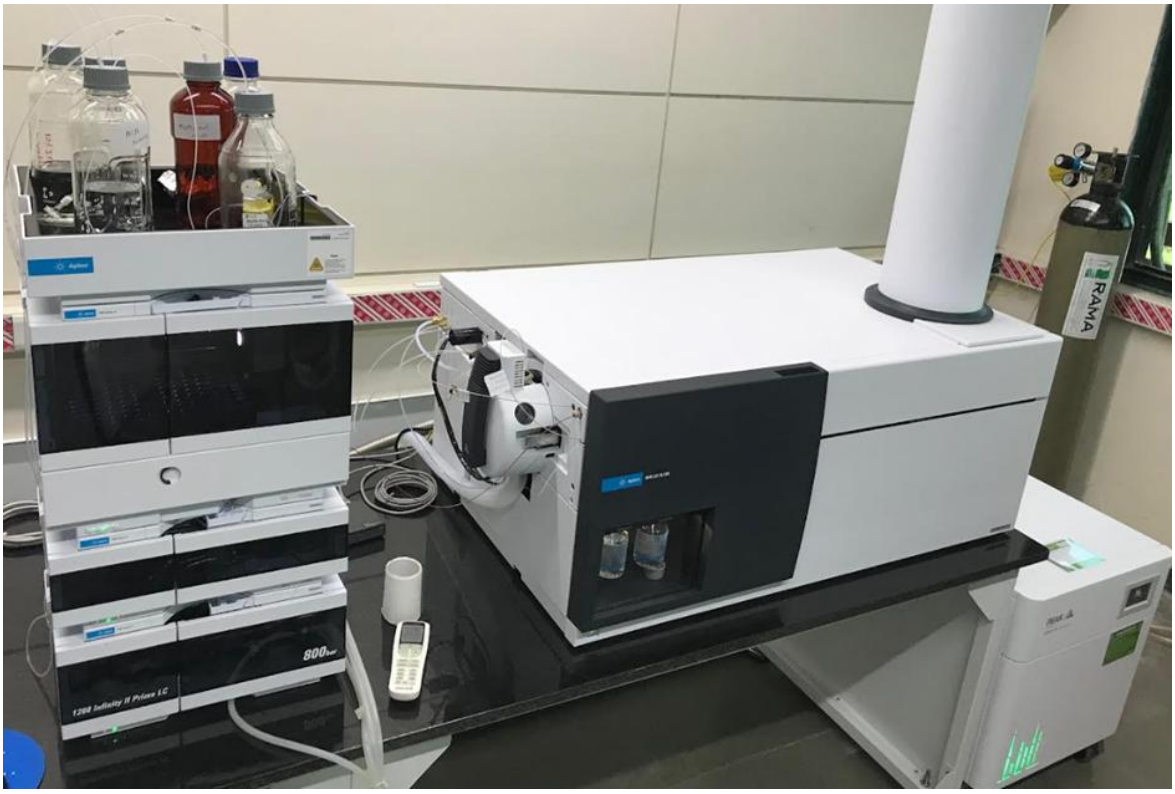
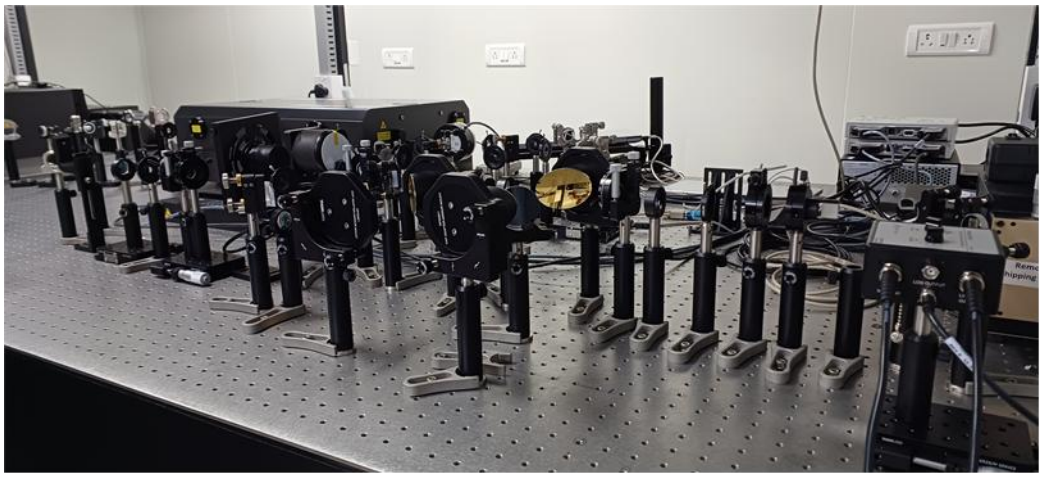
High-performance computing (HPC): A state-of-art centralized high-performance computing (HPC) facility is recently developed in CEBS to support the parallel computation need of the institute. This hybrid CPU/GPU facility has 16 CPU nodes with each node housing 32 processors and one GPU node. The actual computational power for the facility is approximately 30 Terra Flops for both CPU and GPU nodes.

Mass Spectrometer: An Agilent 6545 LC/Q-TOF mass spectrometer is the latest addition from the DPR project, procured in 2023. The machine is in a dedicated room adjacent to the undergraduate laboratory. This mass spectrometer (picture below) is a state-of-the-art quadrupole time-of-flight (Q-TOF) mass spectrometer that performs both high resolution mass spectrometry (HRMS) and high-resolution tandem mass spectrometry (HRMS/MS). It is useful in drug discovery, basic/comparative proteomics and metabolomics research, mass precision for intact protein analysis and identification of structure and sizes of small organic compounds.



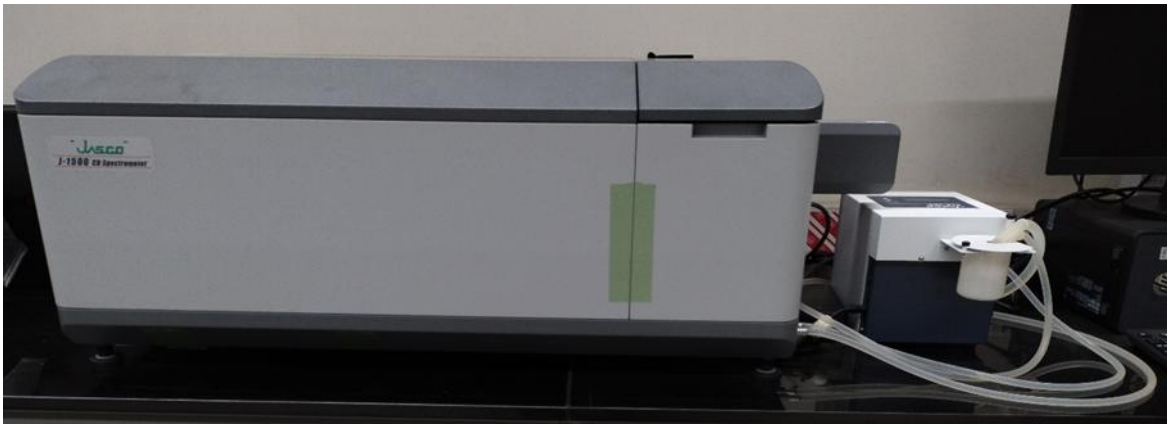
Setting up facilities for ultrafast laser Spectroscopy: Installation of two ultrafast laser spectrometers, namely, the fluoresecence upconversion spectrometer and the tunable pump (350 – 600 nm) and tunable (370 – 1000 nm) probe transient absorption spectrometer has been completed. These spectrometers are now fully operational and capable of recording the transient spectra and photophysical dynamics with time resolution of about 100 fs. Optical set

up of the ultrafast terahertz spectrometer has been completed, software for data acquisition has been procured and installed. The spectrometer is now under testing of its performance.



THz spectrometer

Circular Dichroism: Circular dichroism (CD) is a potent spectroscopic technique that uses the quantum mechanics of how chiral molecules selectively exhibit the differential absorption of circularly polarized light to reveal information about secondary and tertiary structures of proteins and nucleic acids such as DNA and RNA, their interactions and the resulting dynamic alterations. CD is used in the pharmaceutical industry to assess the purity and stability of chiral drug compounds, ensuring they meet regulatory requirements. Overall, CD spectroscopy is a versatile technique with applications in structural biology, chemistry, pharmacology, and material science, providing valuable insights into the chiral properties and structural characteristics of a wide range of molecules.



Circular Dichroism (CD) spectropolarimeter

Differential Scanning Calorimetry: Differential scanning calorimetry (DSC) is a thermal analysis tool that directly investigates the heat energy absorbed or released by a sample as it experiences controlled temperature fluctuations and provides thermodynamic parameters associated with it. DSC measures thermodynamic parameters such as ΔH, T_m and ΔC_p for biomolecules. DSC provides information about thermal stability of proteins, nucleic acids, carbohydrates and lipids. DSC has also applications in various pharmaceutical industry for assessment of drugs.

Differential Scanning Calorimeter (DSC)

Nuclear Magnetic Resonance (NMR): Nuclear magnetic resonance (NMR) spectroscopy is a spectroscopic technique to observe local magnetic fields around atomic nuclei. NMR spectrometer of 400 MHz (Bruker, Switerzand) is recently installed successfully in School of Chemical Sciences, CEBS. A Multinuclear resonance probe with variable temperature for 0 °C to 100 °C. Automatic and manual tuning and matching for many nuclei including ^{1}H,^{13}C,^{15}N, ^{11}B, ^{19}F, ^{31}P, Se etc. is possible. Along with multi-nuclear 1D experiments it can perform other 1D experiments (DEPT 135p, DEPT 90, APT) and 2D (COSY, TOCSY, NOESY, HSQC, DOSY, ROESY) experiments. NMR facility is currently being used by many research groups of CEBS and University of Mumbai.

400 MHz NMR (left) and Single crystal XRD (right) installed in School of Chemical Sciences, CEBS

Single Crystal X-Ray Diffractometer: Single-crystal X-ray diffraction (XRD) is a non-destructive analytical technique which generates data from the X-ray analysis which then are interpreted and refined to obtain the crystal structure. X-ray diffractometer (Xta Lab PRO II, Rigaku), having Mo and Cu sources, is successfully installed in School of Chemical Sciences,

CEBS. Instrument is equipped with cryostat (CrysAlis^{PRO}) to get data at low temperature. Data obtained from this facility provides detailed information about the internal lattice of crystalline substances, including unit cell dimensions, bond-lengths, bond-angles etc. XRD facility can be used for different single crystals of organic, inorganic, organometallic nature. Further it can be used for protein samples. XRD facility is currently being used by many research groups of CEBS and University of Mumbai.

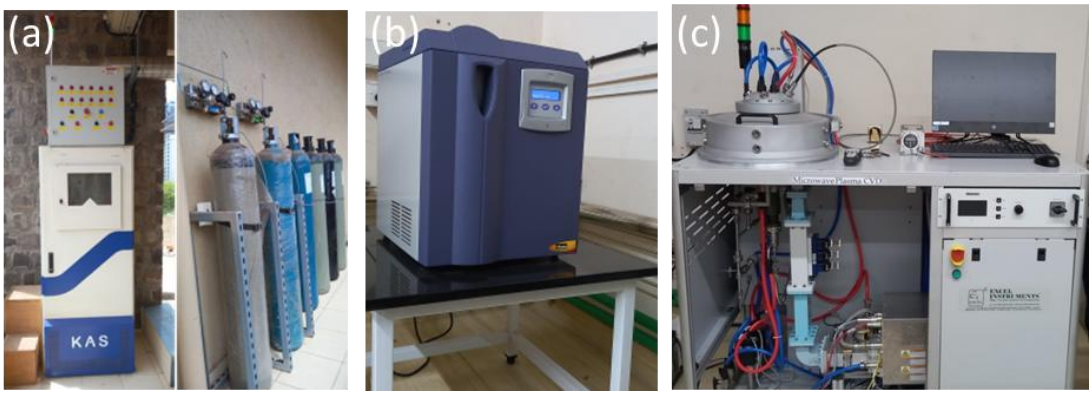
Benchtop X-Ray Diffractometer: Powder X-ray diffractometer (MiniFlex 600C, Rigaku) was installed successfully. This facility can be used to determine crystalline phase identification, quantification, percent (%) crystallinity, crystal size and strain, lattice parameter refinement and molecular structure. It can be used for powder and thin film samples sat room temperature.

Spectrofluoremeter: A highly sensitive spectrofluoremer (FLS 1000, Edinburgh, UK) is installed in School of Chemical Sciences. It can be used to measure both fluorescence and phosphorescence in solution as well as powder samples. Instrument has 450 W Xe lamp, 60 W flash lamp as excitation sources, InGaAs is used as NIR detector. Emission range is from 250 to 1550 nm. Emission studies at variable temperature (0-80 °C) and at 77K can be carried out. Also, instrument can be used to have phosphorescence lifetime beyond 50 µs. This instrument is being used by different research groups of CEBS.

Spectrofluoremeter for fluorescence and phosphorescence studies

Gas chramatograph, FTIR, UV vis spectrometers: School of Chemical Sciences also has facilities of gas chromatography (GC 2030, Shimadzu), FTIR (IR Tracer) and absorption spectrometer (2002 i, Shimadzu). FTIR can be used for samples in powder and liquid form without the requirement of KBr film. UV vis spectrometer can be used in a range of 190- 1500 nm for liquid as well as solid samples.

Microwave plasma chemical vapor deposition: A microwave plasma chemical vapor deposition (MPCVD) technique has been developed to synthesized single crystal diamond (SCD). The facility incorporating various equipments, such as, MPCVD, semiconductor grade gas line system and hydrogen generator is shown below.

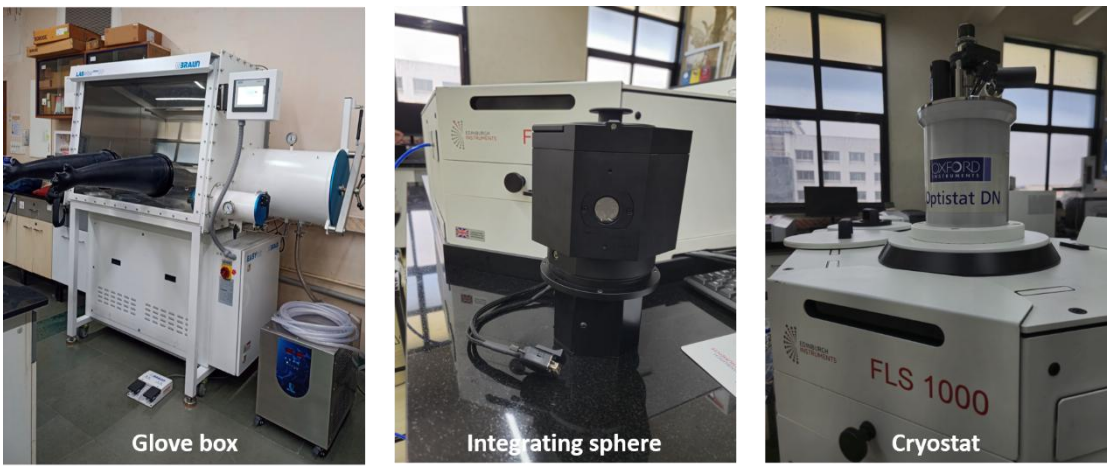


(a) Semiconductor grade (7N purity) gas line supply, (b) Hydrogen generator (5.5N purity) and (c) Microwave plasma chemical vapor deposition (2.45 GHz, 6kW). (Diamond growth facility at UM-DAE CEBS developed through DPR funding of DAE).

Glove box with two ports (MBRAUN make): The glove box of MBRAUN has been successfully installed. It can maintain the oxygen and moisture levels below 1 ppm, thus, providing inert atmosphere for oxygen, air and moisture sensitive reactions, photophysical and electrochemical measurements. We believe this will provide a platform to carry out the ultrasensitive, towards moisture and air, reactions and other experiments.

Cryostat for fluorescence spectrometer: We have installed the cryostat for the measurement of photophysical studies at variable temperature ranging from room temperature to 77K. This can be used with existing fluoremeter to study the temperature dependent steady state as well as excited state dynamics.

Integrating sphere: Integrating sphere (Edinburgh make) is coupled to highly sensitive spectrometer (FLS1000) allows to measure the emissive absolute quantum yield, optical absorption, of novel materials and devices.



Development of the sub-ps time resolved time-domain THz spectrometer has been completed and its performance has been tested.

A custom-fabricated optical window assembly has been installed on a hole in the wall of the clean-room housing the femtosecond laser for transmission of the laser pulse the to the adjoining standard-air laboratory. The femtosecond laser is now available for target experiments in standard-air conditions, in tandem with the beam from an earlier installed nanosecond laser system.