

Specifications For A Nuclear Magnetic Resonance (NMR) Spectrometer

The Naval Research Laboratory (NRL) has a requirement for one 300 MHz nuclear magnetic resonance (NMR) spectrometer. This spectrometer will be used for routine, high sensitivity analysis of liquid samples. The instrument is to replace an existing Bruker AC-300 instrument. This instrument is used by several scientists with a variety of backgrounds, ranging from those with a minimum of operating knowledge to those who are professional spectroscopists. Therefore, its replacement must be versatile, have easy-to-use software, require a minimum of training to be able to operate for routine use, and be highly reliable. The present spectrometer and laboratory are plumbed with dry nitrogen lines for the sample spinning and VT gases. The spectrometer must consist of the following components and meet or exceed the following minimum-specifications:

1. Superconducting Magnet

- a. Field for 300 MHz instrument
- b. Standard bore (54 mm), with an orthogonal design shim stack including at least 17 room temperature shim gradients for producing a homogeneous magnetic field in the sample area of the bore.
- c. Cryogen hold time of at least 3 months for liquid He.
- d. Cryogen hold time of at least 13 days for liquid N₂.
- e. A drift rate of <3 Hz/hr for ¹H when unlocked
- f. The 5 gauss field line will radially extend no farther than 5.6 feet from the center of the magnet.
- g. An antivibration platform or other similar means of support for the magnet will be included.

2. High Resolution Probe

- a. Designed for 5 mm tubes.
- b. Broadband coil tunable from at least ¹⁵N to ³¹P
- c. Either a combined ¹H/¹⁹F coil, or separate ¹H and ¹⁹F coils
- d. ²D lock coil
- e. Coil for gradient pulse spectroscopy
- f. Computer switchable between nuclei without changing cables
- g. Both broadband and ¹H/¹⁹F coils shall be autotunable and automatchable from the computer console.
- h. Must be able to operate from sample temperatures of -100 °C to 150°C, and attain those temperatures with a resolution and precision of <0.5 °C without recabling or replumbing (replumbing of liquid N₂ unit for low temperature excepted).
- i. Designed to be used with dry nitrogen as sample spinning and VT gas
- j. Have 90° pulse widths <20 usec for ¹H, ¹⁹F, ¹³C, and ³¹P

- k. Have signal to noise ratio of >90:1 for ^1H , ^{13}C , and ^{19}F , and >50:1 for ^{31}P and ^{29}Si
- l. Have resolution of <0.45 Hz for ^1H and ^{13}C spinning samples
- m. Have lineshapes <6 Hz and <3Hz at 0.55% amplitude and <12 Hz and <5 Hz at 0.11% amplitude for spinning ^1H and ^{13}C samples respectively at room temperature.
- n. Have spinning sidebands <1% for both ^1H and ^{13}C samples

3. Console/RF Unit

- a. Transmitter or signal generator for ^1H and ^{19}F with a pulsed output of at least 50 watts.
- b. Broadband transmitter or signal generator (9 to 130 MHz range minimum) with a pulsed output of at least 150 watts.
- c. Must be able to vary the intensity of transmitted power over at least a 70 dB range.
- d. Must be able to produce pulse widths from at least 1 μsec to 350 μsec
- e. Pulse amplitude and phase stability of at least 0.1% and 0.1 $^\circ$ respectively
- f. Gradient spectroscopy with the required power supply and amplifier.
- g. Receiver with quadrature detection and at least a 16 bit effective dynamic range.
- h. Digital signal generation and detection
- i. Autolocking and autoshimming
- j. Autotuning and automatching of probes

4. Variable Temperature (VT) Unit

- a. Must control from at least $-150\text{ }^\circ\text{C}$ to $200\text{ }^\circ\text{C}$ in 0.1 $^\circ\text{C}$ increments
- b. Includes a sample cooling accessory for low temperature operation. The accessory will include, but is not necessarily limited to, a liquid nitrogen dewar, a nitrogen evaporator, and an insulated transfer line.
- c. Includes a ceramic spinner in addition to any plastic spinners
- d. Designed for dry nitrogen as the VT gas

5. Sample changer

- a. Must include a computer controlled sample changer that holds at least 6 samples.
- b. Must include at least 1 more plastic spinner than the maximum number held by the sample changer

6. Workstation computer

- a. Must provide a PC, with a Windows 2000 or XP operating system, and a processing speed of at least 2 GHz.
- b. Must provide a hard disk drive with a minimum of 40 GB disk space.

- c. Must include floppy, CD-ROM, and zip-disk drives
- d. Must include ethernet network connections
- e. Must provide at least a 17 inch color monitor

7. Software

- a. Must include operating software for 1D, 2D, and 3D NMR experiments
- b. Must include all common NMR transformations which must at minimum include 1D, 2D, and 3D fourier transformations, S/N enhancement, resolution enhancement, and T1 calculations, and the means to display, overlay, save, and plot spectra, and to plot any part of slice of spectra.
- c. Must be capable of gradient spectroscopy.
- d. Must include the ability for user generated pulse programs
- e. Must be equipped with the vendor's standard menus for all common pulse sequences which at minimum must include ^1H , ^{13}C , ^{19}F , ^{31}P , ^{29}Si , ^{15}N , ^7Li , ^{11}B , ^{119}Sn , COSY, quick COSY (pulsed field gradient spectroscopy), COSY-45, COSY-90, 3-D COSY, T1, DEPT, HETCOR, TOCSY, HMQC, HMBC, COLOC, NOESY, and INADEQUATE.
- f. Must include back-up copies of all software on CD ROM
- g. Must include the ability to convert data into ASCII files for importation to other programs
- h. In addition to the software for operating the NMR instrument, provide either a site license, or at least 8 additional seats of the NMR data processing software.

8. Installation and Training

- a. The price of the spectrometer must include installation at NRL, Washington, D.C. Installation shall include a demonstration that the instrument is in compliance with the specifications.
- b. The price of the spectrometer must include delivery of the instrument to NRL, Washington, D.C. and installation, including installation of the magnet. The price shall include any costs for rigging and liquid He necessary for installation.
- c. At the completion of the installation and demonstration of the specifications, the successful offeror must provide on-location training at NRL for 5 people for a minimum of two days to familiarize the operators with proper operation and care of the instrument.

9. Documentation and Warranty

- a. A full set of all written documentation customarily provided to the public with a commercial item shall be provided. This shall include users manual(s) or equivalent as well as copies of any software, and any manuals for the software included with the system, if customarily provided. This documentation must be received at NRL with the system hardware, unless other arrangements are

agreed to by the authorized Government representative. In addition to the above documentation which is customarily provided, the following specific documentation is required, and shall be included in the price of the spectrometer:

- 1) Shall include all operation and service manuals and schematics in printed form. Electronic copies on CDs that are readable on a windows-based PC are acceptable instead of printed copies.
- 2) Shall include a library of reference spectra that includes the spectra of standard samples so that a comparison can be made between the system's current performance and the reference. A set of tune-up samples and a set of standard samples shall be included.

b. The contractor shall offer the Government at least the same warranty terms, including offers of extended warranties, offered to the general public in customary commercial practice. These warranty terms must be included in the system price. The period of the warranty shall begin upon acceptance.

10. Trade-in

- a. Pricing shall include allowances for trade in of existing AC-300 instrument magnet and console. Existing probes and plotter will not be traded in.