SUPPORTING INFORMATION FOR:

A 3D-Printed High Power Nuclear Spin Polarizer

Panayiotis Nikolaou,*,[†,&] Aaron M. Coffey,[†,□,&] Laura L. Walkup,[‡,#] Brogan M. Gust,[‡] Cristen D. LaPierre,[§,∥] Edward Koehnemann,[⊥] Michael J. Barlow,[¶] Matthew S. Rosen,[§,∥] Boyd M. Goodson,[‡] and Eduard Y. Chekmenev*,[†,□,$,▽]

[†]Department of Radiology, Vanderbilt University Institute of Imaging Science (VUIIS), Nashville, Tennessee 37232, United States
[‡]Department of Chemistry & Biochemistry, Southern Illinois University, Carbondale, Illinois, 62901 United States
[§]MGH/A.A. Martinos Center for Biomedical Imaging, Boston, Massachusetts, 02129United States
[∥]Department of Physics, Harvard University, Cambridge, Massachusetts, 02138United States
[⊥]Mid-Rivers Glassblowing Inc., St. Charles, Missouri, 63304 United States
[¶]University of Nottingham, Nottingham, NG7 2RD, U.K.
[□]Department of Biomedical Engineering, Vanderbilt University, Nashville, Tennessee, 37235 United States
[$]Department of Biochemistry, [▽]Vanderbilt-Ingram Cancer Center, Vanderbilt University, Nashville, Tennessee, 37205 United States

[&]Author Contributions: Both these authors contributed equally to this work

[#]Current Address: Cincinnati Children's Hospital Medical Center, Cincinnati, Ohio, United States

Corresponding Authors:

Eduard Y. Chekmenev, Department of Radiology, Vanderbilt University Institute of Imaging Science, Nashville, Tennessee, 27232 Unites States. Phone: 615-322-1329; Fax: 615-322-0734;

E-mail: eduard.chekmenev@vanderbilt.edu and

Panayiotis (Peter) Nikolaou, Department of Radiology, Vanderbilt University Institute of Imaging Science, Nashville, Tennessee, 27232 Unites States. Phone: 618-203-6912

E-mail: peter.nikolaou@vanderbilt.edu

Overview

This supporting information provides additional information about the SEOP probe designs including 3D CAD drawings showing different angles and views of these VT SEOP probes. Section (a) describes the features of the forced air (FA) VT SEOP probe and various schematic views of the SEOP probe and its components; Section (b) contains information about the thermo-electric (TE) SEOP probe and various schematic views of its components; Section (c) describes the 3D printed OP-cell stem holders; Section (d) provides details about the OP-cell design and the 3D printed former used to assist in its making; Section (e) discusses the 3D printed NMR coil former; Section (f) provides the details about VHG Laser Diode Array (LDA).

a) Forced Air (FA) SEOP VT Probe

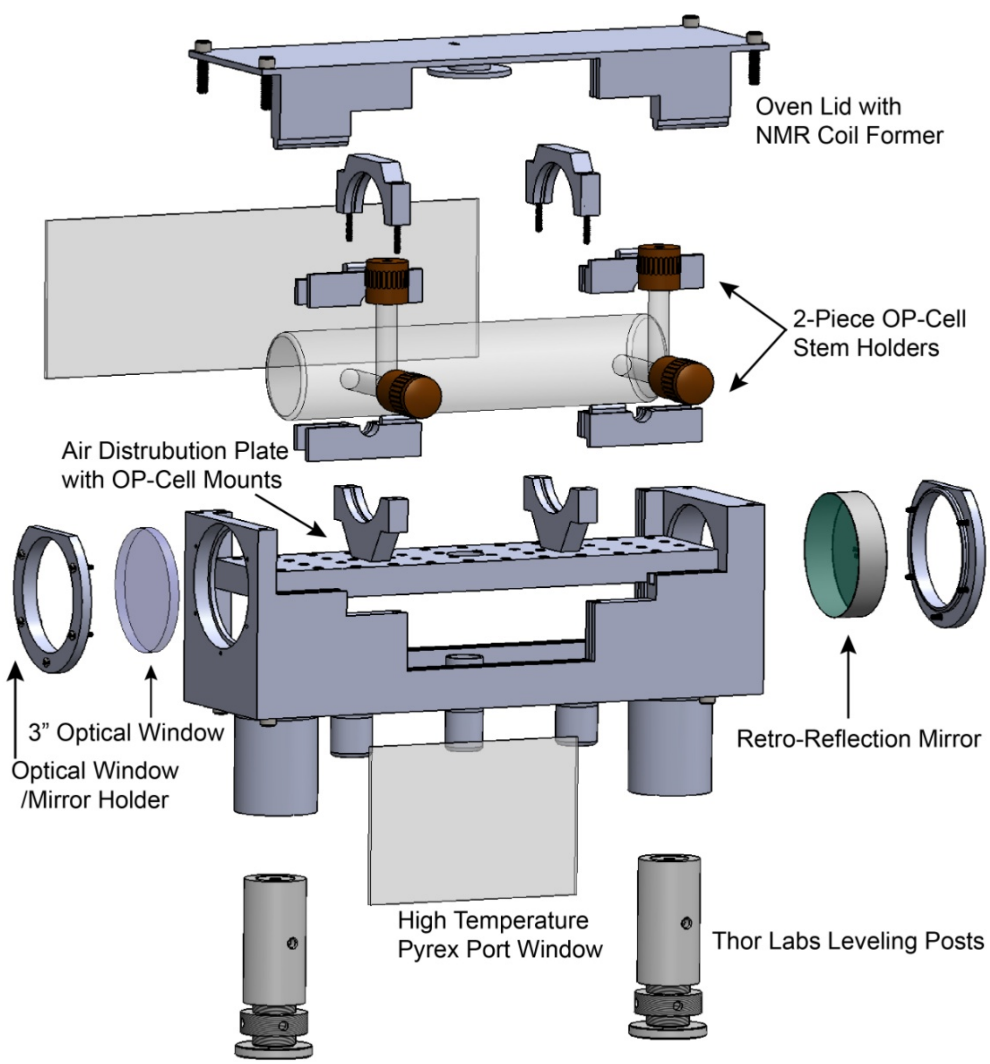

Figure S1. A 3D CAD exploded view drawing of the forced air (FA) VT SEOP probe with labeled components.

The Forced Air (FA) SEOP probe is based on traditional SEOP VT probe/oven designs, with major improvements in simplicity and integrated functionality. Traditionally, a machined probe/oven of this design would require sheets of the desired body material to be cut and machined to form every single wall as an individual piece. The individual pieces would then be held together with nylon or Teflon screws. For instance, compared to 3D printing where the SEOP probe lid is printed as a single piece, the machined version would have to consist of several individual pieces screwed together with the appropriate screw sizes. Furthermore, more intricate pieces such as the OP-cell stem holders would require a highly skilled machinist and several hours to make just a single piece, whereas all four pieces were 3D printed with high precision and accuracy in ~1.5 hrs. The three nozzles (**Fig. 2Sb**) located between the FA VT SEOP probe supporting leg posts (ThorLabs leveling posts) are the SEOP probes heating/cooling gas inlets (outer two) and exhaust outlet (middle one). These are also printed as part of the SEOP probe's main body, which does not require drilling and tapping to screw on nozzles such as a machined version would require. The air distribution plate is hollowed out. Thus, when sitting inside the main body of the SEOP probe, a cavity of 2.5 in x 1 in x 11.5 in is created which serves to distribute the inlet source gas through an array of distribution holes present in the plate (seen best in **Figs. S2 & S3**) in a fashion much like water through a "shower head." The exhaust outlet nozzle feeds through this cavity and the distribution plate itself, thus preventing inlet and outlet gas flows from mixing.

The ThorLabs leveling posts used to support the SEOP probe can be mounted to most breadboards or linear stages using a specially designed mounting clamp (ThorLabs, P/N PF175). The distinctive advantages of this two-post setup are: (i) that lateral movement of the SEOP probe is not hindered (compared to previous four-post designs, where all posts must be un-mounted first to enable movement), thus simplifying horizontal alignment of the SEOP probe with the transmitted laser beam, and (ii) the vertical alignment of the SEOP probe can be adjusted using the leveling posts themselves rather than adjusting the optical breadboard height (a difficult task with a laser table setup).

The NMR coil former is designed to be well centered with the OP-cell, and is printed as a part of the FA SEOP probe lid leaving only a ~2-3 mm air gap from the surface of the OP-cell. Furthermore, a feed-through hole is incorporated into the design allowing the NMR coil wires to exit the SEOP probe. This setup enabled low-field *in-situ* polarimetry via NMR spectroscopy, and eliminates hysteresis due to coil positioning.

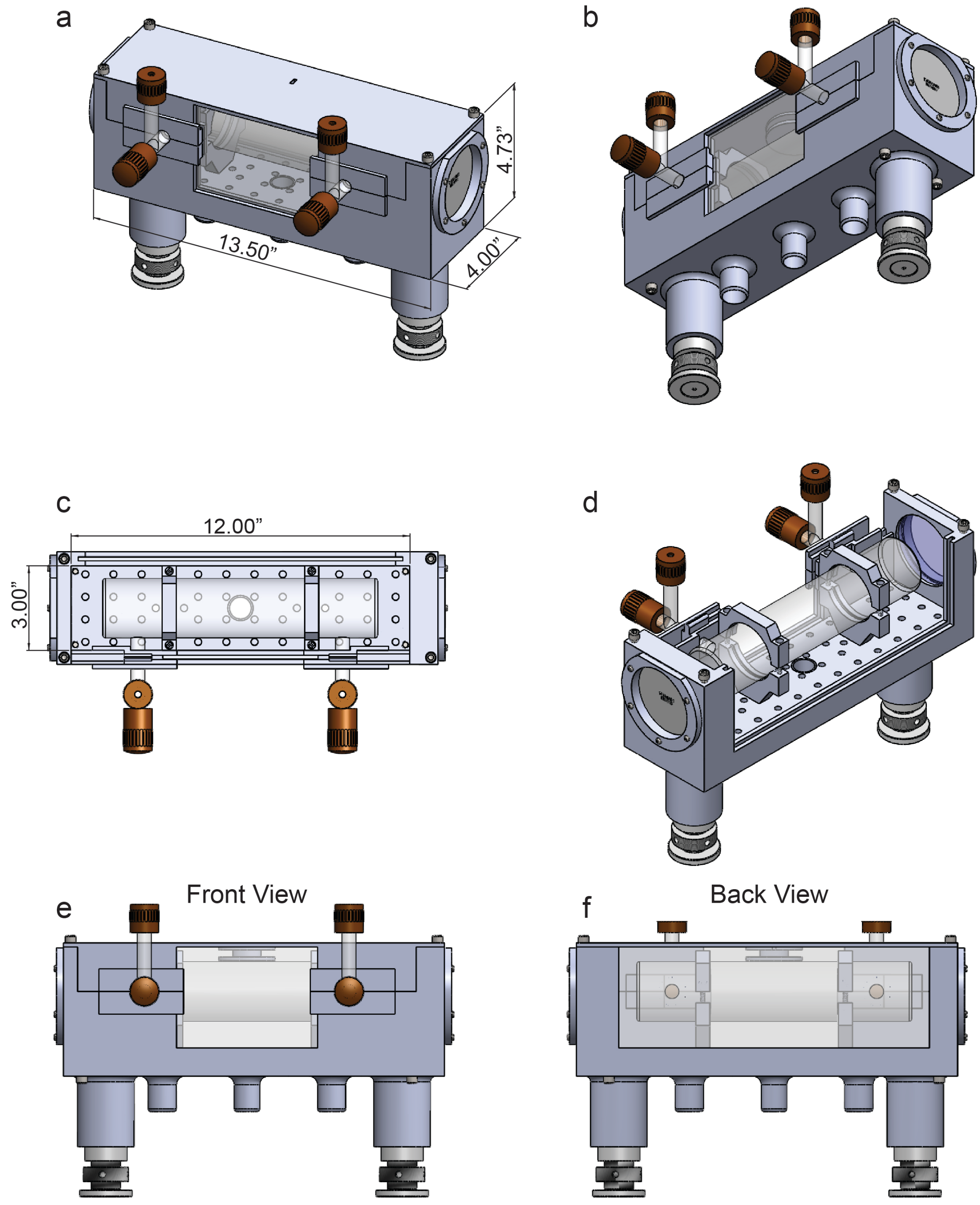

Figure S2. 3D CAD drawing alternative views of the FA VT SEOP probe. **(a)** General outer dimensions of the assembled FA SEOP probe. **(b)** Bottom angled view showing supporting legs and cooling / heating gas inlet and outlet nozzles. **(c)** Top view of FA SEOP probe with lid removed to show internal components and dimensions. **(d)** Angled rear view showing internal components. **(e-f)** Front and back view respectively of the assembled SEOP probe.

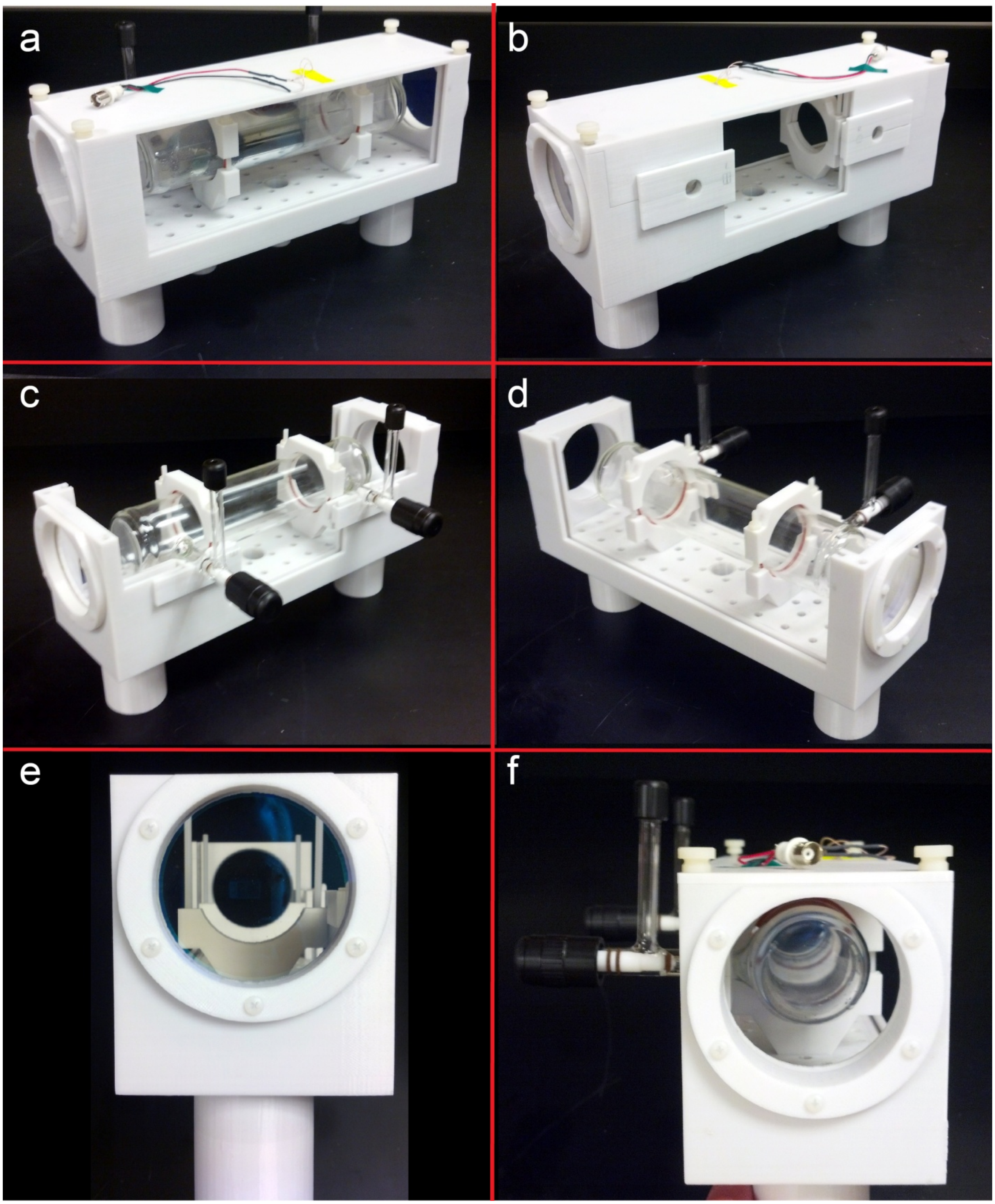

Figure S3. Alternative views of 3D Printed FA VT SEOP probe. **(a)** Back view. **(b)** Front View without OP-cell to show stem holders. **(c)** Frontal top view without lid. **(d)** Back top view without lid. **(e)** Side view without OP-cell **(f)** Side view with OP-cell.

b) Thermo-Electric (TE) VT SEOP Probe

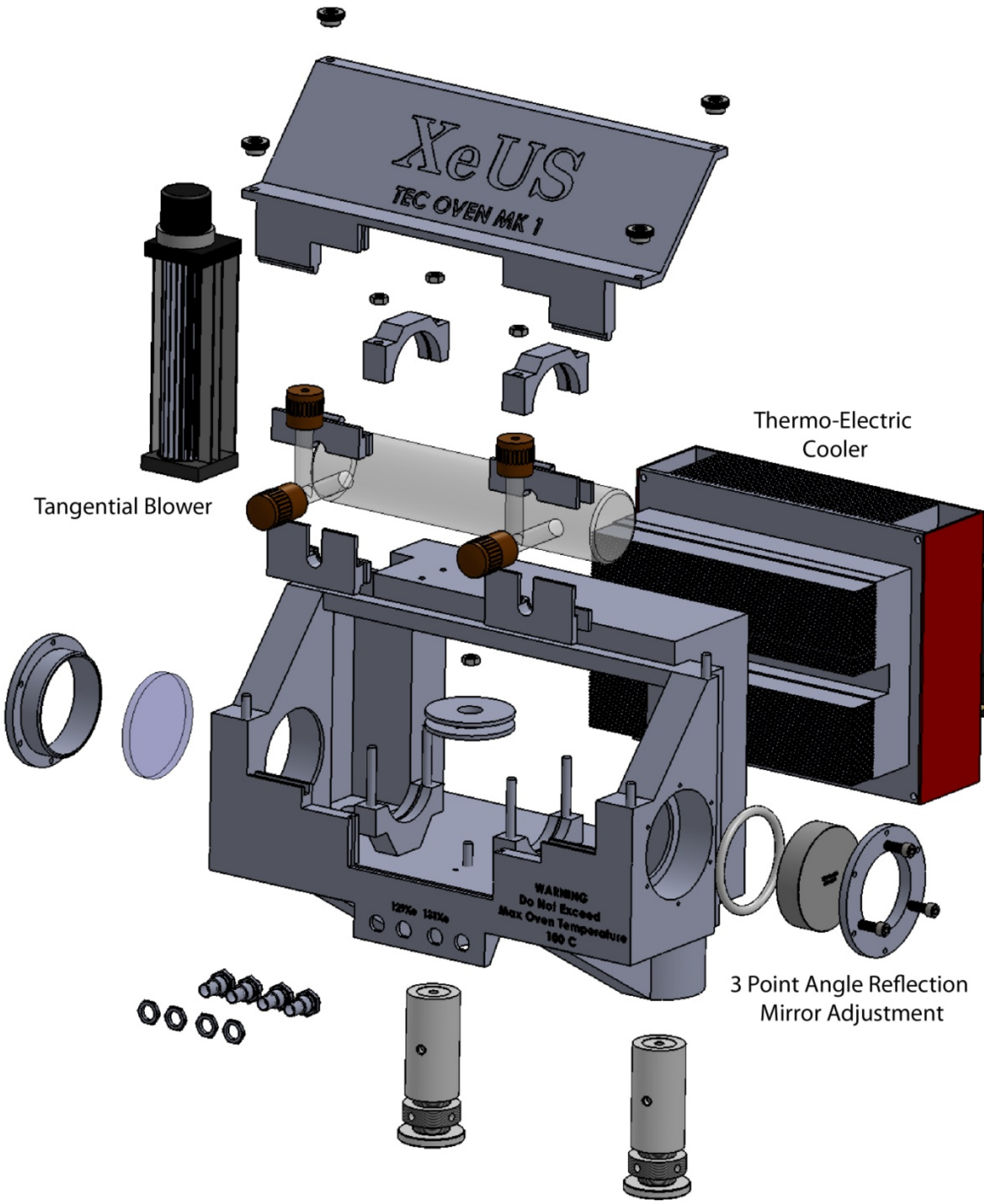

Figure S4. 3D CAD exploded view drawing of the TE VT SEOP probe with labeled components.

Despite the fact that the TE unit has a mass of 14.1 lbs (6.4 Kg), when completely assembled the TE VT SEOP probe is mass-balanced and can stand alone on both leg supports without tipping over or causing strain on the SEOP probe body or associated supports. Strain or unbalance of any SEOP probe could mean either catastrophic failure or difficulty with OP-cell alignment. Furthermore, to ensure the rigidity of this SEOP probe, the base of the probe and the walls surrounding the TE unit were made 1.5 in. and 1 in. thick respectively.

The tangential blower consists of a DC motor with a permanent magnet located inside the black tubular structure (seen in **Fig. S4**). In our first prototype of the TE VT SEOP probe the blower was located on the opposite side of the TEC unit with the motor facing down. It was soon discovered that the RF noise of this motor's built-in brushless motor controller would interfere with low-field NMR polarimetry at 84 kHz. The revised version places the motor far enough from the NMR probe to reduce the electro-magnetic interference. However, to prevent all electromagnetic interference with NMR spectroscopy, the power to both the blower and TE unit is gated off for a few seconds before acquiring. Furthermore, the manufactured TE unit utilized several magnetic nuts, bolts, and screws creating magnetic field inhomogeneities, which was resolved by replacing them with aluminum and Teflon components.

The thermal characteristics of the VT SEOP probe were also tested. Even though the polycarbonate material used to print the probe body can withstand higher heat, it is not recommended to operate in regimes above 100 °C for the OP-cell surface temperature (even though the SEOP probe was tested up to 160 °C with very minor melting of the OP-cell body holders). Even though the SEOP probe does not melt above 100 °C, the PC material begins to degrade when material under stress reaches the Vicat softening point of 138 °C. To improve heat isolation, the interior surface of the TE SEOP probe was covered with a thin layer (1/8 in. thick) of insulating Aerogel (McMaster-Carr, P/N 9590K8). The addition of the insulating Aerogel is a key component, which greatly improved TEC performance in regulating the SEOP probe temperature with very good accuracy, and reduced both heating and cooling times of the OP-cell surface temperature by approximately 3 fold.

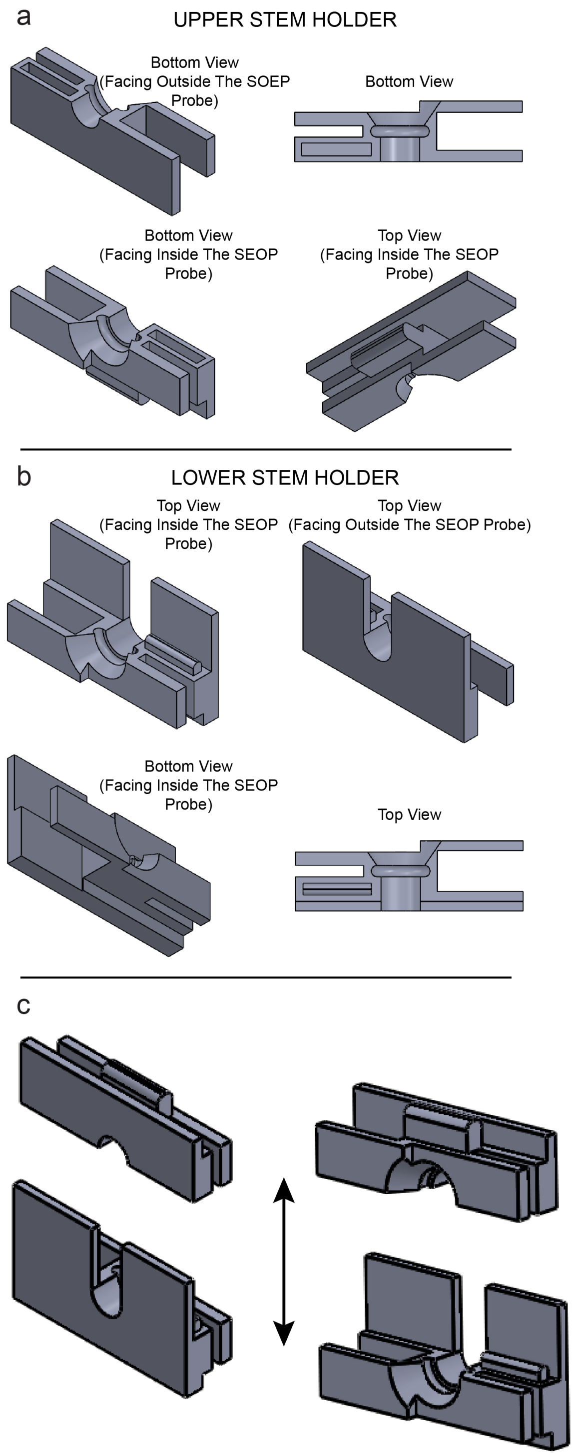

Figure S5. Different views of the stem holder components. (a) Upper stem holder component. (b) Lower stem holder component. (c) The view showing how the upper and lower stem holder components mate.

c) OP-Cell Stem Holders

The Stem holders are the only moving pieces in the SEOP probe design. There are two pieces that make up the Stem holder set: (i) a lower stem holder that mates to the body of the SEOP probe; and (ii) an upper stem holder that mates to the lid. Figure S5a-b displays multiple views of each piece of this two-piece setup. These components have two gaps as seen in the 'Bottom View' of **Fig. S5a** and the 'Top View' of **Fig. S5b**; The enlarged opening allows these components to fit around the SEOP probe wall, while the smaller opening allows the 1/8 in. Pyrex glass window into the opening—thus providing stability while allowing horizontal motion. This ability enables adjustment for perfect fitment of the OP-cell's side stems caused by slight variations from OP-cell to OP-cell in the side stem positioning.

When the OP-cell side stems are attached to the main body of the cell, a conical seam is left at the base of the stem where the two pieces of glass are joined together. In the TE VT SEOP probe designs, the internal volume of the SEOP probe was kept to a minimum to make heating and cooling of the OP-cell more efficient due to minimized heat-flux proportional to probe body surface area. As a result the OP-cell main body is only 0.5 in. away from the SEOP probe body. Therefore, the glass seam may sometimes protrude beyond this distance. To avoid interference with the seam and to ensure good fitment across OP-cells, each stem holder component was designed with half a conical cut out on the side facing the inside of the SEOP probe. This is best seen in 'Bottom and Top view (Facing inside the SEOP probe)' of **Figs. S5a** and **S5b** respectively. The groove located in the middle (left to right) seen in 'Bottom View' of **Fig. S5a** and 'Top View' of **Fig. S5b** was made to allow fitment of a silicone o-ring fit around the outside of the glass side stem that allows the SEOP probe to remain sealed. Furthermore, each has corresponding fillets and channels that allow the components to interlock with each other, the body of the SEOP probe, and the probe lid. Thus there is only one way for these two components to mate together (**Fig. S5**). Finally, the lower stem holder has a taller side wall than the upper stem holder. When the two components mate with each other, the shorter sidewall slides behind the larger one to ensure a complete SEOP probe seal, thus preventing SEOP probe VT air from escaping (best seen in **Fig. S3b**).

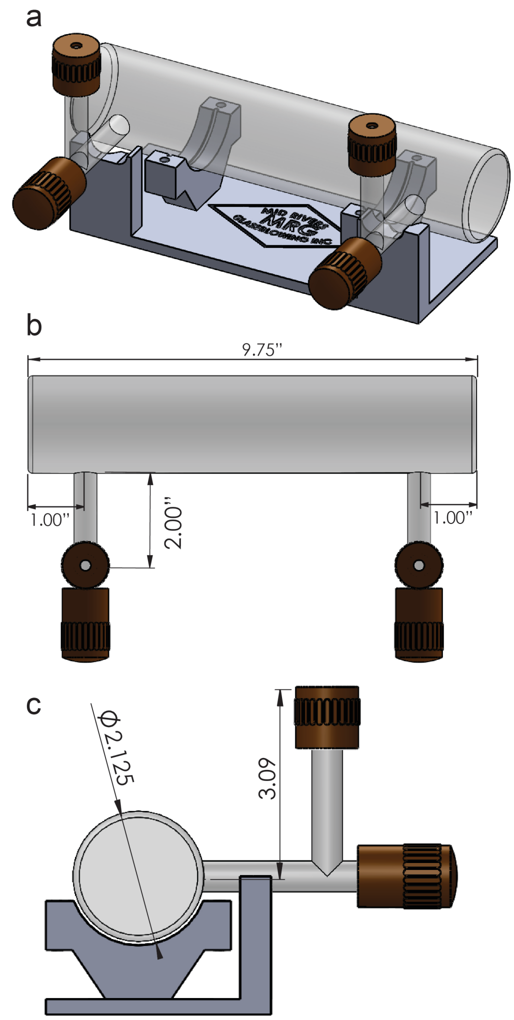

Figure S6. (a) Front view of former with OP-cell (b) Top view of OP-cell with assigned dimensions (c) Side view of former with mounted OP-cell.

d) OP-Cell and 3D Printed OP-Cell Former

The OP-cell is constructed (**Fig. S6b**) from 9.75 in. long tubular glass with a 2 in. inner diameter (ID) and a 2-1/8 in. outer diameter (OD) with optical windows attached on each end, resulting in a 500 mL OP-cell. The side stems are constructed of ½ in. Pyrex tubing joined to Chem-glass pieces. The piece used to seal the OP-cell is a Teflon Stopcock valve (Chem-glass P/N CG-934-01). Attached perpendicular to that valve is a Chem-Thread stem (Chem-glass P/N CG-350-10) containing a compression O-ring used to connect 1/8 in. OD Teflon tubing for gas loading and transfer into and out of the cell.

The 3D printed OP-cell former is a replica design of the base of the TE SEOP probe, but printed with a 1 in. groove in place of the stem holders at the ideal height for the OP-cell side stems to exit the SEOP probe's opening perpendicularly. As mentioned in the main document, scientific glass blowing of custom pieces makes each OP-cell unique. With the aid of the former, inconsistencies of the OP-cells were reduced, allowing reproducing twelve near identical replicas that could be interchanged within, or between each VT SEOP probe design.

The former has a valley cutout groove where the stem holders would be placed, representing the horizontal restrictions placement of the extruding glass. The OP-cell holders provide the vertical alignment needed so that both front and back stems are parallel to each other.

e) NMR Coil Former

The ability to 3D print custom NMR coil formers quickly and easily enhances the ability to reproduce or make a former that can be suited for many applications. The formers used to perform low-field, *in-situ* NMR polarimetry (**Fig. S7**) are 2.5 in. in diameter and ½ in. height, and the central inner portion used to wrap wire has a diameter of 1 in. The hole in the center of the formers (0.26 in.) was made to allow a ¼”-20 threaded rod to pass through the coil and allowing a Teflon nut to bolt it into the TE SEOP probe, thus fixing its position. However, a wire feed-through is also printed into the coil former and TE SEOP probe body allowing the wires to pass to the outside of the SEOP probe. Furthermore, this feature allows these coils to be interchanged with a different coil tuned to a different frequency allowing the study of other xenon isotopes (^{131}Xe) or other noble gases (such as krypton).

f) VHG Laser Diode Array (LDA)

A water-cooled 200 W frequency narrowed Volume Holographic Grating (VHG), or a.k.a. volume Bragg grating (VBG) laser diode array (LDA) developed by QPC Lasers (Sylmar, CA P/N Brightlock Ultra-500 6507-Z002) according to our design requirements is an integral part of the SEOP setup (Fig. 2c). This LDA consists of eight laser diode elements fiber-coupled together to produce a single beam of light. The function of VHGs in LDAs is to work as frequency-selective feedback elements (FSFE) for each individual laser element by reflecting a narrow band of emitted laser light back into the individual laser components, thus forcing them to lase at the injected wavelength. This laser design utilizes “on-chip” volume VHG technology that is manufactured at the wafer level during Metal-Organic Chemical Vapor Deposition (MOCVD). Implementation of such technology results in an order of magnitude narrower (~0.2-0.3 nm) spectral output compared to conventional (broadband) LDAs (~2-3 nm). The improved line width and laser spectral output results in increased photon flux at the correct resonance frequency for Rb absorption (794.8 nm).

The water chiller (KO-Concepts, Titusville, FL; P/N DMC-14) used to cool the LDA allows the spectral output to be fine-tuned over a range of ~1 nm by varying the laser’s diode temperature. The change in temperature directly affects the Bragg gratings of the VHG through expansion (heating) or contraction (cooling), thus increasing or reducing the lasers output centroid wavelength (~0.062 nm/°C) respectively. The wavelength can also be changed (nearly instantaneously) in a similar manner by changing the driving current of the LDA, resulting in a coarse change of ~0.028 nm/amp; the water chiller requires a few minutes for the appropriate temperature change.

Two key innovative feature of this laser are (i) a short, free-standing (~51 mm) solid optical fiber with an 800 µm core that preserves up to 96% of the linear polarization emitted from the laser, and (ii) mating of the solid optical fiber with a custom, integrated, single-piece, detachable optical assembly, which bolts directly onto the laser module. This optical assembly is used to expand, collimate and circularly polarize the emitted laser light to a 2 in. diameter. The new, free-standing, ~51 mm long, 800 µm diameter core fiber and mountable optical assembly have been machined so that when mated, the short fiber is 3 mm away from, and perfectly concentric, with the first expanding lens inside the optical assembly. Soon after the first expanding lens, the beam is directed into a polarizing beam-splitter cube (PBS), which directs most (~96%) of the laser light forward while discarding the other portion into a beam dump. The beam is further expanded to 2 in., collimated, and rendered circularly polarized via a quarter-wave plate. The design allows for the unabsorbed portion of the beam returning from the cell to be discarded into a second beam dump; both beam dumps are thermally managed with two actively air-cooled (via fans) heat sinks. The laser is also equipped with an aiming beam to aid LDA 2 in. beam alignment with the OP-cell. The laser's overall design eliminates the need for separate alignment of an independent optical assembly (and its components) with the LDA module, reduces losses of photon flux throughout the optical path, and greatly facilitates fine alignment with the OP-cell.

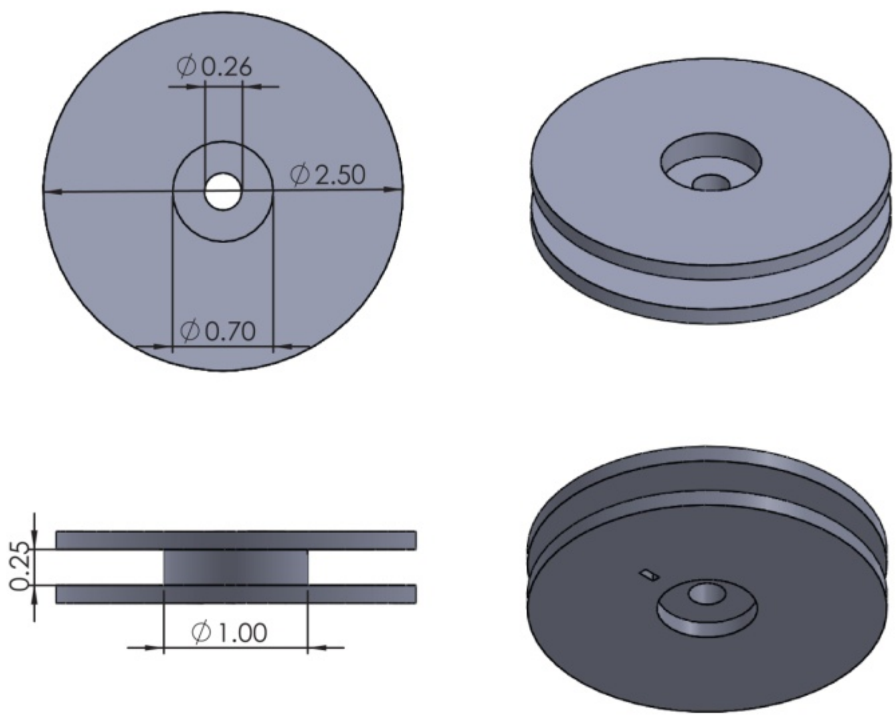

Figure S7. Different views of the 3D NMR Probe former with assigned dimensions.