INDIAN INSTITUTE OF TECHNOLOGY BOMBAY

MATERIALS MANAGEMENT DIVISION

Powai, Mumbai 400076

Technical Specifications for 400 MHz NMR Spectrometer:

1. 400 MHz NMR Spectrometer:

i. Latest version/technology 400 MHz FT-NMR spectrometer for multi-dimensional solution state NMR experiments.

ii. Superconducting magnet system with an operating field of 9.4 tesla with active shielding and standard bore size (54 mm); with field stability of <10 Hz/hour or better.

iii. Shortest possible radial and axial distance of 5 Gauss stray field from the center of the magnet.

iv. Cryogen cooled shim system in addition to room-temperature shims for optimal line shape (please mention the number of cryogen-cooled and room-temperature shim coils); automated gradient shimming capability with associated accessories (software/hardware).

v. Minimum 300 days liquid Helium hold time and long liquid Nitrogen hold time. Please quote for longest hold magnet currently available with compact dewar.Also specify the total liquid He and liquid N_2 hold volume, refill interval and refill volume for liquid He and liquid N_2.

vi. Liquid Helium and Liquid Nitrogen level digital meters with alarms.

vii. All support equipment for cryostat (e.g. liquid He and liquid N_2 transfer line).

viii. Antivibration platform for mounting magnet and specify the lower limit of frequency of vibrations damped.

ix. Specify the number of built-in cryo shims and room temperature shims.

x. Pneumatic sample load/spin/eject system.

2) Console

i. Equipped with two RF channels (please specify the frequency range of operation with best frequency and phase resolution) in addition to lock channel with provisions for deuterium decoupling and observation. Please specify the configuration and bandwidth of all the channels. Minimum 2 channel architecture.

ii. Dual/Multi receiver capability with digital receiver for simultaneous acquisition of multinuclei. Excellent detection capability and elimination of artefacts such as quadrature images with control unit having state of the art technology for signal acquisition, filtering, sampling, multi nuclei acquisition etc.

iii. Gradient experiments such as Pulsed Field Gradient experiments with higher gradient strength, faster shimming should be the capability of the machine. Frequency generation, digital receiver controls with over sampling and digital filters should be quoted appropriately.

iv. Broadband frequency generation for all channels

v. Waveform generators for all channels for pulse shaping (please specify bits and total memory of the shape card).

vi. Quadrature-artifact-free phase sensitive detection.

vii. Receiver control unit for signal acquisition with real-time digital filtering along with oversampling technology – with dual receiver.

viii. Frequency, phase and amplitude shaping capability with individual/simultaneous switching of the parameters in shortest possible duration.

ix. Real time calculation of parameters of pulse sequences.

x. Broad-banded frequency generation for all the channels.

xi. Fast Ethernet based communication system between all the channels.

xii. High-power linear broadband amplifiers of >150 W for X-channel and >50 W for ^{1}H (and/or ^{19}F channel) for double resonance liquid state NMR. Please specify all relevant parameters including power (Wattage), frequency range, duty cycle, maximum pulse duration etc.

xiii. Multinuclear preamplifiers with a ^{2}H preamplifier for lock channel and observation.

xiv. Automatic high-performance gradient shimming for 1D and 2D along with lock, spin and insert / eject.

xv. Lock system should have high precision phase- and field-corrections (please provide documental evidence).

xvi. Built-in tune/match display and add-on filters for noise reduction.

xvii. ADC with high dynamic range and sampling rate. Please specify the resolution of the ADC (in bits) and the maximum sample rate.

xviii. Z-gradient amplifier: at least 30 G/cm.

xix. Pulsed field gradients of any desired shape with high resolution.

xx. Variable temperature set up from -100 °C to +150 °C with a resolution, accuracy and stability better than 0.1 °C.

xxi. State-of-the-art software interface for NMR acquisition and processing.

3) **5 mm double-resonance broadband high-resolution probe** with an actively shielded single axis Z-gradient for observation/irradiation of all NMR nuclei in the range ^{31}P to ^{109}Ag in addition to ^{1}H (please quote for maximum broadband range available); including 1H(19F) and vice versa including 1H-19F correlation 2D expts. sensitive to low gamma nuclei detection; a deuterium lock channel. Variable temperature range from –100 °C to +150 °C; automated tuning and matching.

4) **5 mm double-resonance (13C/1H nuclei) high resolution probe** (13C observe/sensitive) with an actively shielded single axis Z-gradient for observation and a deuterium lock channel. Variable temperature ranges from –100 °C to +150 °C; automated tuning and matching.

5) **Optional:** A 1.7 mm variable temperature triple-resonance probe (for smaller sample quantities) for observation of 1H, 13C and 15N with auto tuning and matching and having pulse field gradient capability with minimum operational temperature range of -50 to +80 °C with all accessories for low and high temperature operations. All the relevant

probe specifications such as 90 deg pulse lengths, sensitivity etc for standard nuclei (1H, 13C, 15N) are to be provided.

Please specify the following:

- Configuration of the coils.
- Pulse widths for ^{1}H, ^{13}C, ^{19}F, ^{31}P, ^{2}H and ^{15}N using standard samples. Please specify the sample used.
- 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 used).
- Maximum gradient strength (at least 30 G/cm).
- Gradient recovery times (not more than 100 μs).
- Decoupling pulse width, power, bandwidth, duty cycle capability on each RF channel.
- Temperatures range over which the probe can be used.
- Compatibility of the magnet/probe with 1.7 mm NMR tubes or its likes.

6) NMR software:

NMR software for spectrometer control, data acquisition and processing, and automatic recording of multiple experiments. Software tools for Structure Analysis, Integration and Deconvolution of 1D, 2D and 3D spectra, NMR simulation, Multiplet analysis, Relaxation data analysis.

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

Additional 2 workstations for data processing having similar configuration as acquisition PC

Minimum 25 or more additional NMR processing licenses for offline processing with regular updates of softwares.

7) **Oil free reciprocating air Compressor** of sufficient capacity and appropriate dryer with filter for supply of dry air with appropriate dew point for smooth operation of pneumatic unit, autosampler and variable temperature unit

8) **Comprehensive Maintenance Warranty** - Comprehensive Maintenance Warranty for five 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.

   Note: Warranty price should be given yearly basis for the 5 years & also quotation should be provided be provided by OEM.

9) **NMR Tubes** - 5 mm standard NMR tubes for the spectrometer – 500 numbers

10) **Sample spinner/holder** - for standard NMR tubes for both low and high temperature – 5 nos.

Other Requirements:

Liquid Helium for installation should be included in the spectrometer price

Optional Requirements:

11) Real-time (online) reaction monitoring kit (syringe pump and capillary)

12) Low temperature accessory

13) Quote for optional autosampler with a capacity of 24 samples or above.

Please provide a list of NMR instruments sold in India.

Note: It is mandatory to quote all items including optional items.