

Technical specifications (updated after pre-bid meeting): NMR (600 MHz) spectrometer

1. Magnet System (standard bore)

Latest technology based stable and actively shielded superconducting magnet (14.1 Tesla) with an operational frequency of 600 MHz for ^1H nucleus in liquid-state NMR, with following specifications:

- i. Shortest possible radial (0.7 m or less) and axial (1.4 m or better) distance for 5 Gauss stray field from the center of the magnet.
- ii. Drift rate of Magnetic field less than 6 Hz/hour
- iii. Liquid Helium hold time of 200 days or more
- iv. All support equipment for cryostat (e.g., Liquid Helium and liquid nitrogen transfer lines).
- v. Digital monitors for liquid Helium and liquid nitrogen levels.
- vi. Anti-vibration legs
- vii. Built-in cryo-shims and room temperature shims; gradient shimming capability and its associated accessory (software/hardware)
- viii. Pneumatic/automatic sample load / spin / eject system
- ix. All supporting equipment for cryogen filling such as Liquid He transfer line, liquid Nitrogen transfer line, etc.

2. Spectrometer console

The console should have deuterium (^2H) lock channel. Further, there should be two independent Radio Frequency channels with best frequency and phase resolution; fast switching time for all parameter without hidden delays.

The console should include:

- i. High-power linear amplifier broadband amplifier 100 W or better for ^1H channel; 500 W, or better, for X channel to provide the shortest possible pulse-widths. Please specify all relevant parameters including power (wattage), frequency range, duty cycle, maximum pulse duration, etc.
- ii. Digital deuterium ^2H lock channel consisting of a deuterium ^2H pre-amplifier. Lock system should have high precision phase and field corrections
- iii. Deuterium Lock channel should be compatible with gradients and automated shimming hardware. The system should be controlled by computer.
- iv. Waveform generators for all channels for pulse shaping
- v. Amplitude, phase and composite pulse decoupling generator
- vi. Pre-amplifiers and filters for noise reduction
- vii. Frequency synthesizers for each channel
- viii. Digital quadrature detector for complete elimination of artefacts in the center of the spectrum.
- ix. Gradient unit with amplifier and accessories for pulse field gradient
- x. Gradient unit for Auto shimming ($1\text{H}/2\text{H}$) to achieve good line shape of sample and to perform all-new gradient pulse program-based experiment with the capability to run DOSY and other gradient experiments having capacity of 50 G/cm, or higher.
- xi. Auto shimming feature for solution-state NMR.

Dr. M. J. ...
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27/08/2024

R. B. Anand
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J. S. ...
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- xii. The console should have all important and necessary components to achieve the NMR probe specifications
- xiii. The console cabinet should have the option, space and electronics for future upgradation to three or four channels

3. Probes:

- i. A state-of-the-art high-sensitive 5 mm broadband probe with the ability to observe ^1H , X, and ^{19}F , with autotune and match. It should have the ability to observe ^{19}F with ^1H decoupling and to perform two-dimensional $^1\text{H}/^{19}\text{F}$ spectroscopy. It should have broadband frequency channel enabling fully automated applications on protons and the widest range of X-nuclei. The probe should allow deuterium detection experiments using short ^2H 90-degree pulses, which is independent of the ^2H lock channel. Operating temperature range at $-100\text{ }^\circ\text{C}$ to $+150\text{ }^\circ\text{C}$ or even improved ranges. The ^1H observe sensitivity in signal to noise ratio should be 1000:1 or more and ^{13}C sensitivity should be 340:1 or more with the standard samples. The ^{19}F sensitivity should be 850:1 or more.
- ii. An additional 5 mm observe probe fitted with an actively shielded single axis Z-gradient, equipped with automatic tuning and matching. The inner NMR coil is tuned to observe ^{13}C . The outer NMR coil is tuned for ^1H decoupling or observation. The sensitivity for ^1H should be 400:1 or more, and ^{13}C should be 290 or more.

4. Auto sampler

An automatic sample handling system with capacity of loading at least 60 samples from front of the magnet at the user level. Equal number of spinners and additional 10 numbers. If variable temperature experiments require different spinners, 5 number of low temperature and 5 number of high temperature spinners should be additionally provided. The NMR data acquisition software should have control for the auto sampler

5. Variable temperature unit having

- i. Temperature range capability: Minus ($-$) $100\text{ }^\circ\text{C}$ to plus ($+$) $150\text{ }^\circ\text{C}$
- ii. High resolution / accuracy / stability of temperature setting (at least $\pm 0.1\text{ }^\circ\text{C}$)
- iii. Accessories for running experiments below ambient temperature

6. Data storage / software / peripherals comprising

- i. A state-of-the art latest model workstation with necessary processing power, memory, dedicated graphics card with complete pre-loaded software / data cards for data acquisition, processing and analyses with necessary perpetual licensed software, and peripherals including a (22-inch) LCD monitor, laser printer should be provided to control in the with the NMR spectrometer and perform the experiments.
- ii. A Network Access Storage (NAS) with a capacity of 60 TB or more data storage should be provided for data transfer and storage.
- iii. An additional workstation with monitor and laser printer should be provided with installed softwares.
- iv. Data processing software should be provided in unrestricted numbers with a perpetual license. The software must be user-friendly and capable of integrating peaks, performing multiplet analysis, deconvolution of 1D, 2D, and 3D spectra, analyzing relaxation and dynamics

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27/8/24
Dr. Myung
27/08/2024

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27/08/2024

RB Aneni
27/8/24
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data, and handling non-uniform sampling. It should include all additional software for diffusion and kinetics experiments. The software must also feature quantification tools, the ability to export data in various formats, and the latest updated processing features.

- v. Any software upgrade (pulse sequence and processing) or new software (pulse sequence and processing) that are released during warranty periods should be given to the user free of cost
- vi. All relevant hardware and software manuals, installation programs stored in CD / DVD / USB etc, along with license files.

7. Initial supply of cryogen for installation

The pre-installation and installation visits should be made by competent engineers at the site of installation at no extra cost to IICB. Vendors have to arrange for all the cryogenics of liquid nitrogen and liquid Helium and related accessories required for charging and installation of the magnet. In case of magnet-quench during the installation or at subsequent times due to any technical reason or failure, the supply (including transport) of the liquid Helium till the magnet is restored to normalcy is the responsibility of the vendor and the entire cost for cryogenics, recharging or replacing the magnet should be borne by the vendor at no additional cost to IICB.

The standard samples used to validate the successful installation should be delivered. The sealed NMR tubes containing the calibration samples should be provided. The vendor has to demonstrate the sensitivity of the quoted probes against the elements as mentioned in their technical brochure/data sheet.

8. Accessories and Consumables:

- i. A compatible online UPS (15 KVA or more), with one hour back up, for the entire NMR Spectrometer
- ii. One set of reference standards should be provided for full operational qualification and instrument performance verification.
- iii. All items for the preventive maintenance kit should be provided by the engineer during installation.
- iv. Essential spare parts for magnet/spectrometer should be provided
- v. Four liquid N₂ Dewars 48-55 L (or above), along with a trolley, for refilling of cryogenics in the magnet.
- vi. A compatible, low noise, 5 HP scroll type (oil, noise, and moisture free) air compressor compatible with the instrument with an additional (min of 90L) stainless-steel buffer tank and two Dryer (one refrigerated air dryer, auto-drain valve, and one active alumina-based pressure swing dryer with suitable connectors fittings and filters).

9. Warranty

Three years comprehensive warranty on all items mentioned above, from the date of complete and satisfactory installation of the spectrometer including:

- i. All parts of the entire instrument from the OEM, additional components including UPS (not considering batteries), air compressor, computer workstations, storage devices
- ii. Regular upgrades to all software during the warranty period

Dr. Myami
27/08/2024

EMR
27/08/2024

3421
27/08/2024

R Banerji
27/8/24
27-08-24

SSG Chakraborty
27-8-24
27/08/24

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Gupta
27/8/24

- iii. Liquid helium supply and refilling: the vender has to ensure that liquid helium is filled periodically during the warranty period for smooth functioning of the instrument to prevent any magnetic quenching and instrument breakdown.
- iv. During the last month of the three-year warranty period, liquid helium should be filled for 100%.
- v. If the instrument is not functional, the service engineer must visit within 48 hours upon.
- vi. In any case, if the machine is down for more than 15 continuous working days during the warranty period, number of days subsequently should be compensated by providing additional extended warranty free of cost.

10. Onsite training

After, successful installation, on-site training to the staff should be provided for 5 days or further required to do all possible representative experiments and for routine maintenance. Further, the vendor should provide a demonstration of all possible experiments that can be performed, data processing of 1D and 2D experiments for structure elucidation to be provided to the general users of IICB for an additional 3 days. Furthermore, an additional 5 days of training should be provided within one year whenever required. This can include advanced training for setting up advanced NMR experiments/special applications using software-installed pulse sequences from the manufacturer.

11. Others

- i. AMC charges for additional five years has to be mentioned. The AMC charges will not be used to determine lowest bidder, and the amount will not be part of the purchase order.
- ii. The OEM has to certify that spares and technical supports are available for 10 years or higher.

Dr. Myami
27/08/2024

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27/08/2024

BBaneyi
27/8/24

Dr. Goshu
27.8.24

EMR
27/08/2024

Dr.
27.08.24

Dr. Ghosh
27/08/24

Dr. Pal
27/8/24