



INDIAN INSTITUTE OF TECHNOLOGY BOMBAY
MATERIALS MANAGEMENT DIVISION
Powai, Mumbai 400076.

Ref. No. 93 (PR No. 1000020780)

RFx. 6100000792

Technical Specification for 600 MHz FT- NMR Spectrometer with liquid probes.

Detailed specifications:

| Item No. 1: | Supply, Installation and commissioning of 600 MHz FT-NMR spectrometer with liquid probes. | |
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| S. No. | | Details |
| 1.1. | Spectrometer Frequency | 600 MHz state of the art liquid-state NMR spectrometer with three channels to carry out high resolution Solution-state NMR experiments such as 1D, 2D and 3D NMR with various combination of selected nuclei, having capabilities for most up-to-date multi-dimensional NMR experiments |
| 1.2. | Super conducting Magnet | <ol style="list-style-type: none">Latest technology based stable and actively shielded superconducting magnetOperating field at 14.1 T (operating frequency of 600 MHz for ^1H)Standard bore size of 54 mmField drift ≤ 10 Hz/hrRoom-temperature shims for optimal line shape (please mention the number of room-temperature shim coils); and automated gradient shimming capability with associated accessories (software/hardware). Shim system cooling during high-temperature experiments should be possibleRadial $\leq 0.8\text{m}$ and Axial distance ≤ 1.5 m for the stray 5 Gauss field from the centre of the magnet. (please specify the overall Magnet dimensions/weight/ceiling height requirements) |

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| | | <ul style="list-style-type: none"> g. Helium hold time ≥ 250 days with alarm function for low helium level and He sensor h. Nitrogen level sensor i. Magnet stand with integrated vibration damping j. All supporting equipment for cryogen filling such as Liquid He transfer line, liquid Nitrogen transfer line, etc k. Special tool kit for magnet |
| 1.3. | Console | <ul style="list-style-type: none"> a. Three or more channel cabinet, with possibility for future up-gradation to four channel b. Broad-Band frequency generation for all channels c. Communication between all channels by appropriate communication system d. Multiple Digital receivers with excellent capability and elimination for artifacts such as signal acquisition, filtering, sampling, parallel multi nuclei acquisition, etc. e. Analog to digital converter (ADC) with bandwidth 5 MHz or more f. Spectral width ≥ 7.5 MHz g. Preamplifier with proper filters for detecting broad range of X-nuclei h. ^2H preamplifier for ^2H observe and decoupling and for lock i. ^1H preamplifier for ^1H and ^{19}F observe and decoupling j. At least one ^1H and 2 broad band amplifiers with minimum power levels of 100W or better for ^1H and 500 W or better for X channels respectively with detection and decoupling capability. k. Variable temperature set up from -150°C to 150°C with a resolution of 0.1°C l. 10A gradient amplifier for pulse field gradient shimming and gradient enhanced spectroscopy m. ^2H lock transceiver n. Pneumatic sample load/spin/eject system o. Variable temperature accessories to cover the entire range of temperatures should be included along with specifications |
| 1.4. | Probes | <ul style="list-style-type: none"> a. 5 mm Room temperature triple resonance probe ($^1\text{H}/^{13}\text{C}/^{15}\text{N}$) probe optimized for ^1H observation and |

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| | | <p>$^{13}\text{C}/^{15}\text{N}$ decoupling (simultaneous irradiation possible) with ^2H locking, Z -shielded gradient and Auto-tuning/matching capability.</p> <p>Please specify the following:</p> <ul style="list-style-type: none"> ● Configuration of the coils. ● Pulse widths for ^1H, ^{13}C, and ^{15}N using standard samples. Please specify the sample used. Typical pulse length for ^1H should be 10 μs or similar ● Best resolution and line-shape (under sample spinning and non-spinning conditions). Please specify the line - widths measured using the standard sample. ● 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 and NMR tube used). ● Maximum gradient strength (≥ 50 G/cm and should have facility to do gradient encoded spectroscopy ● Gradient recovery times (not more than 100 μs). ● Decoupling pulse width, power, bandwidth, duty cycle capability on each RF channel. ● Temperature range over which the probe can be used should be -20°C to $+100^\circ\text{C}$ or better ● Kindly provide printed specification sheet. <p>b. 5mm Room Temperature double-resonance broadband probe optimized for X-nuclei observation with ^1H decoupling and ^1H observation with pulsed-field gradient and ^2H lock and Multiple-solvent suppression capability (2D experiments for e.g. INADEQUATE should be possible along with capability of homonuclear gated decoupling)</p> <p>All specifications as described in part (a) of this section should also be provided</p> <ul style="list-style-type: none"> c. Spinners for room and high temperature operations: 8 numbers d. Spinner for reduced volume sample (3mm) <p>Note: same spinners should be applicable for low and high temperature applications as well. If not, appropriate spinners for both temperature ranges should be included</p> |
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| | | e. Depth gauge |
| 1.5. | Acquisition & Processing | <p>a. Hardware: A compatible high-end workstation with preferable Windows operating system but compatible with Linux OS, minimum of 24 inch LED monitor, CD/DVD read/write drives, USB ports. It should have latest operating system with latest upgraded software for 1D, 2D, and 3D acquisition and processing. PC with minimum Pentium i7 Quad or higher processor, 1TB HDD, > 16GB DDR RAM, 24 inch LCD monitor, Minimum 4 USB ports and two Ethernet ports for data acquisition and internet. Compatible high-end laser jet printer and mouse.</p> <p>b. Software: Unlimited licenses for the most comprehensive latest NMR software to run up-to-date hetero-nuclear multi-dimensional NMR experiments including latest experiments for reconstruction of multi-dimensional NMR study, for control, data acquisition and processing, and automatic recording of multiple experiments should be included. 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 and dynamics data analysis, non-uniform sampling, 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.</p> <p>c. A module that has capabilities to do similarity analysis of complex biological macromolecules in a quantitative manner. Analysis should include deviation in chemical shift and intensity of two spectra, if exist, and provide correlative analysis plot.</p> <p>d. Any software upgrade (pulse sequence and processing) or new software (pulse sequence and</p> |

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| | | processing) that are released during warranty/AMC periods should be given to the user free of cost |
| 1.6 | Installation | <ul style="list-style-type: none"> a. All items for preventive maintenance Kit should be provided by the engineer during installation b. All responsibility/costs should be taken/covered by manufacturer in case of quenching of magnet during installation or later, including all costs for re-charging, cryogenics, and if required complete replacement of magnet c. 100 nos. of NMR tubes (with caps) for standard experiments should be provided d. 50 nos. of 3 mm reduced volume tubes with caps |
| 1.7 | On-site training | <ul style="list-style-type: none"> 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 biological NMR experiments/special applications using software installed pulse sequences from the manufacturer. |
| 1.8 | Comprehensive Warranty | <ul style="list-style-type: none"> a. Comprehensive Warranty for three years for the instrument and accessories (/compressor etc.) from the date of installation. Adequate number of engineer visits (minimum 2) every year should be covered during the warranty period. <p>Note: Warranty price should be given yearly basis for the 3 years & also quotation should be provided by OEM.</p> <p>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 extended warranty free of cost.</p> |
| 1.9 | Other requirements and Conditions | <ul style="list-style-type: none"> a. All the technical details of all the basic items, essential accessories should be produced. b. All standard samples such as line-shape, shimming samples etc. should be included. c. The minimum power required for the operation of spectrometer with all the accessories must be specified in the quote. |

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| | | <ul style="list-style-type: none">d. Specify the pre-installation requirement including the minimum ceiling height, room size etc.e. In case probes need to be sent back for repair, on-site replacement with temporary spare probes should be possible |
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