

INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH TIRUPATI (An Autonomous Institute of National Importance under Ministry of Education, Govt. of India) C/o. Sree Rama Engineering College, Rami Reddy Nagar, Karakambadi Road, Mangalam P.O., Tirupati – 517 507, Andhra Pradesh.

File No: IISERT/PUR/EOI/02/23 Expression of Interest (EOI) for Supply, Installation, and Commissioning of High field high resolution solid and liquid-state NMR spectrometer.

IISER Tirupati is the sixth Institute in the chain of IISERs established by the Govt. of India under the Ministry of Education for imparting quality education in basic sciences and for setting up state-of-the-art research facilities for frontline and cutting-edge research in science.

The permanent campus of IISER Tirupati is situated at Srinivasapuram and Panguru of Yerpedu Mandal. The establishment of IISER paves the way for a unique synergy of one premier educational institute in the country.

The Indian Institute of Science Education and Research Tirupati invites Expression of Interest (EOI) for the Supply, Installation, and Commissioning of High field high resolution solid and liquid-state NMR spectrometer at IISER Tirupati Main Campus.

An Online pre-indent conference is proposed to be held on 23-Nov-2023 with the prospective manufacturers, their authorized channel partners or agents/suppliers, and system integrators to discuss with the Technical Committee on the aspects of technology, design, specification, clientele, and other related issues for Supply, Installation, and Commissioning of High field high resolution solid and liquid-state NMR spectrometer



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Utility of 600 MHz NMR Spectrometer:

600 MHz Nuclear Magnetic Resonance (NMR) spectrometer is a powerful analytical tool widely used in the field of chemistry, biochemistry, and structural biology. The high magnetic field strength of 600 MHz provides several advantages, enhancing the utility of the spectrometer for various applications:

- 1. **Increased Sensitivity:** The higher magnetic field strength leads to greater sensitivity in NMR measurements. This increased sensitivity allows for the detection of signals from less abundant nuclei and facilitates the study of samples with lower concentrations.
- 2. **Improved Resolution:** The higher field strength contributes to enhanced spectral resolution. This is particularly valuable when dealing with complex samples, such as proteins or large organic molecules, where distinct signals may overlap at lower field strengths.
- 3. **Advanced Structural Analysis:** The improved resolution and sensitivity of a 600 MHz NMR spectrometer enable detailed structural analysis of organic compounds, small molecules, and biomolecules. This is crucial for understanding molecular conformations, interactions, and dynamics.
- 4. **Protein NMR Studies:** In structural biology, protein NMR studies benefit significantly from a 600 MHz instrument. The higher field strength allows researchers to obtain high- quality spectra of larger proteins, facilitating the determination of three-dimensional structures and the characterization of protein dynamics.
- 5. **Metabolomics and Small Molecule Studies:** In metabolomics research, where the goal is to identify and quantify metabolites in biological samples,



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a 600 MHz NMR spectrometer provides improved sensitivity and resolution. This aids in the precise analysis of complex mixtures and the identification of subtle chemical shifts.

Quantitative NMR Analysis: Higher field strengths enhance the accuracy of quantitative NMR analyses. Researchers can obtain more precise measurements of concentrations and study chemical reactions in real-time with improved reliability.

6. **Multi-Nuclear Capability:** A 600 MHz NMR spectrometer can accommodate the study of multiple nuclei, including commonly used nuclei like proton, carbon-13, nitrogen-15, and others. This versatility allows researchers to gain a comprehensive understanding of the molecular composition and dynamics of their samples.

In summary, a 600 MHz NMR spectrometer is a valuable instrument in scientific research, providing enhanced sensitivity, resolution, and versatility for a wide range of applications in chemistry, biochemistry, and structural biology. It empowers researchers to explore the intricacies of molecular structures, interactions, and dynamics with precision and efficiency.

The brief description and requirements for High field high resolution solid and liquid-state NMR spectrometer are provided below:

High field high resolution solid and liquid-state NMR spectrometer

1. Magnet System (standard bore)

Testa actively shielded super-conducting magnet with an operational frequency of 600 MHz for 'H nucleus in liquid-state NR with following specifications.



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- Shortest possible radial and axial distance for 5 Gauss stray field from the center of the magnet. Please specify overall Magnet dimensions and ceiling height requirements,
- Drift rate of Magnetic field less than 10 Hz/hour
- Liquid Helium hold time of at least 150 days or higher
- Please specify the total liquid Helium and N₂ hold volume, refill interval and refill volume.
- All support equipment for cryostat (e.g., Liquid Helium and liquid nitrogen transfer lines).
- Digital monitors for liquid Helium and liquid nitrogen levels.
- Anti-vibration legs (please specify the lowest frequency damped).
- Built-in cryo-shims and room temperature (ultra) shims; gradient shimming capability and its associated accessory (software/hardware)
- Pneumatic sample load / spin / eject system

2. Console

Three or more RF channels (specify the frequency range of operation) with best frequency and phase resolution; fast switching time for all parameter without hidden delays. Please specify the configuration and bandwidth of each channel. The console should include:

- Waveform generators for all channels for pulse shaping
- Amplitude, phase and composite pulse decoupling generator
- Pre-amplifiers and filters for noise reduction
- High-power linear amplifier broadband amplifier 400 W or better for 1H channel.
 400 W or better for ¹³C/¹⁵N and 100 W or better for 2H to provide the shortest possible pulse widths. Please specify all relevant parameters including power (wattage), frequency range, duty cycle, maximum pulse duration, etc.
- Frequency synthesizers for each channel



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- Digital quadrature detector for complete elimination of artefacts in the center of the spectrum.
- Transmitter controllers for each channel (event duration < 25 ns)
- Digital 2H lock channel consisting of a pre-amplifier. Lock system should have high

precision phase and field corrections (please provide documental evidence)

- ADC with high dynamic range and sampling rate. Please specify the resolution of the ADC (in bits) and the maximum sample rate
- Gradient unit with amplifier and accessories for pulse field gradient

3. Variable temperature unit having

- Broad temperature range capability (desired -150°C to 200°C)
- High resolution 1 accuracy / stability of temperature setting (at least ± 0.1°C)
- Accessories for running experiments in solid and liquid samples below ambient temperature

4. Probes

1. Multinuclear Z-gradient based broad band probe (5 mm) with automatic tuning and matching facility for observation of 1H nuclei with 19F decoupling or 19F observe with 1H decoupling and for observation of nuclei in the range of 31P to 15N or better. with 1H decoupling/observe. Best signal to noise (S/N) ratio values for each nuclei on standard test samples.

2. Triple resonance Indirect Probe (H-C-N) 5 mm Z gradient with automatic Tuning and matching facility

3. Probes should be equipped for variable temperature experiments -20 °C to +100 °C or better range with suitable attachment.

4. CP-MAS Probe for Solid sample analysis and its accessory (10 spinners and additional rotors and caps- 2 caps for every rotors)



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5. HR-MAS Probe for Semi-solid and soft matter analysis

6. Cryogenic Probe along with all its accessories:

5 mm triple resonance (1H/13C/15N) cryogenic probe with 2 H locking, Z shielded gradient and Auto -tuning capability. Please provide the following information: (i). Configuration of the coils, (ii). Nuclei whose RF coils/pre amplifiers are cryo -cooled (iii). Pulse widths for ¹H, ¹³C, ²H and ¹⁵N using standard samples. Please specify the sample used. (iv). Best resolution and line shape (under sample spinning and non-spinning conditions). Please specify the line -widths measured using the standard sample. (v). Best Signal -to -noise (S/N) ratio values for each nuclei of the probe measured using standard samples (Please provide data and mention the sample used). S/N should be measured using samples in regular 5 mm thin walled tubes. (vi). Salt tolerance. Please provide S/N and pulse width values of all nuclei at: (i) low (< 20 mM) and (ii) high (> 150 mM) salt concentrations. Please provide any accessory required for performing experiments with high salt containing samples. (vii). Maximum gradient strength (\geq 50 G/cm). (viii). Gradient recovery times (not more than 100 us). (ix). Decoupling pulse width, power, bandwidth, duty cycle capability on each RF channel. (x). Temperature range over which the probe can be used (desired 0 to -80 °C). (xi). Tuning accessory for auto -tuning capability (xii). Compatibility of the cryoprobe with 3 mm NMR tubes or its likes

4. Auto sampler

An automatic sample handling system with capacity of loading at least 60 samples along with 60 spinners.

5. Data storage/ software / peripherals comprising



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1. One high performance state-of-the-art workstation with tools/software/data cards for data acquisition, processing, plotting, structure verification, spectral simulation and multiple analyses of 1D and 2D (HSQC, TOCSY, COSY, HETCOR, NOESY, HMBC, DOSY, DQF COSY, J-resolve). One work station should be equipped with Linux/Windows based software for data collection and processing.

2. LCD monitor (27 inch), Laser printer.

3. NMR software for acquisition and processing including pulse sequence program.

4. All required documents, manuals, installation CDs/DVDs etc. for hardware and software.

5. Data processing software should be compatible with Windows operating system on any PC or Laptop.

6. Special software like molecular structure determination, Dynamic centre etc.

7. An additional work station for data storage

8. Unlimited multi-user licenses for the complete software package required for data processing.

6. Warranty

Five-year comprehensive on-site warranty on all items mentioned above from the date of complete and satisfactory installation of the spectrometer including;

- All parts and labor
- Free maintenance and service
- Regular upgrades to all software during warranty period
- The manufacturer has to take all responsibilities (including financial, insurance, etc.) for shipping and installation during this period.

In case, the machine is down for more than 1 week during the warranty period, number of days accordingly should be compensated by providing additional



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extended warranty free of cost.

7. Please quote the shortest possible delivery time of the complete system.

A delivery / installation time of less than twelve months from the time of placing the order is desirable.

8. Initial supply of cryogen for installation

The liquid helium required for installation should be provided by the NMR supplier. All responsibility / costs should be taken / covered by the manufacturer in case of quenching of magnet during installation, including all costs for re-charging, cryogenics, and if required complete replacement of magnet,

9. Consumables and Accessories:

- A compatible online UPS of necessary wattage, with one hour back up, three phase output for NMR electronics.
- A suitable oil-free air-compressor complete with dryer and proper ratings/specification capable of catering to all the needs.
- One set of reference standards should be provided for full operational qualification and instrument performance verification.
- All items for preventive maintenance kit should be provided by the engineer during installation.
- 1000 of 5 mm and 100 of 3 mm NMR tubes for 600 MHz spectrometer should be provided.
- Essential spare parts for magnet / spectrometer.
- One liquid N₂ Dewar's 200 L (or above) for refilling of cryogens in the magnet.
- One liquid He Dewar 200 L (or above) for refilling of cryogens in the magnet.



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At least 60 numbers of 5 mm spinners (regular temperature), 4 numbers of 5 mm spinners (low temperature), 4 numbers of 5 mm spinners (high temperature) and 10 numbers of 3 mm spinners.

10. Onsite training

Initial on-site training to the staff for 2-3 weeks or as long as required to do all possible representative experiments and for routine maintenance. This can include advanced training for setting up biological NMR experiments/special applications using software installed pulse sequences from the manufacturer.

11. General information:

1. The technical specifications should be quoted in the same manner as described in the technical specifications desired in the tender. A compliance report should be attached in this regard.

2. Vendor should provide a certificate that the spares will be provided in future for a period of ten years.

3. The vendor should provide the total number of installations of 600 MHz NMR instruments installed by the Vendor in India.



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Prospective manufacturers, their authorized channel partners or agents/suppliers, and system integrators are invited to attend a pre-indent meeting with the Technical Committee to discuss all the aspects of the High field high resolution solid and liquid-state NMR spectrometer including technology, design, features, specification, equipment, and clientele. They are also invited to make a presentation on their company portfolio and expertise, proposed specifications, and a list of accessories required for the as per NMR, the above-mentioned application and requirements of the Institute.

All prospective bidders are requested to kindly send their requests and profiles through email at <u>purchase@iisertirupati.ac.in</u> so as to reach the latest by 22nd Nov 2023.

Date and Time of the Online pre-indent conference:23rd Nov 2023 at 03:30

PM. The Pre-indent conference will be conducted via Google Meet/Any other virtual mode.

Contact for information:

Technical & Commercial contact:

Deputy Registrar (Admin & Purchase)

Indian Institute of Science Education and Research (IISER), Tirupati

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Note:

- **1.** This notice is applicable to those firms who have experience in the Supply, Installation, and Commissioning of High field high resolution solid and liquid-state NMR spectrometer for "Expression of their Interest" to participate in the preparation of specifications and thereafter in the bidding process.
- **2.** The Pre-indent conference will be conducted via Google Meet/Any other virtual mode. Kindly ensure you have an active broadband internet connection for the conference.