

## **INDIAN INSTITUTE OF TECHNOLOGY BOMBAY**

## MATERIALS MANAGEMENT DIVISION Powai, Mumbai 400076.

Ref No.84 (PR.No 1000017908)

RFx No. 6100000761

## **Technical Specification for 400MHz NMR Spectrometer**

Item No. 1:	Supply, Installation and Commissioning of 400 MHz FT-NMR Spectrometer with Solid + Liquid Probe.	
S. No.		Details
1.1.	Spectrometer Frequency	400 MHz state of the art solid-state NMR spectrometer with two channels to carry out high-resolution Solid-state NMR experiments such as 1D, 2DNMR with various combination of selected nuclei, having capabilities for most up-to-date multidimensional NMR experiments
1.2.	Superconducting Magnet	<ul> <li>a. Latest technology based stable and actively shielded superconducting magnet</li> <li>b. Operating filed at 9.4 T (operating frequency of 400 MHz for ¹H)</li> <li>c. Shim coil – cryogen cool and room temperature</li> <li>d. Stray field at least 0.5 meters in radial and 1.0-meter n axial</li> <li>e. Helium hold time &gt;300 dayswith alarm function for low helium level</li> <li>f. Nitrogen level sensor</li> <li>g. Magnet stand with Air spring and damped isolator / Vibration-proof platform with vibration damping accessory for vertical damping</li> <li>h. All support equipment for cryogen filling the magnet such as Liquid He transfer line, liquid Nitrogen transfer line, etc.</li> <li>i. High-performance cryo and room temperature shim system for optical line shape.</li> <li>j. Special tool kit for magnet</li> </ul>

		k. An efficient shimming system to obtain excellent line
		shape in solid-state configuration.
1.3.	Console	<ul> <li>a. Two or more channel cabinet for future up-gradation</li> <li>b. Broadband frequency generation for all channels</li> <li>c. Communication between all channels by an</li> </ul>
		appropriate communication system  d. Multiple Digital receiverswith excellent capability and elimination for artifacts such as signal acquisition,
		filtering, sampling, multi nuclei acquisition, etc. e. Analog to digital converter (ADC) with bandwidth 5 MHz or more.
		f. Preamplifier with proper filters for detecting a broad range of nuclei <sup>31</sup> P to <sup>109</sup> Ag
		g. At least one <sup>1</sup> H and one broadband amplifier with power levels of 200W or better for <sup>1</sup> H and 500 W or better for X channels respectively with detection and
		decoupling capability.  h. Variable temperature set up from -150 °C to 200 °C with a resolution of 0.1 °C.
		i. 10A gradient amplifier for pulse field gradient
		shimming and gradient enhanced spectroscopy
		j. 2H lock transceiver(in case of liquid-state probe
		usage)
		k. Pneumatic sample load/spin/eject system preferably for both solid and liquid samples.
1.4.	Probe	a. Solid-state CP MAS broadband Probe of 4mm
		diameter with MAS $\geq$ 12 kHz spinning speed. Nuclei <sup>1</sup> H, <sup>2</sup> H, <sup>7</sup> Li, <sup>13</sup> C, <sup>15</sup> N to <sup>31</sup> P, etc.
		Please specify the following:
		<ul> <li>Configuration of the coils.</li> </ul>
		• X-channel should be tunable from <sup>31</sup> P to <sup>15</sup> N.
		<ul> <li>Best resolution and line-shape using the standard sample.</li> </ul>
		<ul> <li>Best Signal-to-noise (S/N) ratio values for each nucleus of the probe measured using standard samples (Please provide data and mention the sample used).</li> </ul>
		<ul> <li><sup>1</sup>H &amp; <sup>19</sup>F high power decoupling for up to 50ms.</li> <li>Solid-state NMR measurement Temperature range -50 °C to +200 °C along with required accessories.</li> </ul>
		• Tuning accessory for auto-tuning capability for all X-nuclei is preferred.

		Automated magic angle adjustment is preferred.
		<ul> <li>Kindly provide a printed specification sheet.</li> </ul>
		Timely provide a printed specification sheet.
		b. Liquid state Broadband Probe to cover nuclei <sup>1</sup> H, <sup>13</sup> C,
		<sup>15</sup> N, <sup>19</sup> F, <sup>11</sup> B, <sup>31</sup> P, etc.
1.5.	Acquiring &	a. <b>Hardware:</b> A compatible high-end workstation
	Processing	with preferable Windows operating system,
	system	minimum of 24 inches LED monitor, CD/DVD
		read/write drives, USB ports. It should have the
		latest operating system with the latest upgraded
		software for 1D, 2D, and 3D acquisition and
		processing.
		b. PC with minimum Pentium i9 Quad or higher
		processor, 1TB SSD, > 16GB DDR4 RAM, 24 inch
		LCD monitor, Minimum 4 USB ports and two
		Ethernet ports for data acquisition and internet. c. <b>Software</b> : Most comprehensive latest NMR
		software to run up-to-date hetero-nuclear multi-
		dimensional NMR experiments including latest
		experiments for the reconstruction of multi-
		dimensional NMR study, for control, data
		acquisition and processing, and automatic
		recording of multiple experiments. The package
		should include all the latest pulse sequences for
		multi-dimensional & multi-receive NMR
		experiments available with the vendor. The
		licensed software modules should include tools for
		Structure Analysis, Integration and Deconvolution
		of 1D, 2D and 3D spectra, NMR simulation,
		Multiplet analysis, Relaxation data analysis, etc.  Automatic setup with acquisition, analysis and
		quantification of the NMR samples. High-end
		graphic tools for plotting one- and multiple-
		dimension spectra, for drawing structure and for
		making presentations on NMR experiment.
		Structure elucidation software.
		d. Any software upgrade (pulse sequence and
		processing) or new software (pulse sequence and
		processing) that are released during warranty
4.6		periods should be given to the user free of cost.
1.6	Installation	a. All items for preventive maintenance Kit should
		be provided by the engineer during installation
		b. Minimum 50 nos. of liquid NMR tubes with caps
		should be provided. c. Minimum 20 nos. of4 mm Zirconia rotors with
		caps suitable for standard and variable temperature
		caps surrable for standard and variable temperature

		experiments (up to max offered temperature) should be provided. Additionally, supply a minimum of 5 nos. of each Vespel, Kel-F and ZrO <sub>2</sub> rotor caps for 4 mm Zirconia rotor.  d. Sample packing kit (2 nos) and Cap remover (2 nos) should be provided.  e. In case magnet-quench during the installation or at subsequent times due to any technical reason or faulty design or failure, the manufacturer will take the complete responsibility of the supply (including transport) of the spares andconsumables, till the magnet is restored to normal and the entire costs for cryogenics, recharging or if required replacing the magnet will completely be taken care by the manufacturer
1.7	On-site training	completely be taken care by the manufacturer.  a. 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 variable temperature NMR experiments/special applications using software installed pulse sequences from the manufacturer.
1.8	Warranty	a. The entire instrument and the components should be under a complete comprehensive warranty period of 3 years. This includes the replacement of damaged parts, engineering/service support, consumables at the cost of the supplier.  In case, the machine is down for more than 1 week during the warranty period, the number of days accordingly should be compensated by providing an additional extended warranty free of cost.
1.9	Other requirements and Conditions	<ul> <li>a. All the technical details of all the basic items and essential accessories should be produced.</li> <li>b. The minimum power required for the operation of the spectrometer with all the accessories must be specified in the quote.</li> <li>c. Specify the pre-installation requirement including the minimum ceiling height, room size, etc.</li> <li>d. Standard samples for calibration of available nuclei in solid-state mode should be included.</li> </ul>