute of Technology Kanpur
- **Dr. Ahin Roy**, Indian Institute of Technology Kharagpur

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(BITS Pilani-Pilani Campus)

Email for Queries: aasm@pilani.bits-pilani.ac.in

Organized by: Department of Chemistry, BITS Pilani-Pilani Campus

innovate achieve lead

Program Schedule

Day 1 (October 15, 2022, Saturday)

08:00 am – 08:20 am: Formal Welcome and Inauguration

08:20 am – 08:30 am: Address by the Director, BITS Pilani, Pilani Campus: Prof. Sudhirkumar Barai

08:30 am – 08:40 am: Address by the Head of the Department of Chemistry, BITS Pilani, Pilani Campus: Prof. Indresh Kumar

08:40 am – 08:50 am: Address by the Guest of Honour: Prof. G. R. Chaudhary, Panjab University

08:50 am – 08:55 am: Vote of Thanks

08:55 am – 09:15 am: High Tea

Session 1: Chair: Prof. S. C. Sivasubramanian, BITS Pilani, Pilani Campus

09:15 am – 10:45 am: Resource person's talk 1: Theory, concepts, and applications of 1D ^{1}H NMR spectroscopy by Prof. Diwan S. Rawat, Delhi University

10:45 am – 11:00 am: Tea break

11:00 am – 12:30 pm: Resource person's talk 2: Theory, concepts, and applications of 1D NMR spectroscopy of non-^{1}H based nuclei by Prof. Ramesh Ramapanicker, Indian Institute of Technology Kanpur

Session 2: Moderator: Prof. Rajeev Sakhuja, BITS Pilani, Pilani Campus

12:30 pm – 01:00 pm: Q&A discussion panel on 1D NMR spectroscopy: Two Resource Persons of Day 1

01:00 pm – 02:30 pm: Lunch break

Session 3: Hands-on-training

02:30 pm – 05:30 pm: Hands on training on sample preparation, 1D NMR experiments and analysis

05:30 pm – 06:00 pm: Tea

Day 2 (October 16, 2022, Sunday)

Session 1: Chair: Prof. Indresh Kumar, BITS Pilani, Pilani Campus

09:00 am – 10:30 am: Resource person's talk 1: Theory, concepts, and applications of 2D NMR spectroscopy in chemistry by Prof. N. Suryaprakash, Indian Institute of Science, Bangalore

10:30 am – 11:00 am: Tea break

11:00 am – 12:30 pm: Resource person's talk 2: Theory, concepts, and applications of NMR spectroscopy in biophysics by Prof. P. K. Madhu, Tata Institute of Fundamental Research, Mumbai

Session 2: Moderator: Prof. Paritosh Shukla, BITS Pilani, Pilani Campus

12:30 pm – 01:00 pm: Q&A discussion panel on 2D NMR techniques: Two Resource Persons of Day 2

01:00 pm – 02:30 pm: Lunch break

Session 3: Hands-on-training

02:30 pm – 05:30 pm: Hands on training on sample preparation, 2D NMR experiments and analysis

05:30 pm – 06:00 pm: Tea

Day 3 (October 17, 2022, Monday)

Session 1: Chair: Prof. Madhushree Sarkar, BITS Pilani, Pilani Campus

09:00 am – 10:30 am: Resource person's talk 1: Theory, concepts, and applications of High-Performance Liquid Chromatography by Prof. Parasuraman Jaisankar, Indian Institute of Chemical Biology Kolkata

10:30 am – 11:00 am: Tea break

11:00 am – 12:30 pm: Resource person's talk 2: Theory, concepts, and applications of Gas Chromatography by Prof. R. Ravi Krishna, Indian Institute of Technology Madras

Session 2: Moderator: Dr. Partha Addy, BITS Pilani, Pilani Campus

12:30 pm – 01:00 pm: Q&A discussion panel on advancements and applications of chromatographic techniques: Two Resource Persons of Day 3

01:00 pm – 02:30 pm: Lunch break

Session 3: Hands-on-training

02:30 pm – 05:30 pm: Hands on training on sample preparation, chromatographic experiments, and analysis

05:30 pm – 06:00 pm: Tea

Day 4 (October 18, 2022, Tuesday)

Session 1: Chair: Prof. Ajay Kumar Sah, BITS Pilani, Pilani Campus

09:00 am – 10:30 am: Resource person's talk 1: Theory, concepts, and applications of mass spectrometry techniques that utilize spray method-based ion sources by Prof. SVK Kumar, Tata Institute of Fundamental Research Mumbai

10:30 am – 11:00 am: Tea break

11:00 am – 12:30 pm: Resource person's talk 2: Theory, concepts, and applications of mass spectrometry techniques that utilize gas phase method and desorption method-based ion sources by Prof. Soumen Kanti Manna, Saha Institute of Nuclear Physics, Kolkata

Session 2: Moderator: Prof. Prashant U. Manohar, BITS Pilani, Pilani Campus

12:30 pm – 01:00 pm: Q&A discussion panel on advancements and applications of mass spectrometric techniques: Two Resource Persons of Day 4

01:00 pm – 02:30 pm: Lunch break

Session 3: Hands-on-training

02:30 pm – 05:30 pm: Hands on training on sample preparation, mass spectrometric experiments and analysis

05:30 pm – 06:00 pm: Tea

Day 5 (October 19, 2022, Wednesday)

Session 1: Chair: Prof. Bharti Khungar, BITS Pilani, Pilani Campus

09:00 am – 10:30 am: Resource person's talk 1: Theory, concepts, and applications of steady-state absorption and fluorescence spectroscopy by Prof. Anindya Datta, Indian Institute of Technology Bombay

10:30 am – 11:00 am: Tea break

11:00 am – 12:30 pm: Resource person's talk 2: Theory, concepts, and applications of time-resolved fluorescence spectroscopy by Prof. Sobhan Sen, Jawaharlal Nehru University

Session 2: Moderator: Prof. Inamur R. Laskar, BITS Pilani, Pilani Campus

12:30 pm – 01:00 pm: Q&A discussion panel on ultraviolet-visible (UV) and fluorescence techniques and applications: Two Resource Persons of Day 5

01:00 pm – 02:30 pm: Lunch break

Session 3: Hands-on-training

02:30 pm – 05:30 pm: Hands on training on sample preparation, UV and fluorescence experiments, and analysis

05:30 pm – 06:00 pm: Tea

Day 6 (October 20, 2022, Thursday)

Session 1: Chair: Prof. Ram K. Roy, BITS Pilani, Pilani Campus

09:30 am – 11:00 am: Resource person's talk 1: Theory, concepts, and applications of infrared (IR) spectroscopy by Dr. B. M. Krishna Mariserla, Indian Institute of Technology Jodhpur.

11:00 am – 11:30 am: Tea break

11:30 am – 01:00 pm: Resource person's talk: Theory, concepts, and applications of Raman spectroscopy by Prof. Jyotishman Dasgupta, Tata Institute of Fundamental Research, Mumbai

Session 2: Moderator: Prof. Shamik Chakraborty, BITS Pilani, Pilani Campus

01:00 pm – 01:30 pm: Q&A discussion panel on advancements and applications of IR and Raman techniques. Two Resource Persons of Day 6

01:30 pm – 02:30 pm: Lunch break

Session 3: Hands-on-training

02:30 pm – 05:30 pm: Hands on training on sample preparation, IR and Raman experiments, and analysis

05:30 pm – 06:00 pm: Tea

Day 7 (October 21, 2022, Friday)

Session 1: Chair: Prof. Anil Kumar, BITS Pilani, Pilani Campus

09:00 am – 10:30 am: Resource person's talk 1: Resource person's talk 1: Theory, concepts, and applications of transmission electron microscopy (TEM) by Dr. Ahin Roy, Indian Institute of Technology Kharagpur

10:30 am – 10:50 am: Tea break

10:50 am – 12:20 pm: Resource person's talk 2: Resource person's talk: Theory, concepts, and applications of scanning electron microscopy (SEM) by Dr. Indranath Chakraborty, Indian Institute of Technology Kharagpur

Session 2: Moderator: Prof. Surojit Pande, BITS Pilani, Pilani Campus

12:20 pm – 12:50 pm: Q&A discussion panel on advancements and applications of SEM and TEM: Two Resource Persons of Day 7

12:50 pm – 02:00 pm: Lunch break

Session 3: Hands-on-training

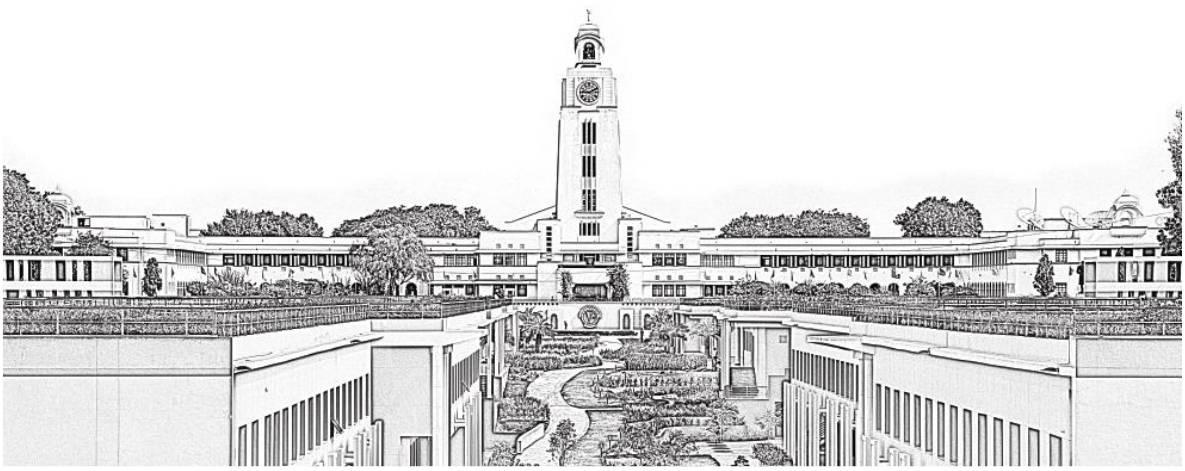
02:00 pm – 04:45 pm: Hands on training on sample preparation, SEM experiments, and analysis

04:45 pm – 05:00 pm: Feed back

Session 4: Valedictory function

05:00 pm – 05:10 pm: Address by the Dean of Administration, BITS Pilani, Pilani Campus: Prof. S. K. Verma

05:10 pm – 05:30 pm: High Tea



Hands-on-training experiments

Day 1: 1D-Nuclear Magnetic Resonance (NMR) Spectroscopy

Day 2: 2D-Nuclear Magnetic Resonance (NMR) Spectroscopy

Objectives

The objective of this experiment is to get hands-on experience in using NMR techniques and analyze the 1D and 2D spectra of organic compounds.

Upon completing this experiment, you should:

- know the basic components of NMR instruments
- understand the mechanism of action

About NMR instrument

The heart of the NMR magnet system is a superconducting magnet located inside the helium vessel (**Fig. 1**), which is filled with liquid helium. The helium vessel is surrounded by a nitrogen vessel filled with liquid nitrogen. The outer casing, the room temperature (RT) vessel.

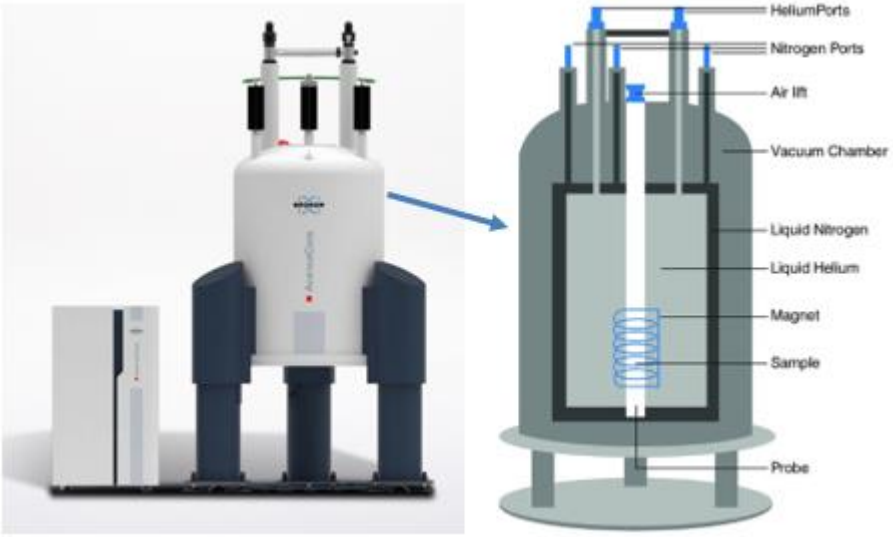


Fig. 1 A representative image of an NMR instrument.

Steps to follow prepare an NMR sample are provided below.

1. Find a clean, dry NMR tube.
2. Choose an appropriate NMR solvent (deuterated solvent) in which your compound is completely soluble.
3. Dissolve the compound (10-12 mgs) with 0.5 ml of selected NMR solvent.
4. Put the solution into the NMR tube by filtering with a cotton pad to avoid solid particles.
5. Acquire your spectrum.

Day 3: High-Performance Liquid Chromatography (HPLC)

Objective

The objective of this experiment is to get hands-on experience in using HPLC techniques and analyze a mixture of organic compounds with quantitation therein.

Upon completing this experiment, you should:

- know the basic components of the HPLC instrument
- understand the mechanism of action and its variables that affect separation
- understand the basic methods of calibration of this chromatographic analysis
- know how to analyze HPLC chromatograms of organic molecules

About HPLC

High-performance liquid chromatography is one of the most powerful tools in analytical chemistry. It can separate, identify, and quantitate the compounds that are present in any sample that can be dissolved in a liquid. Today, compounds in trace concentrations as low as parts per trillion [ppt] may easily be identified. HPLC can be and has been, applied to just about any sample, such as pharmaceuticals, food, nutraceuticals, cosmetics, environmental matrices, forensic samples, and industrial chemicals. HPLC is basically a highly improved form of column chromatography. Instead of a liquid being allowed to drip through a column under gravity, it is forced through under high pressures of up to 400 atmospheres that makes it much faster. It also allows us to use very small-sized particles having a much greater surface area for significant interactions between the stationary phase and the molecules flowing past it. This allows a much better separation of the components of the mixture. The major improvement over column chromatography is the use of appropriate detection methods which are extremely sensitive and automated nowadays thus making HPLC a highly reliable and efficient analytical tool.

HPLC Separation Modes

In general, three primary characteristics of chemical compounds can be used to create HPLC separations. They are: 1. Polarity, 2 Electrical Charge, 3 Molecular Size.

Types of HPLC

Component	Reverse Phase	Normal Phase
Definition	Reverse phase HPLC is a chromatographic technique in which we use a hydrophobic stationary phase	Reverse phase HPLC is a chromatographic technique in which we use a hydrophilic stationary phase
Stationary Phase	Nonpolar (silica modified with hydrophobic long chains)	Polar (mainly pure silica)
Mobile phase	Polar	Nonpolar
Components in the mobile phase	An aqueous blend of water with a miscible, polar organic solvent, such as acetonitrile or methanol.	Organic solvents such as hexane, ethyl acetate, etc.
Column	Column difficult to damage	Column easy to damage
Analytes	Carries polar analytes at the beginning and can be eluted by decreasing the polarity of the mobile phase.	Carries non-polar analytes at the beginning and can be eluted by increasing the polarity of the mobile phase.
Retention time	Higher reproducibility of retention time	Higher reproducibility of retention time
Uses	Approximately 70% because of its broad applicability, and reproducibility.	Not that much in use

The HPLC instrument (**Fig. 2**) is constituted of several components as discussed below.

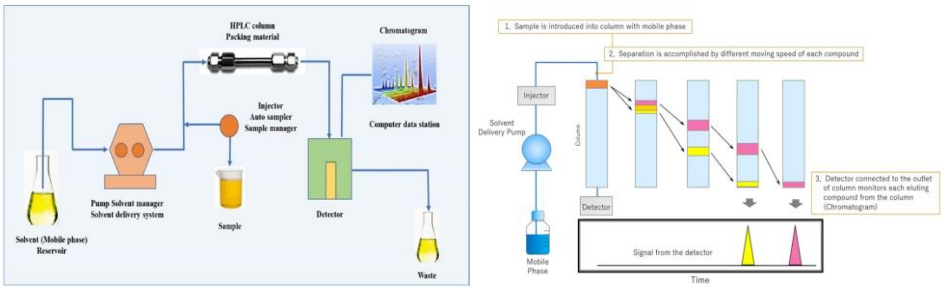


Fig. 2 Basic design of an HPLC instrument.

1. **Pump -** The pump is positioned in the upper stream of the liquid chromatography system and generates a flow of eluent from the solvent reservoir into the system. High-pressure generation is a "standard" requirement of pumps besides which, it should also be able to provide a consistent pressure at any condition and a controllable and reproducible flow rate.
2. **Injector –** An injector is placed next to the pump. The simplest method is to use a syringe, and the sample is introduced to the flow of eluent. The most widely used injection method is based on sampling loops. The use of an autosampler (auto-injector) system is also widely used that allows repeated injections in a set scheduled time.
3. **Column –** The separation is performed inside the column. The recent columns (**Fig. 3**) are often prepared in a stainless-steel housing since stainless is tolerant toward a large variety of solvents.
4. **Detector –** Separation of analytes is performed inside the column, whereas a detector is used to observe the obtained separation. The composition of the eluent is consistent when no analyte is present. While the presence of an analyte changes the composition of the eluent. What the detector does is measure these differences. This difference is monitored as a form of an electronic signal. There are different types of detectors available.
5. **Recorder -** The change in eluent detected by a detector is in the form of an electronic signal, and thus it is still not visible to our eyes. So, a computer-based data processor (integrator) is required for data acquisition with features like peak-fitting, baseline correction, automatic concentration calculation, molecular weight determination, etc.
6. **Degasser –** The eluent used for analysis may contain gases such as oxygen that are non-visible to our eyes. When gas is present in the eluent, this is detected as noise and causes an unstable baseline. Degasser uses special polymer membrane tubing to remove gases.
7. **Column Heater –** The LC separation is often largely influenced by the column temperature. To obtain repeatable results, it is important to keep consistent temperature conditions.

Fig. 3 HPLC columns.

Experimental plan

Determination of the purity and quantity of a given compound (α-amino nitrile) in the given solution.

1. Prepare the standard solution of the pure compound (in 0.2 mmol, 0.4 mmol, 0.6 mmol, 0.8 mmol, 1 mmol in 10 mL solvent) in methanol.
2. Inject each sample in HPLC and plot a calibration curve.
3. Prepare an unknown sample by arbitrary mixing of standard samples and inject in HPLC.
4. Obtain the purity of the compound by observing its retention time and the concentration of the compound from the calibration curve.

Day 4: High-Resolution Mass Spectrometry (HRMS)

Objectives

The objective of this experiment is to get hands-on experience in using the HRMS instrument for the analysis of masses of organic compounds.

Upon completing this experiment, you should:

- know the basic components of HRMS instruments
- understand the mechanism of action of the instrument
- understand how to analyze HRMS data of the organic compound

About HRMS

High-resolution mass spectrometry (HRMS) uses mass spectrometers capable of high resolution, as well as high mass accuracy measurements than the conventional method (for example, in the conventional method both propane and ethanol show m/z of 44. But, in HRMS propane and ethanol show 44.0624 and 44. 0261 respectively). This instrument is capable of distinguishing compounds with the same nominal mass and determining elemental compositions through accurate mass analysis.

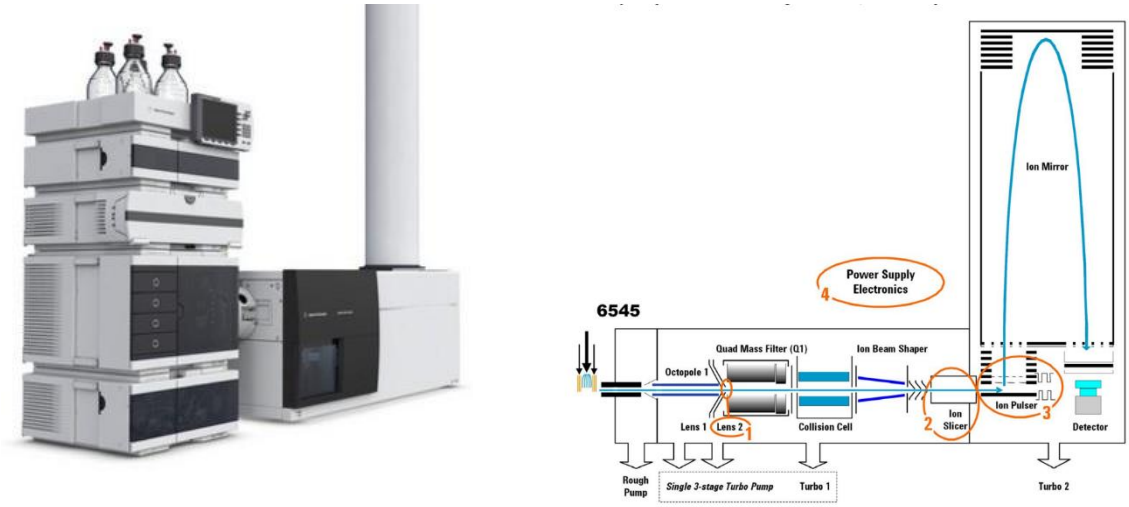


Fig. 4 A representative image of an HRMS instrument (left) and a schematic diagram of working principles of the instrument (right).

The HRMS instrument (**Fig. 4**) is constituted of several components as discussed below.

1. Ion source - A sample is ionized with either a positive charge or a negative charge

Methods of ionization

a. ESI (Electrospray ionization)- This technique used in mass spectrometry to produce ions using an electrospray in which a high voltage is applied to a liquid to create an aerosol. It is especially useful in producing ions from macromolecules because it overcomes the propensity of these molecules to fragment when ionized.
b. APCI (Atmospheric pressure chemical ionization)- This is a soft ionization method similar to chemical ionization where primary ions are produced on a solvent spray. The main usage of APCI is for polar and relatively less polar thermally stable compounds with a molecular weight of less than 1500 Da.

Modes in HRMS instrument are summarized below.

Positive Mode	Negative Mode
Positive ionization is the process that forms positively charged ions. $GH^+ + M \longrightarrow MH^+ + G$	Negative ionization is the process that forms negatively charged ions. $GH^- + M \longrightarrow MH^- + G.$

2. Mass analyzer - The mass analyser (**Fig. 5**) is the heart of the mass spectrometer, which takes ionized masses and separates them based on mass-to-charge ratios. There are several general types of mass analyzers, including magnetic sector, time of flight, quadrupole, and ion trap. The quadrupole consists of four parallel metal rods and each opposing rod pair is connected together electrically. One pair of raids is applied

with a radio frequency (RF) voltage while another one has applied with a direct current (DC) voltage. At a given DC and RF combination, only the ions of a particular m/z show a stable trajectory and can be transmitted to the detector, while other ions with unstable trajectories don't pass the road, because the amplitude of their oscillation becomes infinite. By changing DC and RF in time, usually at a fixed ratio, ions with different m/z values can be transmitted to the detector one after another.

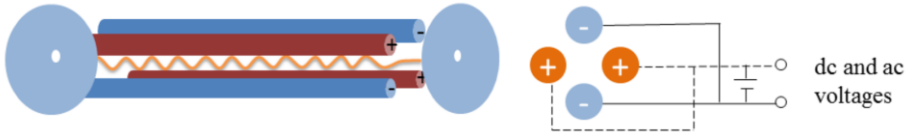


Fig. 5 A schematic diagram of the mass analyser of an HRMS instrument.

In Agilent 6545 Q-TOF mass spectrometer, the quadrupole mass analyzer and the hexapole collision cell are simply used as ion guides to transport ions. During HRMS/MS analysis, the quadrupole mass analyzer selects precursor ions that are fragmented in the hexapole collision cell into product ions, which are then impelled to the TOF mass analyser, at an angle perpendicular to the original path.

3. Detector - Located at the end of the flight path records the arrival time and the number of incoming ions. The square of the flight time is proportional to the m/z.

Experimental plan

1. Determine the mass of given compounds (pyridine carboxaldehyde and toluidine) and compare their masses.
2. Prepare the solution by dissolving 1-2 mg of the given organic compound in a minimum amount to a suitable solvent then dilute it to 1 mL using ACN. Further dilute 30 µL of the standard solution with 1 mL ACN and then repeat the process one more time.
3. Filter the resultant solution through a 0.22 µM syringe filter in a 2 ml glass vial.
4. Place the sample on an auto-sampler and record the mass of the sample.

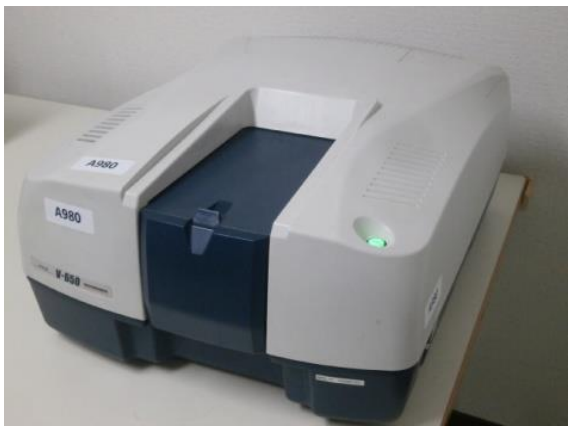
Day 5: Ultraviolet-Visible (UV-Vis) Spectroscopy

Objectives

The objective of this experiment is to get hands-on experience in using the UV-vis spectrophotometer for the analysis of absorption spectra of organic compounds.

Upon completing this experiment, you should:

- know the basic components of UV-vis spectrophotometer
- understand the mechanism of action of the instrument
- understand how to analyze UV-vis spectra of molecules



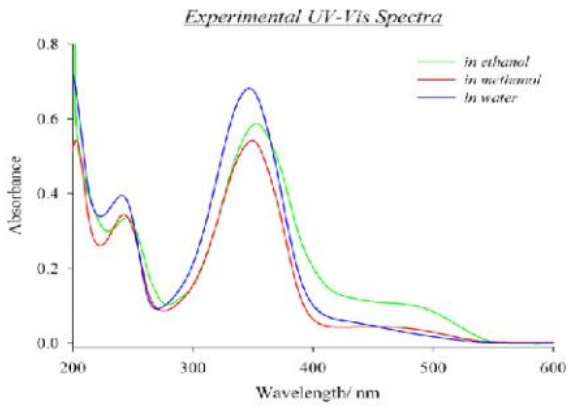


Fig. 6 A representative image of an UV-vis spectrophotometer (left) and representative examples of absorption spectra (right).

About UV-vis spectroscopy

UV-Visible spectroscopy is an analytical technique that measures the discrete wavelengths of UV or visible light absorbed by or transmitted through a sample compared to a reference or blank sample. This property is influenced by the sample composition, potentially providing information on what is in the sample and at what concentration. When matter absorbs ultraviolet radiation, the electrons present in it undergo excitation. This causes them to jump from a ground state (an energy state with a relatively small amount of energy associated with it) to an excited state (an energy state with a relatively large amount of energy associated with it). It is important to note that the difference in the energies of the ground state and the excited state of the electron is always equal to the amount of ultraviolet radiation or visible radiation absorbed by it.

Instrumentation

Jasco V-650 instrument will be used for training. It is a double-beam spectrophotometer with a photomultiplier tube detector. The high sensitivity of the photomultiplier tube detector enables accurate measurements of low-concentration samples. By controlling the high voltage applied to the PM tube, the dynode feedback circuit allows a wider dynamic range. Low stray light slit settings provide excellent linearity of up to 4 absorbance units. A schematic presentation of the instrument is depicted in **Fig. 7**. The light from the light source is focused and then it enters the monochromator. It is dispersed by the grating in the monochromator and focussed on the exit slit. The light that passes through the exit slit is monochromated. This light is split into two beams by a sector mirror, one going to the sample to be measured and the other to the reference samples such as solvent. The beams that pass through the sample and the reference are incidented on the detector.

Spectrophotometer Specifications

- **Light Source:** A Deuterium lamp with a wavelength range from 187-350 nm for use in the UV region and a Halogen lamp with a wavelength range from 330-2700 nm for use in the VIS/NIR region.
- **Optical System:** Consists of a single monochromator having 1200 lines/mm plane grating.
- **Sample Holders:** Quartz Cuvettes are used to hold the sample and reference.
- **Detector:** Photomultiplier tube detector

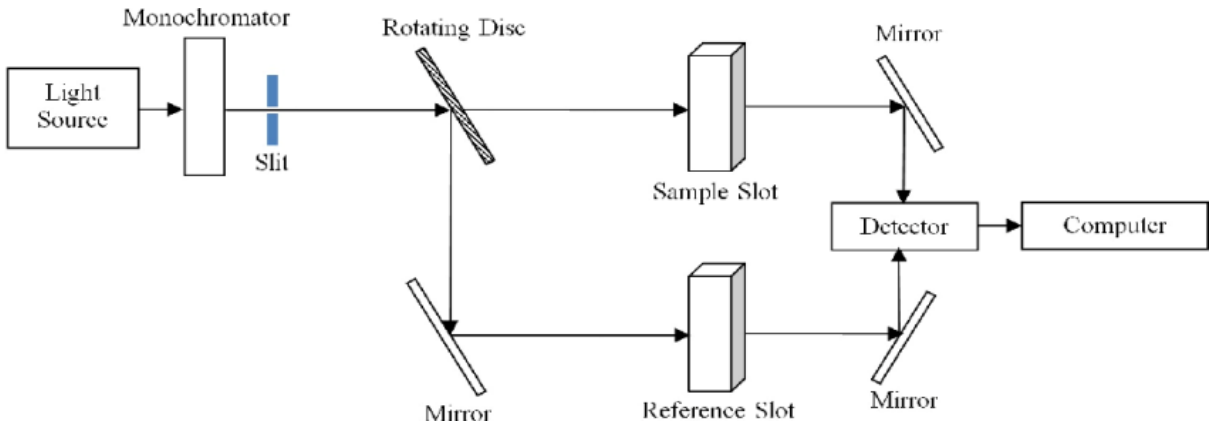


Fig. 7 A schematic representation of an UV-vis spectrophotometer.

Experimental plan

1. Prepare the solution of the sample (Rhodamine-B dye) in distilled water.
2. Do the baseline correction by taking the distilled water in both the cuvettes (in reference and the sample cuvette).
3. Then, record the spectra of the sample by taking its solution in the sample cuvette (reference cuvette with distilled water).

Day 5: Steady-State Fluorescence Spectroscopy

Objectives

The objective of this experiment is to get hands-on experience in using the fluorometer for the analysis of fluorescence spectra of organic compounds.

Upon completing this experiment, you should:

- know the basic components of fluorometer
- understand the mechanism of action of the instrument
- understand how to analyze fluorescence spectra of molecules

About fluorescence spectroscopy

Fluorescence, a type of luminescence, occurs in gas, liquid, or solid chemical systems. Fluorescence is brought about by absorption of photons in the singlet ground state promoted to a singlet excited state. The spin of the electron is still paired with the ground state electron, unlike phosphorescence. As the excited molecule returns to ground state, it involves the emission of a photon of lower energy, which corresponds to a longer wavelength, than the absorbed photon. **Fig. 8** is a schematic of a typical filter fluorometer that uses a source beam for fluorescence excitation and a pair of photomultiplier tubes as transducers. The source beam is split near the source into a reference beam and a sample beam. The reference beam is attenuated by the aperture disk so that its intensity is roughly the same as the fluorescence intensity. Both beams pass through the primary filter, with the reference beam being reflected to the reference photomultiplier tube. The sample beam is focused on the sample by a pair of lenses and causes fluorescence emission. The emitted radiation passes through a second filter and then is focused on the sample photomultiplier tube. The electrical outputs from the two transducers are then processed by an analog to digital converter to compute the ratio of the sample to reference intensities, which can then be used for qualitative and quantitative analysis. To obtain an emission spectrum, the excitation monochromator is fixed, and the emission monochromator varies. To obtain an excitation spectrum, the excitation monochromator varies while the emission monochromator is fixed.

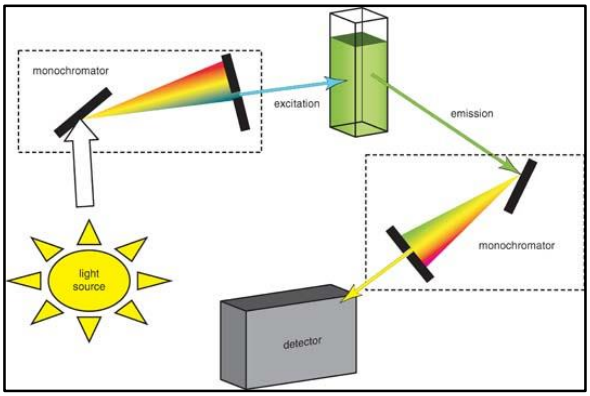


Fig. 8 A schematic representation of an UV-vis spectrophotometer.

Experimental Plan

Reagents:

[1] 1000 mL 0.1 N sulfuric acid solution

0.1 N sulfuric acid to be prepared from concentrated sulfuric acid (98%). Show calculations. Use distilled water for the solution.

[2] Quinine sulfate solution

Stock solution A: Weigh 10 mg of quinine sulfate powder and transfer to a 100 mL standard flask. Add about 50 mL of 0.1 N sulfuric acid and shake well to dissolve. Make up the volume to 100 mL with 0.1 N sulfuric acid, mix well. Dilute this solution whenever is required depending on the experiment.
Stock solution B: Pipette out 10 mL of the above solution to another 100 mL standard flask and dilute to 100 mL with 0.1 N sulfuric acid. This is 10 ppm solution of quinine solution.
Stock solution C: From the above, take 10 mL and dilute to 100 mL (with 0.1 N sulfuric acid) in another standard flask. This is 1 ppm solution.

Experiment

1. Record absorption spectrum of Stock solution A. Use proper reference solution. Determine $\lambda_{max,abs}$ from the absorption spectrum.
2. Record fluorescence emission spectra of the prepared solutions [Test tube no. 1, 2, 3, ...] by exciting at $\lambda_{max,abs}$.
3. Record fluorescence emission spectra of one of the solutions used in step 2 by exciting at wavelengths ±10 nm of $\lambda_{max,abs}$ (at least four such emission spectra).
4. Record the fluorescence spectra of quinine sulfate solution in presence of quencher, acrylamide.

Day 5: Time-Correlated Single-Photon Counting (TCSPC)

Objectives

The objective of this experiment is to get hands-on experience in using the TCSPC instrument for the analysis of time-resolved fluorescence properties of fluorescent molecules.

Upon completing this experiment, you should:

- know the basic components of TCSPC instrument
- understand the mechanism of action of the instrument
- understand how to collect fluorescence lifetime data of fluorescent molecules

About TCSPC

Time-correlated single-photon counting (TCSPC) is a well-established and common technique for fluorescence lifetime measurements, it is also becoming increasingly important for photon migration measurements, optical time domain reflectometry measurements and time of flight measurements. The principle of TCSPC is somewhat unique (**Fig. 9**). The sample is excited with a pulse of light, which is the waveform that would be observed when many fluorophores are excited and numerous photons are observed. However, for TCSPC the conditions are adjusted so that less than one photon is detected per laser pulse. In fact, the detection rate is typically 1 photon per 100 excitation pulses. The time is measured between the excitation pulse and the observed photon and stored in a histogram. The *x*-axis is the time difference and the *y*-axis the number of photons detected for this time difference. When much less than 1 photon is detected per excitation pulse, the histogram represents the waveform of the decay. If the count rate is higher the histogram is biased to shorter times. This is because with TCSPC only the first photon can be observed. At present the electronics are not fast enough to measure multiple photons per pulse when the lifetimes are in the nanosecond range. Multiple photons per pulse can be measured for decay times near a microsecond or longer. Specialized electronics are used for measuring the time delay between the excitation and emission. The experiment starts with the excitation pulse that excites the samples and sends a signal to the electronics. This signal is passed through a constant function discriminator (CFD), which accurately measures the arrival time of the pulse. This signal is passed to a time-to-amplitude converter (TAC), which generates a voltage ramp that is a voltage that increases linearly with time on the nanosecond timescale. A second channel detects the pulse from the single detected photon. The arrival time of the signal is accurately determined using a CFD, which sends a signal to stop the voltage ramp. The TAC now contains a voltage proportional to the time delay (Δt) between the excitation and emission signals. As needed the voltage is amplified by a programmable gain amplifier (PGA) and converted to a numerical value by the analog-to-digital converter (ADC). To minimize false readings the signal is restricted to given range of voltages. If the signal is not within this range the event is suppressed by a window discriminator (WD). The voltage is converted to a digital

value that is stored as a single event with the measured time delay. A histogram of the decay is measured by repeating this process numerous times with a pulsed-light source.

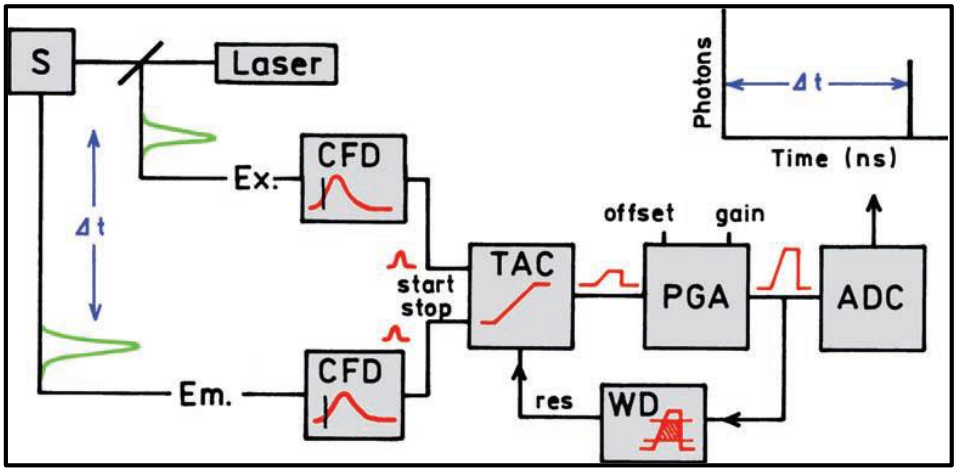


Fig. 9 A schematic representation of a TCSPC instrument.

Experimental Plan

Reagents

[1] PyTr solution Preparation.

Stock solution: Prepare 10^{-3} M solution of compounds. Weigh 3.5 mg of PyTr (M. Wt. 350) powder and transfer to a 10 mL standard flask. Add 10 ml of tetrahydrofuran (THF) and shake well to dissolve. Dilute this solution whenever is required depending on the experiment.

Experiment

1. Record absorption spectrum of Stock solution A. Use proper reference solution. Determine $\lambda_{max\ abs}$ from the absorption spectrum.
2. Record fluorescence emission spectra of the prepared solutions and determine the $\lambda_{max\ em}$.
3. Using absorption and emission value maxima, suitable excitation source, Record the fluorescence lifetime of the sample by taking the reference of Ludox as a IRF sample.

Day 6: Fourier-transform Infrared (FTIR) Spectroscopy

Objectives

The objective of this experiment is to get hands-on experience in FT-IR spectrometer for the analysis of infrared frequencies of molecules.

Upon completing this experiment, you should:

- know the basic components of IR spectrometer
- understand the mechanism of action of the instrument
- understand how to collect IR data of molecules

About FT-IR spectroscopy

Fourier transform infrared spectroscopy (FTIR) is a broadly used technique to identify the functional groups in the materials (gas, liquid, and solid) using the beam of infrared radiation. Infrared spectroscopy measures the absorption of IR radiation made by each bond in the molecule and, as a result, gives a

spectrum that is commonly designated as % transmittance versus wavenumber (cm^{-1}). A diverse range of materials containing the covalent bond absorbs electromagnetic radiation in the IR region. The IR region is at lower energy and higher wavelength than the UV-visible light and has higher energy or shorter wavelength than microwave radiations. For the determination of functional groups in a molecule, it must be IR active. An IR active molecule is one that has a dipole moment. When the IR radiation interacts with the covalent bond of the materials having an electric dipole, the molecule absorbs energy, and the bond starts oscillating back and forth. Therefore, the oscillation which caused the change in the net dipole moment of the molecule should absorb IR radiations.

Fig. 10 A representative image of an FT-IR spectrometer (left) and a representative example of IR spectrum (right).

Fourier Transform InfraRed (FTIR) spectrophotometer measures an infrared spectrum by Fourier-transform of an interferogram. The typical FTIR spectrometer consists of an IR light source, interferometer, sample compartment, detector, amplifier, and computer (**Fig. 11**).

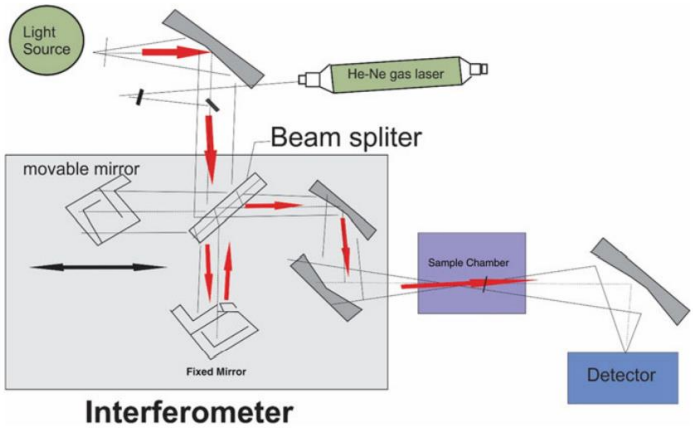


Fig. 11 A schematic representation of a FT-IR spectrometer.

Background Scan

A single-beam spectrum obtained without a sample is called a background spectrum, which is the characteristic of the instrument and the measuring environment. In this spectrum, the characteristic bands around 3500 cm^{-1} and 1630 cm^{-1} are attributed to atmospheric water vapor, and the bands at 2350 cm^{-1} and 667 cm^{-1} are ascribed to atmospheric carbon dioxide. Therefore, the background spectrum must always be run when analysing a sample by FTIR.

Three methods are available for solid samples

1. KBr pellet method
2. Nujol mull method
3. Compound dissolved in a solvent method

Other modes of IR measurement

ATR-FTIR

The ATR (Attenuated Total Reflection) units are designed as horizontal crystals with fastening usefulness, guaranteeing good contact between the sample and solids. In the case of liquid or viscous material, a small drop of the sample is sufficient for its measurement. Crystal constituents are mostly made up of zinc selenide (ZnSe), diamond, and germanium.

For liquid and "soft" sample analysis, ZnSe is appropriate because it is an inexpensive material; however, scratches are made on ZnSe and can only be used between pH 5 and pH 9. For the study of highly absorbing-colored samples such as rubbers and carbon black, germanium material is the choice due to its high refractive index. Similarly, for high-surface sensitivity, like thin layers, Ge is perfect because of its low penetration depth. Diamond is chemically inert and an ideal substance for manufacturing crystal surface materials. Although making the crystal material from diamond is quite expensive, however, the reliability of the instrument due to the high resistance of diamond to cut and scrap and its complete insolubility make diamond an ideal material for ATR-FTIR crystal formation. The stepwise procedure for an ATR is as follows: (i) clean the crystal (e.g., with cellulose tissue and isopropanol); (ii) then measure the instrument background within the ATR unit; and (iii) after that, place the sample on the crystal confirming the good contact, record the sample, and save the document.

Experiment plan

1. The pellet will be prepared by grinding the sample (Zeolite) with dried KBr and then applying pressure using a hydraulic press.
2. Background spectra will be recorded using a bare KBr pellet.
3. Compound mixed KBr pellet will be used to record the spectra, followed by the analysis of the spectra.
4. By the ATR method, we can directly record the spectra of the sample (Zeolite).

Day 6: Raman Spectroscopy

Objectives

The objective of this experiment is to get hands-on experience in Raman spectrometer for the analysis of Raman signals of molecules.

Upon completing this experiment, you should:

- know the basic components of Raman instrument
- understand the mechanism of action of the instrument
- understand how to collect Raman data of molecules

About Raman spectroscopy

Raman spectroscopy belongs to the category of vibrational spectroscopy. This means that it analyses a sample chemically by using light to create (excite) molecular vibration and interpreting this interaction afterward. It is based on the inelastic scattering of light that occurs when the matter is irradiated by light. As the change of wavelength is very small compared to the wavelength of the irradiating light, the change of wavelength is most easily observed when using monochromatic light sources. After this (monochromatic) light has interacted with the sample, a very small part of it has changed its wavelength. This change is called: the Raman effect. We can now collect that light and can use it to gain information about the sample. A representative image of a Raman spectrometer is shown below (**Fig. 12**).

Fig. 12 A representative image of a Raman spectrometer.

The Raman effect

For a better understanding it is important to know that when photons (light) "strike" matter, most of the scattered light remains unchanged in its wavelength. For example, if you point a green laser pointer at a wall, you will always see a green dot. The scattered light obviously has the same color, and this phenomenon is called Rayleigh scattering. However, also inelastic scattering processes can occur, which then lead to the emission of light with a different wavelength. This usually happens in relation to molecular vibration. This scattering phenomenon, which was predicted by Adolf Smekal in 1923 and discovered by C.V. Raman in 1930, is called the Raman effect.

Using the Raman effect for spectroscopy

Discovering and understanding the Raman effect opened the door to a new kind of spectroscopy. However, Raman spectroscopy did not really take off until the discovery of the Laser since the use of monochromatic light plays an important role. Raman spectroscopy is based on the interaction of light with the chemical bonds of a substance. These yield detailed information about chemical structure, polymorphism, crystallinity, and molecular dynamics. Thus, the sample is irradiated with a laser, and some of the scattered light is analyzed with a spectrograph (dispersive or FT technology). In the end, we obtain a Raman spectrum that shows us characteristic signals or "bands" for the material under investigation. Raman is a universal sampling technique and therefore works for both inorganic and organic materials. However, since it is based on the rather weak Raman effect, other spectroscopic effects and certain material properties can critically interfere. In the case of sample fluorescence, the sample won't yield a nice Raman spectrum. However, a switch to near-infrared (NIR) lasers and FT-Raman technology is a viable solution. Another, more significant problem is strongly absorbing (e.g. black) samples, for example, carbon-filled polymers. To acquire Raman spectra, you just must focus the Laser on the sample you want to investigate. That sample, however, must not show fluorescence to the Laser used for excitation. If that is the case, the fluorescence will cover most of the Raman effect since it is so weak in comparison. After the laser light has irradiated the sample, the scattered light is passed through a filter (to get rid of any light from the excitation laser). Then it is directed onto a grating, which distributes the inelastic parts like a prism and according to wavelength. In the end these rays are directed to a CCD sensor which then outputs a spectrum depending on the intensity. Below are the Raman spectra of a dimethicone sample (blue) compared to a reference from a spectral library (**Fig. 13**). In the beginning, we mentioned that a Raman spectrum contains certain "bands" or signals. These are unique for certain functional groups and often also for substances. They provide information about the chemical composition of the substance but also about crystallinity, polymorphism, or changes in pressure and temperature. A Raman spectrum is a powerful tool for materials research, the development of new pharmaceuticals, and wherever chemical microanalyses down to the nanometer range are required. Raman can analyse samples down to 0.5 µm (500 nm).

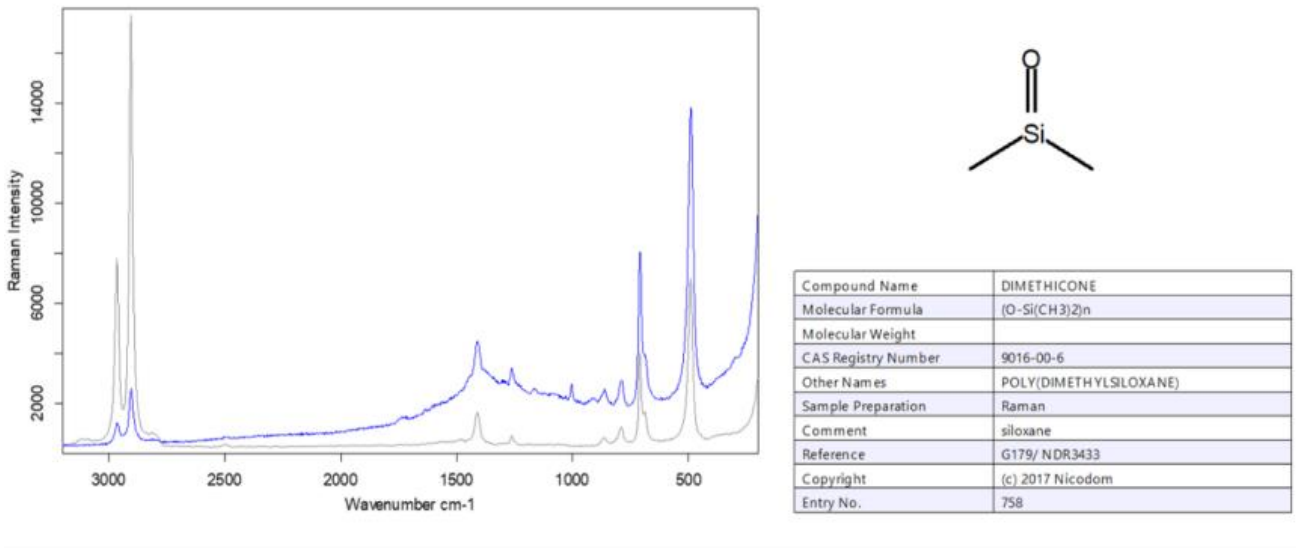


Fig. 13 A Raman spectrum of dimethicone sample.

Application

Raman spectroscopy can be used in all areas where non-destructive (microscopic) chemical analysis and imaging are required. It delivers answers to qualitative and quantitative analytical questions. In general, Raman is easy to use and quickly provides key information to characterize the chemical composition and structure of a sample. Basically, it matters little whether the samples are solid, liquid, or gaseous. Here are some applications of Raman spectroscopy:

- Pharmaceuticals
- Geology and mineralogy
- Semiconductors
- Material Research
- Life-science

Operating procedure

A. Calibration

1. Calibration standards are placed on top of the sample holder. There are three calibration standards: Polymer and Silicon Wafer. Only a Silicon wafer would be used for auto-calibration.
2. Load the slide of calibration standards onto the sample holder
3. Focusing: Use Joystick to find the edge of the Si wafer and fine-focus it by rotating Joystick. Turn coarse focus to minimize bright spot size. Bright Spot For planar translation of XY stage. For focusing. Rotate counter-clockwise to move the objective farther from the sample and vice versa. After finding the edge, rotate Joystick 1/8 counter-clockwise and change the objective to 50X. Find edge and fine focus it. (You may adjust the intensity of white light to change brightness and contrast.) After finding the edge, rotate Joystick 1/8 clockwise counter-clockwise again and change the objective to 100X. Find edge and fine focus it. (You may adjust the intensity of white light to change brightness and contrast.) Move away from the edge and find a position on the Si wafer to do the calibration.
4. After choosing the position for calibration, click the red 'Stop' icon to turn off the video camera (Note: At this time, the 'Stop' icon would turn grey, indicating no system activity exists, such as imaging, mapping, or scanning). The image you saw before clicking `Stop` would be captured and kept. You can save the frozen image by clicking on the 'Save File button.

B. Sample measurement

1. After calibration put your sample (Aspirin) on the slide (e.g., flat film of powder sample, selection loaded on silicon or other substrates)

2. Focusing: The focusing part can be done the same as done during calibration.
3. Acquisition Parameters: At the bottom of the LabSpec6 interface, you can choose grating (1800g/mm or 600g/mm), Laser (532nm or 633nm, Ensure the one you select is turned on.), and filter (vary from 0.01% to 100%. The number represents the amount of light transmitted. 100% means no filtering.) On the hand right-hand side of the LabSpec6 interface, you can choose the 'Acquisition' tab to manage acquisition settings.
4. After giving Title, choosing Laser, grating, and filter, and setting acquisition parameters such as spectral range, objective, acquisition time, and accumulation numbers, you can run the measurement.
5. File Management: To save or open files, click on the 'Save As' icon or the 'Open File' icon on the top of the software interface.
6. Shutting down:
   a. After saving your data, close all the files by clicking on the 'Cross' following file names under the 'Browser' tab.
   b. Close LabSpec6 software by clicking on the 'Cross' at the top left corner.
   c. Lift objectives and take away your samples.
   d. Clean the working area.

Day 7: Scanning-electron microscopy (SEM)

Objectives

The objective of this experiment is to get hands-on experience in SEM instrument for the analysis of SEM images of molecules.

Upon completing this experiment, you should:

- know the basic components of SEM instrument
- understand the mechanism of action of the instrument
- understand how to collect SEM data of samples

About SEM instrument

The Scanning electron microscopes (SEM) is a type of electron microscope which uses an electron beam to image samples with a resolution down to the nanometer scale. The SEM works on the principle of applying kinetic energy to produce signals on the interaction of the electrons. The electrons are emitted from a filament and collimated into a beam in the electron source. The beam is then focused on the sample surface by a set of lenses in the electron column. The interaction between electrons and matter result in production of various signals. When high energy electrons reach the sample, several electron and X-ray signals are generated. These are used to view crystallized elements and photons These include:

- Backscattered electrons (BSE)
- Secondary electrons (SE)
- Diffracted backscattered electrons

SE and BSE are used to produce an image. BSE come from deeper regions of the sample, while SE originate from the specimen and play the primary role of detecting the morphology and topography of the specimen. Therefore, BSE and SE carry different types of information. BSE images show high sensitivity to differences in atomic number: the higher the atomic number, the brighter the material appears in the image. SE imaging can provide more detailed surface information.

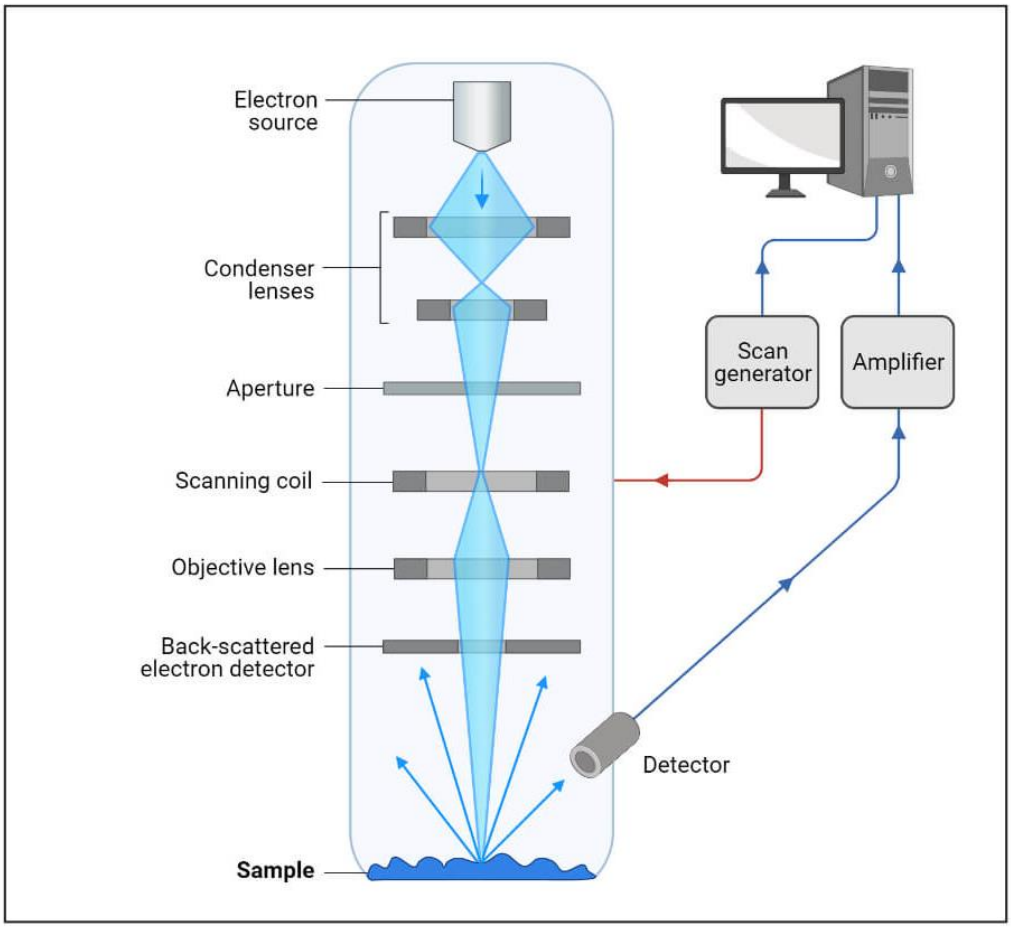


Fig. 14 A schematic representation of a FESEM instrument.

Parts of Scanning Electron Microscope

The major components of the Scanning Electron Microscope include (**Fig. 14**):

- Electron Source – This is where electrons are produced under thermal heat at a voltage of 1-40kV. The electrons condense into a beam that is used for the creation of an image and analysis. There are three types of electron sources that can be used *i.e.,* Tungsten filament, Lanthanum hexaboride, and Field emission gun (FEG)
- Lenses – It has several condenser lenses that focus the beam of electrons from the source through the column forming a narrow beam of electrons that form a spot called a spot size.
- Scanning Coil – they are used to deflect the beam over the specimen surface.
- Detector – It's made up of several detectors that can differentiate the secondary electrons, backscattered electrons, and diffracted backscattered electrons. The functioning of the detectors highly depends on the voltage speed, the density of the specimen.
- The display device (data output devices)
- Power supply
- Vacuum system

Coating of the samples:

It is commonly necessary to coat the sample with a thin layer of gold or gold-palladium alloy to prevent charging of the surface, to promote the emission of secondary electrons so that the specimen conducts evenly, and to provide a homogeneous surface for analysis and imaging.

Applications of SEM

It is used in a variety of fields including industrial uses, nanoscience studies, biomedical studies, microbiology

- Used for spot chemical analysis in energy-Dispersive X-ray Spectroscopy.
- Used in the analysis of cosmetic components which are very tiny in size.
- Used to study the filament structures of microorganisms.
- Used to study the topography of elements used in industries.

Advantages of the SEM

- They are easy to operate and have user-friendly interfaces.
- They are used in a variety of industrial applications to analyse surfaces of solid objects.
- Some modern SEMs can generate digital data that can be portable.
- It is easy to acquire data from the SEM, within a short period of time of about 5 minutes.

Experimental plan

1. Sample (Cadmium Indium Sulfide - $CdIn_2S_4$) will be coated with conducting metal using a sputter coater.
2. Sample (Cadmium Indium Sulfide - $CdIn_2S_4$) will be loaded into the instrument.
3. Imagining of the following sample will be done.

Photo Gallery

Inaugural ceremony: Director, BITS Pilani, Pilani Campus; Head of the Department of Chemistry, BITS Pilani, Pilani Campus; Convenor, co-convenor, and participants are lighting the lamp during the inaugural function.

- Director, BITS Pilani, Pilani Campus and the Head of the Department of Chemistry, BITS Pilani, Pilani Campus are providing inaugural speech.
- A group photo in presence of the participants.
- Class room teaching
- Resource person felicitation

- Resource persons' felicitations

- Resource persons' felicitations

- Hands-on-training

- Hands-on-training

- Hands-on-training
- Valedictory function
- Distribution of certificates to participants
- High tea

List of participants

No.	Name	Email ID	Designation	Affiliation
1	Kesar Singh	kesarsingh84@gmail.com	Research scholar	Dr. Harisingh Gour Central University, Sagar, Madhya Pradesh
2	Lokesh Kumar Tripathi	lokeshtripathi16@gmail.com	Research scholar	Kumaun University, Nainital
3	Paramjit Singh	singhparam10@gmail.com	Research scholar	Jamia Millia Islamia, New Delhi
4	Rajendra Patel	rajendrapatel2187@gmail.com	Research scholar	Central University of Gujarat
5	Jitendra kumar	jitendrakumar_2k20phdac05@dtu.ac.in	Research scholar	Delhi Technological University
6	Pushpender	Pushpenderlamba0799@gmail.com	Research scholar	Guru Jambheshwar University of Science and Technology, Hisar
7	Sheel Ratna	sheelratna222@gmail.com	Research scholar	Babasaheb Bhimrao Ambedkar University, Lucknow
8	Gaman Kumar	gamankumar977@gmail.com	Research scholar	Central University of Haryana
9	Sahil	sahilphy0407@gmail.com	Research scholar	University of Petroleum and energy studies, Dehradun
10	Azam Raza	araza@myamu.ac.in	Research scholar	Aligarh Muslim University, Aligarh, U.P.
11	Jagdish Chandra Jat	jatjagdish45@gmail.com	Research scholar	Sangam University, Bhilwara
12	Abhishek Singh Yadav	2020phdbt001@curaj.ac.in	Research scholar	Central University of Rajasthan
13	Dr. Ranveer Singh	chemdrranveersingh2015@gmail.com	Assistant Professor	MLB Govt.College, Nokha (Bikaner) Rajasthan

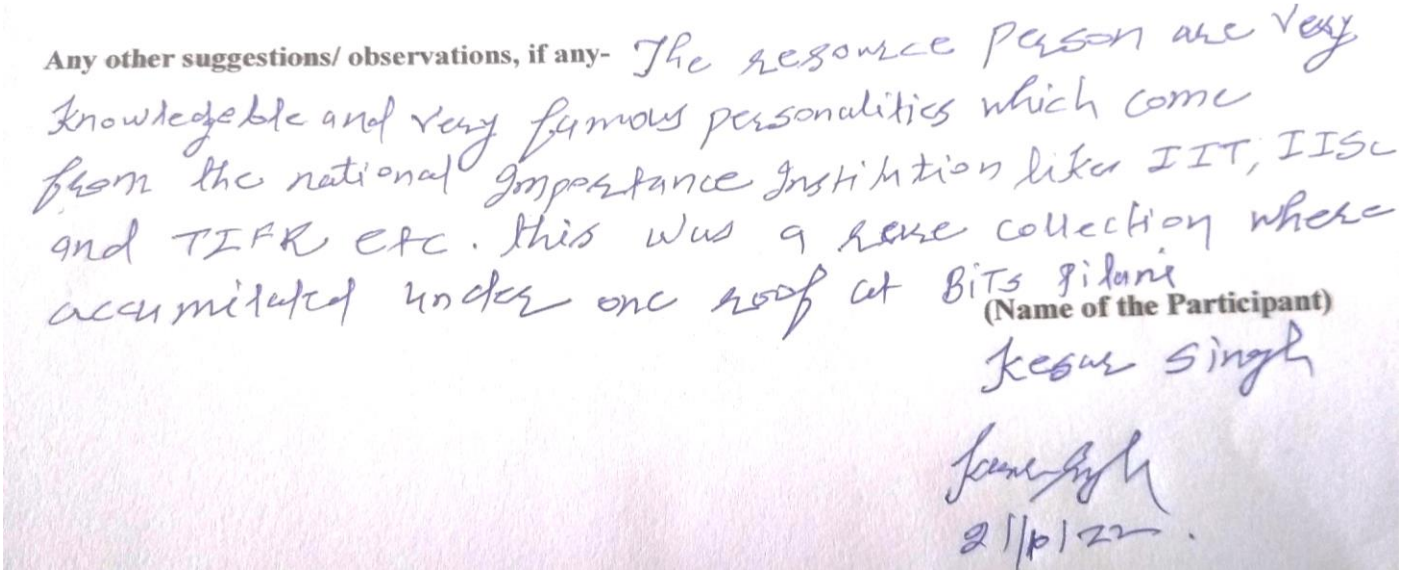
14	SHUMAILA MASOOD	shumailamasood0@gmail.com	Research scholar	Jamia Millia Islamia, New Delhi,India
15	Rajnee Yadav	yadav.rajnee307@gmail.com	Research scholar	Amity University Haryana
16	Nupur Sinha	nupur.sinha.22pd@bmu.edu.in	Research scholar	BML Munjal University, NH 48, Kapriwas, Gurugram-122413
17	Shailja Pandey	shailja.06040890020@ipu.ac.in	Research scholar	Guru Gobind Singh Indraprastha University, New Delhi
18	Isha Gupta	ishikagupta443@gmail.com	Research scholar	Maharshi Dayanand University, Rohtak
19	Suman Mahala	sumammahala2018@gmail.com	Research scholar	Central University of Rajasthan
20	Sakshi	sakshisonidops@gmail.com	Research scholar	Dr. Harisingh Gour University, Sagar, M.P.
21	Kanchan Guru	kanchanguru21@gmail.com	Research scholar	Manipal University Jaipur, Jaipur
22	Babita kumari	babitakumari2389@gmail.com	Research scholar	Maharaja ganga singh university, bikaner
23	Neha Abbasi	nehaabbasi@gmail.com	Research scholar	Jamia Millia Islamia, New Delhi,India
24	Manu	manu_2k20phdac01@dtu.ac.in	Research scholar	Delhi Technological University
25	Abhiruchi yadav	abhiruchi27a@gmail.com	Research scholar	Central University of Haryana
26	Meenakshi Tanwar	minaxi8787@gmail.com	Research scholar	Delhi Technological University
27	Ram Prasad	p20190430@pilani.bits-pilani.ac.in	Research scholar	BITS Pilani, Pilani Campus
28	Shivani	p20190446@pilani.bits-pilani.ac.in	Research scholar	BITS Pilani, Pilani Campus

29	Annu	p20200436@pilani.bits-pilani.ac.in	Research scholar	BITS Pilani, Pilani Campus
30*	Manisha	p20200015@pilani.bits-pilani.ac.in	Research scholar	BITS Pilani, Pilani Campus

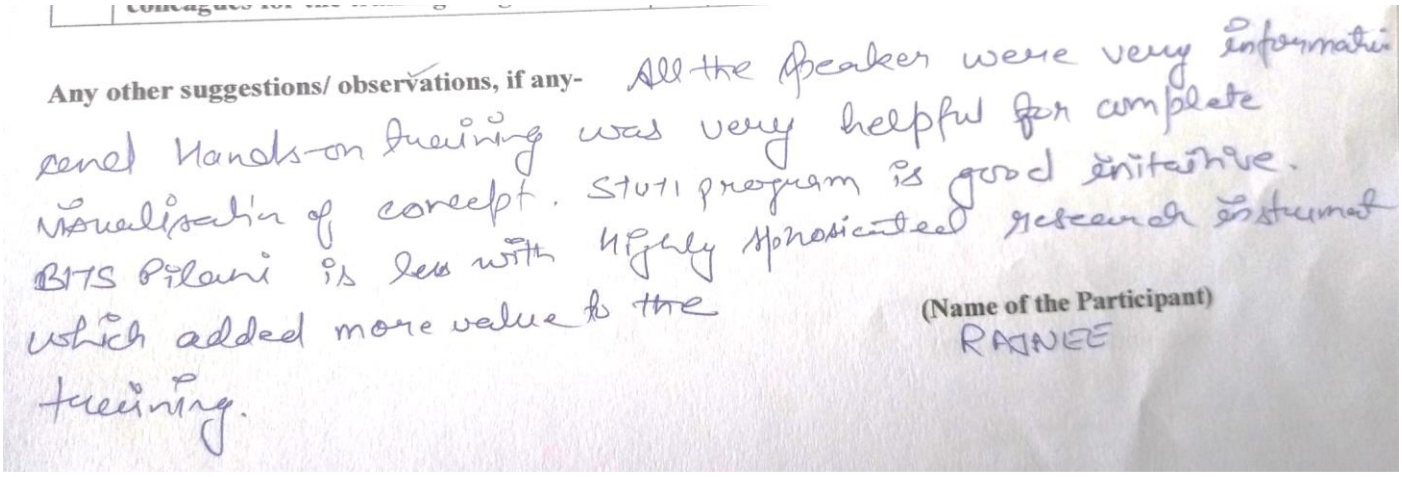
*One additional internal candidate due to the absence of an external candidate

Participants' Feedback

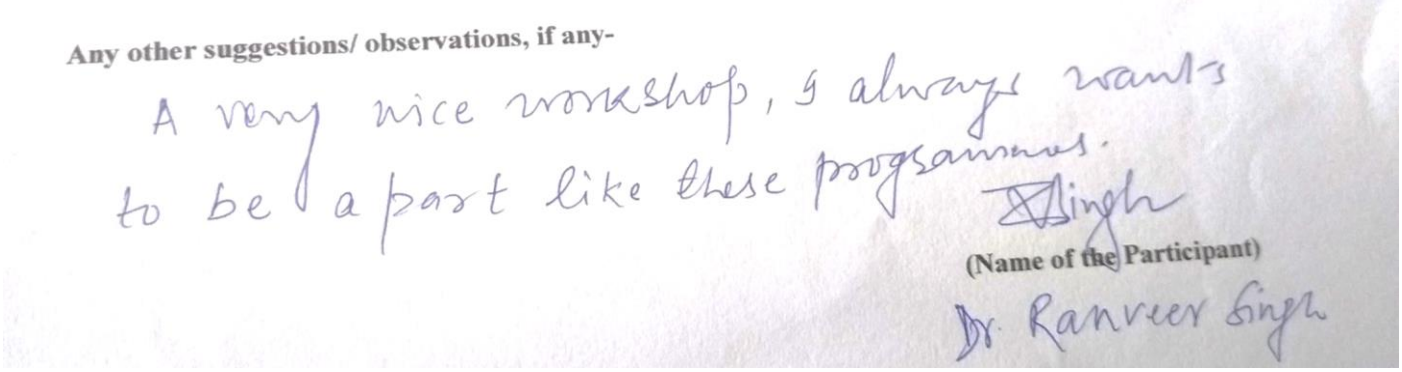
We received extremely positive and encouraging feedback from all the participants. The depth of the resource talks and the quality of the hands-on-training have been greatly appreciated. We provide below snapshots of few feedbacks.


Any other suggestions/ observations, if any- The resource person are very knowledgable and very famous personalities which come from the national importance institution like IIT, IISc and TIFR etc. this was a rare collection where accumilated under one roof at BITS Pilani

(Name of the Participant)
Kesar Singh
21/12/22.

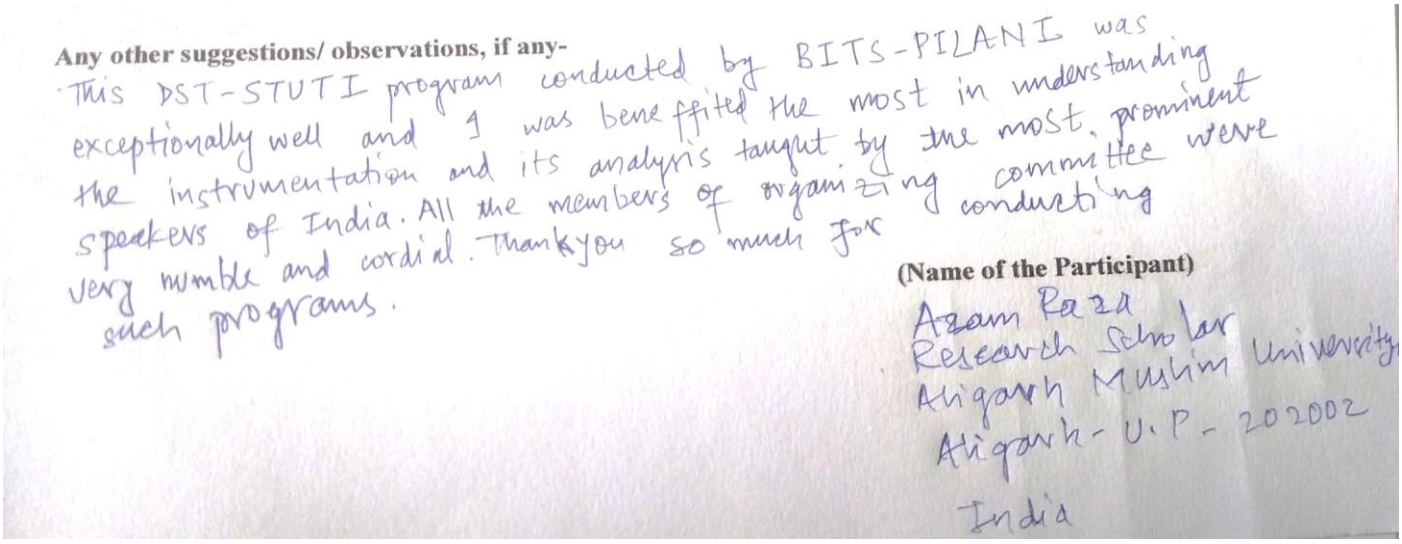

Any other suggestions/ observations, if any- All the speaker were very informati
eand Hands-on training was very helpful for complete
visualisation of concept. Stuti program is good initiative.
BITS Pilani is lea with highly sophisticated research instrumat
which added more value to the
training.

(Name of the Participant)
RANJEE


Any other suggestions/ observations, if any-

A very nice workshop, I always wants to be a part like these programmes.

(Name of the Participant)
Dr. Ranveer Singh



Any other suggestions/ observations, if any-
This DST-STUTI program conducted by BITS-PILANI was exceptionally well and I was benefitted the most in understanding the instrumentation and its analysis taught by the most prominent speakers of India. All the members of organizing committee were very humble and cordial. Thankyou so much for conducting such programs.

(Name of the Participant)
Azam Raza
Research Scholar
Aligarh Muslim University
Aligarh - U.P - 202002
India

Acknowledgements

We are grateful to the DST, New Delhi and SAIF, Panjab University, Chandigarh for giving us the opportunity to host the one-week long hands-on-training program. We thank all the participants, all resource persons, all volunteers, all organizing committee members, advisory board members, all students, staffs, and faculty colleagues of our Department of Chemistry, BITS Pilani, Pilani Campus. Our sincere thanks are due to our leadership team for their constant encouragement and support. The program would not have been successful without the enormous help and support from our estate management unit, reprography unit, instrumentation unit, guest house, cafeteria, and travel departments. We sincerely thank all of them.

Department of CHEMISTRY

Established: 1944

UGC DRS-SAP & DST-FIST Sponsored

An Overview

BITS Pilani
Pilani Campus

Contact us

Head, Department of Chemistry,
Birla Institute of Technology and Science Pilani
Pilani Campus, Rajasthan, 333031, INDIA
Phone: (01596) 255629/ 255279
Web: http://www.bits-pilani.ac.in/pilani/pilaniChemistry/Home

BITS Pilani
Pilani Campus

50 years of igniting young minds

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About us

One of the oldest & ever-evolving department having a vision to excel in teaching & research. Active research in the frontier areas of both fundamental and applied chemistry has been appreciated nationally & globally over past decades. The department continues to grow and attain new paradigms in chemistry education in the country.

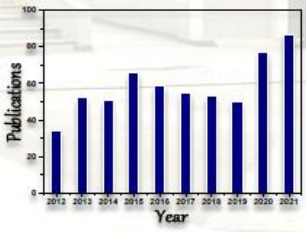
Faculty Members	21
Ramanujan Fellow	1
DST Women scientist	1
Ph.D. Scholars	65
M.Sc (Hons.) Students- per year (4 Yr. Integrated M. Sc Program)	72
Government Sponsored Projects (last 5 years)	29 (893.9 Lacs)
Industry Sponsored Projects	2 (54.8 Lacs)
Publications (last 5 years)	252
H index	54
Average Citations/year	2000
Average Impact Factor	3.53

MSc Chemistry program

Student-Faculty Ratio ~ 17
Placement 97%

PhD Program:

Number of PhD Students registered: 65



Thrust areas of research

1. Green Chemistry and Catalysis
2. Organic and Medicinal Chemistry
3. Synthetic Chemistry & Materials Science
4. Theoretical and Computational Chemistry
5. Photochemistry and Gas Phase Spectroscopy

Courses Offered

- General Chemistry
- Chemistry Laboratory
- Physical Chemistry I, II, III, IV
- Organic Chemistry I, II, III, IV
- Inorganic Chemistry I, II, III
- Colloid and Surface Chemistry
- Instrumental Methods of Analysis
- Chemical Experimentation I, II
- Biophysical Chemistry
- Numerical Methods in Chemistry
- Polymer Chemistry
- Electrochemistry
- Supramolecular Chemistry
- Magnetic Resonance
- Organic Chemistry & Drug Design
- Nanochemistry
- Green Chemistry and Catalysis
- Photochemistry and Laser

Spectroscopy

- Electron Correlation in Atoms & Molecules
- Frontiers in Organic Chemistry
- Biochemical Sensors
- Statistical Thermodynamics
- Chemistry of Life Processes
- Heterocyclic Chemistry
- Bioinorganic Chemistry
- Solid State Chemistry
- Electronic Structure Theory
- Chemical Applications of Group Theory
- Atmospheric Chemistry
- Sustainable Chemistry using renewables
- Introduction to Computational Chemistry Lab

Instrumentation Facilities

- FT-NMR (400 MHz)
- FT-IR
- Fluorimeter
- HPLC
- UV-Vis
- CHI Potentiostat
- GC, GC-MS, LC-MS
- Polarimetry
- TR fluorescence
- Microwave CEM Discover
- DSC
- HRMS (DST FIST)
- TCSPC system (DST FIST)
- Ball Mill
- Belsorp Mini II
- High Performance Computation

Library: Online access of ACS, RSC, Wiley-VCH, Elsevier, Taylor & Francis etc. journals.

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