NASA Astrobiology Early Career Collaboration Award Report on Probing Shielding Tensor Components of Amino Acids using Nuclear Magnetic Resonance

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Abstract

This report outlines the work performed during the two visits to National High Magnetic Field Laboratory (Maglab) funded by NASA Astrobiology Early Career Collaboration Award.

Visit I (08/06/23 - 08/12/23)

Single crystals of N-Acetyl-L-Valine (*L-NAV*) were grown at Western Michigan University (WMU) to be used for the Single Crystal Nuclear Magnetic Resonance (SCNMR) analysis. The SCNMR goniometer probe was designed and constructed at the Maglab.

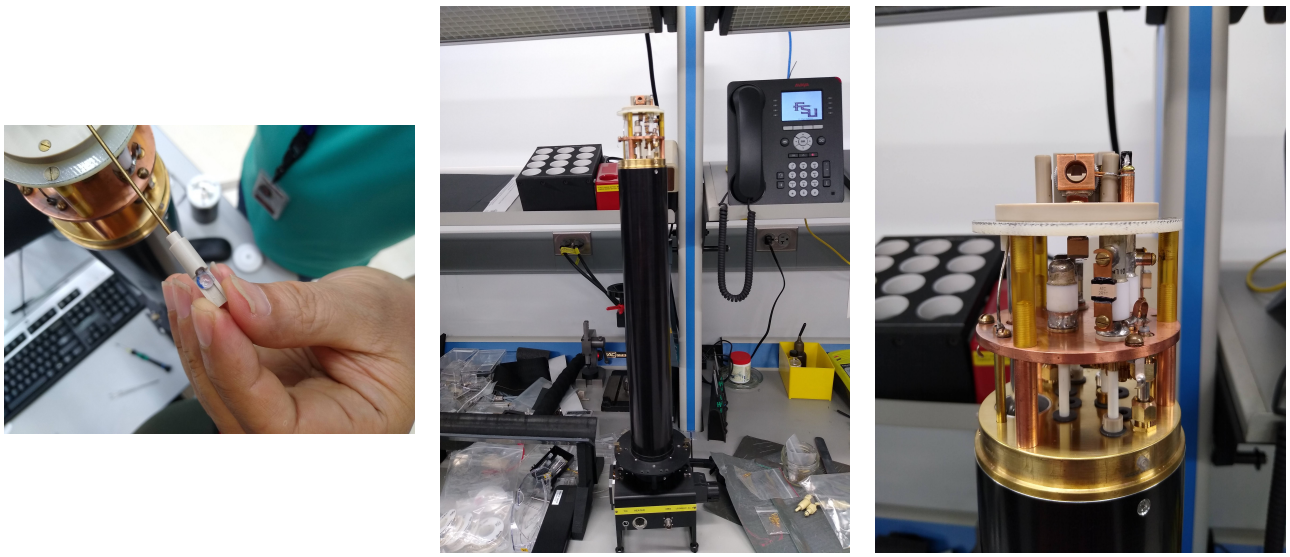

Figure 1: *Left: L*-NAV crystal on goniometer. The crystal is marked for reference. *Center:* SCNMR goniometer probe to be used in 14.1 Tesla NMR magnet. *Right:* Close up view of probe showing its components. On the top is the coil where sample is placed.

The initial aim of our project was to measure the shielding tensor components for ^{14}N in amino acids. The signals from the nucleus were not detected even after several attempts. It could be due to very low gyromagnetic ratio of ^{14}N ($\gamma = 1.934 \times 10^7\,\mathrm{rad\,T^{-1}\,s^{-1}}$), resulting in its low sensitivity. This made us switch our focus to other nuclei and other chiral samples.

Visit II (11/08/23 - 11/15/23)

For future experiments, *B,B,B*-8-hydroxyquinoline-*bis*-isopineylcampheyl-boron (8-HQ(ipc)$_2$B) sample having both boron (B) and nitrogen (N) as chiral centers was chosen. The selection of sample was

based on the presence of ^{11}B which has much higher gyromagnetic ratio ($\gamma = 8.584 \times 10^7$ rad T^{-1} s^{-1}) than ^{14}N. The crystals of the sample of both chirality were grown. Also, the samples of alanine (both *D* and *L*) and glycine (achiral) were enriched with ^{17}O. Selection of ^{17}O (spin = 5/2) was made as it meets the primary objective of the project to measure the shielding tensor components of quadrupolar nuclei (spin > 1/2) in amino acids.

Figure 2: *Left:* 8-HQ(ipc)$_2$B crystals harvested for experiment. *Center:* Glycine crystals enriched with ^{17}O. *Right:* *L*-alanine crystal on goniometer. The crystal is marked for reference.

On the second visit to Maglab, successful detection of ^{11}B and ^{17}O nuclei was done. We could take high quality data with our samples. Each crystal was rotated from -15° to 195° in interval of 15°. The data was collected for rotation of samples in three orthogonal directions. The data will be used to find the shielding tensor components of ^{11}B and ^{17}O in chiral samples. As outlined in the proposal, the results will be used to verify the model that uses the effect of tensor components of amino acids to explain the preferential selection of L-amino acids. That model could explain the origin of the homochirality of amino acids on Earth.

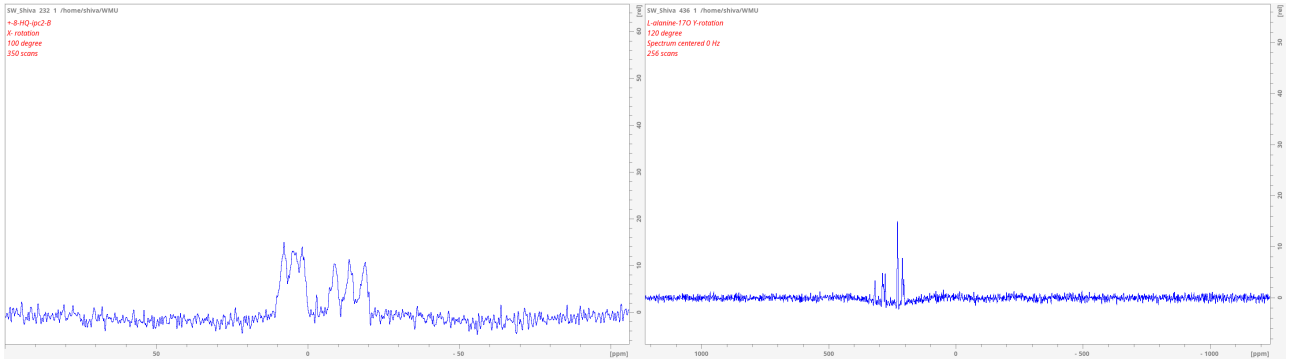

Figure 3: *Left:* Signal for ^{11}B detected in the experiment. *Right:* Signal for ^{17}O detected in the experiment.