Requirements / Specification Document

Use this document to detail specifications/requirements for an item and/or ancillary services. ⓘ

TITLE: **BENCHTOP EPR/ESR SPECTROMETER** ⓘ

Requesting Lab/Division/Group: Physical Measurements Lab/Applied Physics Division/Magnetic Imaging Group
NB686080-26-01894

General Statement of Need ⓘ

The Magnetic Imaging Group (MIG) is requesting a benchtop electron paramagnetic resonance (EPR) spectrometer (also known as electron spin resonance (ESR)) to enhance its capabilities to provide measurements to the magnetic resonance community. This spectrometer would provide new measurements as well as track new species that are not possible in existing nuclear magnetic resonance (NMR) or magnetic resonance imaging (MRI) experiments. This spectrometer would allow for studies of spin species in free radiacal configureations as well as nano-particle composites. At present, the MIG does not have this capability in its group and limits the ability to observe certain species in samples. Electron paramagnetic resonance, also known as electron spin resonance, is a technique that allows for the observation of electrons in configurations such as metals, free-radicals, and as ions in solution. Understanding of spectral position, peak splitting, and g-factor can be very important for understanding the local environment of an electron. This information can be used in further research such as hyperpolarization, material stability, and material sysnthesis. Ongoing research at NIST requires a EPR/ESR system capable of experiments in the X-band range of radiofrequqncy with temperature control, rotational control, and light illumination. The MIG would like to acquire a new benchtop EPR/ESR spectrometer capable of providing these measurements. This project would provide new electron paramagnetic measurements. These additions would bring improved measurement capabilities to the MIG and provide provide flexibility for future work. This project is designed to add a benchtop EPR/ESR spectrometer to the existing suite of magnetic resonance tools owned by MIG. This system will allow for the study of electron spins in radical species, metallic species, nanoparticles, and other various systems. This new capability will enchance the work of our group to the NIST mission of providing quantitative and precise measurements for the magnetic resonance community. In acquiring a benchtop EPR/ESR spectrometer, the MIG will enhance the capabilities of the research group as well as its abilities to study samples as part of its work with the magnetic resonance community. This system will improve the available systems of study as well as stability of solutions containing metal ions. This system will help understand the behavior of electrons in metal films, nanoparticles, and stable radical species.

Items and/or Ancillary Services ⓘ

Item 1: Benchtop EPR/ESR Spectrometer
Quantity: One (1)
Specifications:
1. Operational frequency with the X-band (8 to 12 GHz) of radiofrequency.
2. Sensitivity: 5 x 10^10 spins/mT (or 5 x 10^9 spins/G).
3. Weak pitch signal-to-noise ratio: 600:1 or better.

4. Microwave power: REQUIRED: 10 uW to 100 mW, Recommended: as low as 1 uW and/or as high as 200 mW.
5. Field Homogeneity within sample region: ±5 uT (50 mG) or better.
6. Field Stability 1 uT/h (10 mG/h).
7. Magnetic Field sweep range: REQUIRED: -10 to 650 mT (-100 to 6500 G), Recommended: -1000 to 6500 mT or better.
8. Modulation frequency: REQUIRED: 10 kHz to 100 kHz, Recommended higher frequency if possible.
9. Resonator: Unloaded Q of 5000 or better.
10. Warranty: REQUIRED: 3 years from date of acceptance, Recommended: 5 years from date of acceptance.
11. Software to run spectrometer as well as software for off-spectrometer data processing and analysis. Spectrometer software must be Windows 11 compatible and run on Dell Workstation PC (provided by NIST, will have at least 32 GB RAM and 1 TB solid state drive). Software must run locally and not depend on cloud support/operation. Software for spectrometer operation should include automated calibration and tuning, data processing in single data set and batch data set work flows, and quantification workflows. Off-spectrometer data processing software to have same options as spectrometer software for data processing (e.g. single and batch work flows, data fitting routines). Software to be able to export data sets to common file structure such as CSV or provide data file structure to be able to be loaded into other processing programs or custom software in languages such as Python.
12. Standard Sample Set to be included that measures quantities of G-factor, Magnetic Field Sweep, Hyperfine Splitting, and Signal-to-Noise ratio/Instrument Sensitivity.

Separately Priced Options and Services:
Item 2: Liquid Nitrogen Variable Temperature Control System
Quantity: One (1)
Specifications:
1. Attachment to Benchtop EPR/ESR spectrometer for temperature control of the sample while in the spectrometer.
2. Controllable by software from Benchtop EPR/ESR with synchronization for serialized experiments with temperature control.
3. REQUIRED: Temperature range of 95 K (or lower) to 450K (or greater).
4. Recommended/Preferred: Temperature range of 95 K (or lower) to 550 K (or greater).
5. REQUIRED: Temperature stability ±0.2 K.
6. Required: Support desk for configuration of Liquid Nitrogen Storage Dewar, transfer lines, and other required components as appropriate for Benchtop EPR/ESR spectrometer

Item 3: Optical Irradiation System / Photochemistry System
Qty: 1
Specifications:
1. Attachment to Benchtop EPR/ESR spectrometer for light illumination of the sample while in the spectrometer.
2. Controllable by software from Benchtop EPR/ESR with synchronization for serialized experiments with exposure control.
3. REQUIRED: wavelength of 350 nm to 750 nm.
4. Recommended/Preferred: Interface with Optical Fiber cables such as SMA 905 to allow other

light source options.
Item 4: Automated Goniometer
Qty: 1
Specifications:
1. Attachment to Benchtop EPR/ESR spectrometer to control rotation of the sample while in the spectrometer.
2. Controllable by software from Benchtop EPR/ESR with synchronization with spectrometer software so serialized experiments of angle are possible.
3. REQUIRED: Rotation of 0 degrees to 360 degrees with step size resolution of 0.1 degrees [List any other item(s) or service requirements here using the same format above.]

Service Requirements / Item Specifications

Section ⓘ	Requirements/Specifications ⓘ
Planning Considerations ☒ N/A	☐ List any visits required to allow potential vendors to see site specific constraints. [Explain requirement here] ☐ US citizen required on-site (foreign nationals require preregistration 30 days prior) ☐ Vendor rep on-site more than three days ☐ Other considerations: [List other considerations to ensure an accurate quote]
Shipping & Delivery ☐ N/A	Item to be shipped to NIST via NIST UPS or Fedex Frieght Codes to be provided by TPOC or Admininistrator of TPOC **Shipping criteria:** ☐ Partial delivery acceptable ☐ Direct delivery to building required [Explain need for requirement here] Building has: ☐ Loading dock ☐ Containerization preference: [Choose container] Other requirements: [List any other requirements here] **Delivery date criteria:** ☒ Delivery of goods, installation, and training shall be completed no later than: 20 Weeks ☐ Deliver no earlier than: [Insert date here] ☐ Other: [List other shipping, delivery, or specil requirements]
Electronic Media ☐ N/A	Any software and manuals are to be provided to TPOC ☒ Software ☒ Electronic manuals ☒ License Key ☐ Other: [List any other Electronic Media requirements here] Karl.stupic@nist.gov
Installation ☒ N/A	[Enter installation requirements by item here.] ☐ Vendor technician on site ☐ Rigging ☐ Uncrating / Unpackaging ☐ Removal of packaging material

	☐ Equipment set up ☐ Start-up services ☐ Turn key installation ☐ Other [Enter details here.] Note: When installation is required, TPOC or COR shall be the coordination point.
Facility / Utility Considerations ☒ N/A	[List site specific utility considerations by item here.] ☐ OFPM Work Order Number(s) [List any Work Order Number(s) here] ☐ Power available Voltage: [Enter voltage here] (V) Max Current: [Enter max current draw here] (A) Phase: [Choose phase] Frequency: [Typically 60Hz] (Hz) NEMA Plug Type: [Enter plug type here] (i.e.: NEMA L5-20P) Environment: [Choose environment] Other power consideration: [List any other power considerations here] ☐ Utility connections: [List relevant available utilities, pressure(s), and flowrate(s)] ☐ Other considerations: [List other considerations to ensure an accurate quote]
Warranty ⓘ ☐ N/A	Base Manufacturer Warranty is acceptable [If you require an Extended Manufacturer Warranty, describe the warranty requirements per item here.] What is included? ☒ Labor ☒ Parts ☐ Travel ☐ Cost and liability for returns ☐ Other: [Enter other requirements here] ☒ Warranty length: Three years minimum, Five years preferred Period Length:[Ex. month, 6 month, year etc.]
Training ☒ N/A	[Training requirements (who, when, what, where) here. If on-site, is travel necessary?] ☐ On-site ☐ Off-site location: [Enter location(s) here] ☐ Number of trainees: [Enter number of trainees here] Scope of training: ☐ Operations ☐ Maintenance ☐ Troubleshooting ☐ Safety ☐ Other: [Enter other scope requirements here] ☐ Training materials to be provided: [Describe requirement here] ☐ Other: [Enter other training requirements here] Note: When training is required, TPOC or COR shall be the coordination point.

Inspection and Acceptance ☐ N/A	[Enter inspection requirements per item here] ☐ Planned government acceptance testing (7 business days) ☒ Gov't acceptance expected to take longer than 7 business days: 15 Days ☐ Inspection and acceptance plan: [Explain here] ☐ Other: [Enter other requirements here]
Maintenance ⓘ ☒ N/A	[Describe your maintenance requirements per item here] Period Length: [Ex. month, 6 month, year etc.] What is included? ☐ Labor ☐ Spare parts ☐ Consumables ☐ Travel ☐ Cost and liability for returns ☐ Software updates ☐ Manuals ☐ Service plan length: [Enter service plan length here] ☐ Other: [Enter other requirements here] ☐ Requirements: [Enter requirements here] (i.e.: onsite within 72 hours, etc.) ☐ Option Period 1 ☐ Option Period 2 ☐ Option Period 3 ☐ Option Period 4
Government Furnished Material / Equipment ☒ N/A	[List any government furnished material/equipment per item here] ☐ Samples for testing ☐ Government equipment which will leave gov't site (TPOC must coordinate with division property custodian) Serial Number: [Enter Serial Number here] Description: [Enter description here] NIST property number: [Enter NIST property number here] ☐ Other: [Enter other details here]
Travel ☒ N/A	[Describe any travel requirements per item here] ☐ Explain: [Explain here] ☐ Other: [Enter other requirements here] *Vendor: To the maximum extent possible, include as part of appropriate sections above (maintenance, repair, etc.). Otherwise, it will be a separate line item, reimbursable per the Federal Travel Regulation.*

Provide suggestions to improve this form by clicking here.