

## Specifications for 500 MHz FT NMR Spectrometer

Supply and installation of high resolution, broad band 500 MHz FT-NMR spectrometer for liquids and solids applications having the following specifications:

### I. Spectrometer

- a. Operation Frequency : 500MHz( $^1\text{H}$ )
- b. Observation Nuclei :  $^1\text{H}$ ,  $^{19}\text{F}$   $^{15}\text{N}$  to  $^{31}\text{P}$  (broad band),  $^6\text{Li}$ ,  $^{29}\text{Si}$ ,  $^{51}\text{V}$ ,  $^{119}\text{Sn}$
- c. Decoupling frequency:  $^1\text{H}$  as standard

### II. Superconducting magnet

- a) Standard bore size (54 mm)
- b) Operation field of 11.746 Tesla with minimum field drift <6Hz/hr
- c) Compact shielded magnet (specify the dimensions with operational height) with radial 5 G line  $\leq 0.6$  m and axial 5 G line  $\leq 1.2$  m

#### **d) Suitable vibrating damping accessory for acquiring artifacts free data (Specify the damp-frequency limit)**

e) All support equipment for cryogen filling of the magnet. (Liquid Helium transfer lines, liquid Nitrogen transfer-lines, liquid Nitrogen transfer tubes, O rings, coupling attachments, shorting plug, top cover for magnet bore, other spares etc.)

f) Helium and Nitrogen level meters and indicators

g) **Liquid Helium hold time  $\geq 360$  days** (specify the refill volume and total volume of helium)

h) Liquid Nitrogen minimum hold-time of  $\geq 14$  days (Specify the refill volume and total volume of Nitrogen)

i) High performance cryo- and room temperature shim system for optimal line shape

**j) External Disturbance Suppression (EDS) 99%**

### III. Console

- a) Minimum 2 channel architecture with up gradation possibility
- b) Broad band frequency generation for all channels
- c) Communication between all channels by appropriate communication system
- d) Dual/Multi receiver capability with digital receiver of excellent detection capability and elimination of artifacts such as quadrature images with control unit having state of the art technology for signal acquisition, filtering, sampling, multi nuclei acquisition etc.

- e) Analog to digital converter (ADC) with bandwidth 5 MHz or more.
- f) Preamplifier for multinuclear observation, 2H lock, all necessary filters for noise and artifact reduction.
- g) Frequency, phase and amplitude shaping capabilities with simultaneous switching of the parameters possible in  $\leq 25$  ns.
- h) Linear broadband amplifiers with minimum power levels of 100 W and 500 W for 1H and X, respectively for double resonance liquid state NMR experiments (and solid-state upgradation in future) and decoupling.
- j) Field gradient unit of  $> 50$  G/Cm strength and control for execution of Gradient spectroscopy, Gradient shimming generation of PFG of desired shape, high quality PFG based solvent suppression, DOSY experiments etc.
- k) A high end Work station: with latest configuration (minimum of 8 GB RAM, at least 1 TB hard disk capacity or more with 24" LED display or better, latest available processor, colour printer and other necessary accessories)

#### IV. Software

- a) Latest available Windows based software for NMR acquisition and data processing.
- b) User Licences – 20Nos., Free updates for the entire warranty period.
- c) Software for interpretation and report making automatically.
- d) Automatic setup with acquisition, analysis and quantification of the NMR samples.
- e) Structure elucidation software, NMR library for structural determination, Cmc assist software and Nus software should be provided.**

#### V. Sample Holder:

Automatic sample changer (Auto sampler) with a capacity of minimum 24 or more NMR samples with necessary accessories including spinners.

#### VI. Probes

- a) Liquid Probe** - 5 mm variable temperature probe for observation of  $^{19}\text{F}$ ,  $^1\text{H}$ ,  $^{15}\text{N}$  and X nuclei ( $^{31}\text{P}$  to  $^{109}\text{Ag}$ ),  $^{51}\text{V}$ ,  $^{119}\text{Sn}$  with auto tuning and matching and having pulse field gradient capability with minimum operational temperature range of  $-150$  to  $+150$  °C with all accessories for low and high temperature operations. All the relevant probe specifications such as  $\pi/2$  pulse lengths, sensitivity etc for standard nuclei ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{15}\text{N}$ ,  $^{119}\text{Sn}$ ,  $^6\text{Li}$ ,  $^{29}\text{Si}$  etc.) are to be provided.
- b)** To study natural products and/or samples of low amount/quantity, **a 1.7 mm variable temperature triple-resonance probe** for observation of  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$  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.

**c) Solid State probe - High Spinning Speed MAS probe upto 15 kHz (As optional)**

- i. Broad band double resonance magic angle spinning probe of 4 mm diameter to achieve a spinning speed of up to 15 kHz and to cover a range of nuclei, 15N-31P + proton decoupling (Provide probe specifications) **or** probe with capability for nuclei 1H, 31P, 7Li, 11B, 23Na, 27Al, 13C, 79Br, 207Pb, 29Si, 6Li, 15N, 19F.
- ii. 90° pulse widths and power for 1H, 13C and 15N. Please also specify maximum duration of r.f. irradiation for each nuclei, duty cycle, etc.
- iii. Best resolution and line shape. Please specify line widths achievable
- iv. Signal to noise ratio for each nuclei
- v. Specify temperature range achievable
- vi. Include additional accessories that may be required for the probe.

**d) Any other dual channel probes**

**Please Note, either [a] or [b] or [c] or [d] or Any Combinations among a – d or All May be considered for purchase. Hence, Price should be quoted item wise.**

**VII. Essential Accessories**

- 1) Oil free air compressor of sufficient capacity (Make: ATLAS COPCO) with low noise level and appropriate filters for supply of dry air with appropriate dew point for smooth operation of the pneumatic unit, auto-sampler and variable temperature unit of the spectrometer.
- 2) UPS of required capacity (Make: NUMERIC) with 1-hour backup for uninterrupted power supply for functioning of the spectrometer
- 3) 5 mm standard NMR tubes **FOR LIQUID SAMPLES** suitable for the spectrometer- 200 in number
- 4) 5 mm spinners for low and high temperature experiments: 50 Nos.
- 5) 50 litre Capacity liquid Nitrogen containers – 10 numbers
- 6) Liquid Nitrogen transfer device from the container to magnet [May be of Local purchase] : 2 Nos.**
- 7) Liquid helium transfer line: 1 No**
- 8) Filling contract agreement of Liquid Helium for 3 years from the date of installation should be quoted.**

**VII. Other requirements and Conditions**

- a) Standard samples, (<sup>51</sup>V, <sup>6</sup>Li, <sup>119</sup>Sn, <sup>29</sup>Si etc.) for testing and calibration should be provided
- b) Suitable cabinet (s) to store probes, spares and accessories should be provided.

- c) Air conditioners of required capacity (Make :OGeneral or Hitachi)
- d) Price may be quoted item wise wherever possible and with CIF Karaikudi. Minimum delivery time may be quoted.
- d) Standard warranty for 3 Years from the date of installation and AMC Charges **for the 4<sup>th</sup> and 5<sup>th</sup> years should be quoted.**
- e) On-site training for operation and maintenance should be given after the installation.
- f) Periodical visit of application specialist for on-site training and implementation of latest NMR experiments.
- g) Consumables like Liquid Helium, Helium gas and Liquid Nitrogen and nitrogen gas etc., required for installation and topping off the magnet should be provided.**
- h) All the technical details of all the basic items, essential accessories and optional items should be provided.
- i) Hard copy/soft copy of the service and operational manuals for all the modules of the spectrometer, peripherals, optional items and accessories must be supplied with the spectrometer.
- j) Specify the pre-installation requirement including the minimum ceiling height, room size etc. Requirement for installation of the main equipment, accessories and supportive infrastructure like UPS and Air conditioners which including Civil, Electrical, Mechanical (Crane) should be provided by the vendor **which includes man power.**
- k) Training for 2 personnel at manufacturing site should be quoted along with the instrument.
- l) User list in India is to be provided. An undertaking to the effect that the quoted system will be supported (by spares and service) for a minimum period of 10years from the date of installation.