Appendix A: Technical Specification
RFP 633764
High Performance Digital 400 MHz Solutions Nuclear Magnetic Resonance (NMR) Spectrometer Console & Probes
March 10, 2021

Battelle Memorial Institute, Pacific Northwest Division (Battelle), Management & Operating Contractor of the U.S. Department of Energy's Pacific Northwest National Laboratory (PNNL), requires a 400 MHz Nuclear Magnetic Resonance (NMR) Spectrometer console, probes and shim stack replacements for an existing magnet.

NMR Console/Probe Specifications

The 400 MHz NMR console and probes shall consist of the following main components which must be compatible with one another.

1. Console

The console shall be capable of the highest level solution state NMR experiments with accessories and components (adaptors, Variable Temperature (VT) control, preamps, relays, filters, components, pulse shaping, gradient pulses, total pulse programming control and delivers precisely timed RF events) that allow these consoles to interface with an existing magnet: Oxford 400/54, project # 130410, Magnet No: S0108, DLN0108508 (magnet manual will be provided upon request).

Each channel shall be highly stable and the console shall include a ^{2}H lock channel. The following components and/or requirements shall be included/met:

1.1. Two (2) broadband low power (1 Volt peak to peak) RF channels – two fully broadbanded low power RF channels with expansion capability up to ≥ 3 channels shall be provided. Outputs of the two channels shall be capable of operating in synchronous or fully asynchronous modes. Blanking of high-power transmitters shall be controlled independently of rf pulse outputs and data acquisition trigger.

1.2. Pulse programmer-controlled frequency-jumping (or the phase equivalent) capabilities for each rf output channel (<0.5 μs for a ≤5 MHz jump). The frequency jump hardware shall provide for phase continuity of the rf phase after frequency jumps.

1.3. Independent pulse-shaping capability for all rf output channels with ≥79 dB amplitude control and ≤3° phase variation over the entire amplitude dynamic range, and ≤100 ns amplitude switching time.

1.4. Pulse programmer with ≤20 ns time resolution, ≤50 ns minimum timing event, and no hidden or indeterminate delays, including within multidimensional acquisitions.

1.5. ≥4 user assignable TTL-level control lines with BNC outputs for triggering of external devices within a pulse program.

1.6. Console schematics or technical documentation for all console hardware. Documents shall be sufficiently detailed to allow maintenance and repair of the instrument hardware by Battelle personnel as necessary and appropriate.

1.7. High power transmitters/amplifiers

1.7.1. Channel 1: highband, with $^{1}H/^{19}F$ observe, spinlock and decouple capability (≥300W), amplifier shall be class AB operation with high speed (≤1 μs) blanking switch.

1.7.2. Channel 2: broadband observe, spinlock and decouple capability (i.e. 30-400 MHz, ≥ 300 W), channel shall be class AB operation with high speed (≤1 μs) blanking switch.

1.8. Phase sensitive receiver with digital signal processing

1.8.1. One (1) receiver

1.8.2. ≥20 bits effective dynamic range at 5 kHz and ≥18 bits effective dynamic range at 500 kHz.

1.8.3. ≥3.3 MHz receiver bandwidth.

1.8.4. ≥ 54 dB user settable gain.

1.8.5. Real-time display of data acquisition in averaged or single-scan modes.

1.8.6. Broadband detection capability.

1.8.7. RT preamplifiers for each RF channel, to have a noise figure of < 1.5 dB

1.10. VT capability - Computer-controlled liquid sample temperature management from -40°C to +150°C with 0.1°C resolution for solutions. Must include all preconditioning gas controller(s) (e.g. - 60°C FTS unit), temperature stacks/exhaust means, gas flow controls, exchangers and containers required for continuous operation between at least -60°C-+150°C. Actual temperature range may be limited by individual probes.

1.11. High performance triple-axis liquid-state pulsed-field gradient (PFG) capability (to support at least 40 G/cm – z-axis) and to include software to support automated gradient shimming for all z-gradient related (axial) shims as a minimum requirement. Actual G/cm will depend on individual probes.

1.12. ^{2}H Lock Channel with blanking capability.

1.13. Filter Kits - 100 W

1.13.1. High-pass 400 MHz

1.13.2. Band-pass ^{13}C, ^{15}N, ^{31}P

1.13.3. Low-pass 250 MHz

1.14. Shim insert for existing magnet

1.14.1. A room temperature shim insert and all accompanying components that is compatible with the existing magnet (as noted in section 1) that shall thereby allow the probes listed in this document to be shimmed to industry standards compatible with high resolution small molecule structure elucidation using the console and software listed in this specification document.

2. Software/Computer system

The following components and/or requirements must be met:

2.1. Host computer shall be Unix based (Red Hat Enterprise Linux or equivalent)

2.2. Software/computer system/site license (or equivalent) for all relevant software including user manuals.

2.2.1. Site license must cover a minimum of 5 workstations to include the spectrometer.

2.3. Tools for analysis of dynamics and diffusion data (e.g. inverse Laplace transform)

3. Probes

The following probes or a sufficient number of probes shall be provided to meet the frequency ranges listed in console subsections listed above. The ^{1}H RF homogeneity of probes, measured as the peak intensity ratios of 450°/90° pulses, when shimmed to lineshape standard (0.3% CHCl3 in acetone-d6) or DSS linewidth specifications should be ≥ 80%.

3.1. 5mm X optimized double resonance probe (BBO) designed for broadband X observation from ^{109}Ag to ^{31}P

3.1.1. Pulse widths for ^{1}Hmust be < 11us, for ^{19}F <20us, for ^{31}P <10 us, for ^{13}C <10 us, and for ^{15}N <25us.

3.1.2. ^{1}H sensitivity must be > 500/1 in 0.1 % ethylbenzene standard.

3.1.3. ^{19}F sensitivity must be > 500/1

3.1.4. ^{31}P sensitivity must be > 200/1

3.1.5. ^{13}C sensitivity must be > 200/1 in 10 % ethylbenzene standard.

3.1.6. ^{15}N sensitivity must be > 20/1

3.1.7. ^{13}C spinning lineshape must be <0.2/2/4 Hz

3.1.8. ^{1}H non-spinning lineshape must be <0.8/7/14

3.2. 10 mm X optimized double resonance probe (BBO) designed for broadband X observation from ^{109}Ag to ^{31}P.

3.2.1. Pulse widths for ^{1}H must be < 30 us, for ^{31}P <30 us, for ^{13}C <15 us, and for ^{15}N <40us.

3.2.2. ^{31}P sensitivity must be > 300/1

3.2.3. ^{13}C sensitivity must be > 500/1 in ASTM standard.

3.2.4. ^{15}N sensitivity must be > 60/1

3.2.5. ^{13}C spinning lineshape must be <0.2/3/7 Hz