Adding Solid-State ^{17}O NMR to the Tool Box for Studies of Organic and Biological Molecules

Jiahui Shen[1], Victor Terskikh[2], Jochem Struppe[3], Alia Hassan[3], Martine Monette[3], Ivan Hung[4], Zhehong Gan[4], Andreas Brinkmann[2], Gang Wu[1]

1. Queen's University; 2. National Research Council Canada; 3. Bruker BioSpin; 4. National High Magnetic Field Laboratory.

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Nuclear magnetic resonance (NMR) spectroscopy is a powerful technique for chemists to obtain detailed information about chemical bonding and molecular structure. However, most successful NMR applications for studying organic and biological molecules to date rely on the detection of "NMR friendly" spin-1/2 nuclei such as ^{1}H, ^{13}C, and ^{15}N. Another key element in organic and biological molecules, oxygen, has rarely been used in NMR studies, largely for two reasons. First, the only NMR-active oxygen isotope, ^{17}O, is exceedingly hard to find in nature (its natural abundance is a mere 0.037%). Second, *^{17}O has an unusual nuclear spin number (I = 5/2), and thus belongs to a special class of nuclei known as quadrupolar nuclei that yield more complex NMR spectra. As such, it is much harder to obtain high-quality, high-resolution NMR spectra for quadrupolar nuclei than for spin-1/2 nuclei*.

This research team has developed a synthetic strategy to introduce ^{17}O-labels onto all oxygen-containing functional groups in D-glucose, which increases the ^{17}O NMR signal intensity by a factor of 1000 over its natural abundance level. To further boost the sensitivity, the MagLab users employed two state-of-the-art NMR technologies. One was to perform the measurement on the most powerful NMR magnet in the world, the MagLab's 35.2T Series Connected Hybrid. The other was to use a new probe recently developed by Bruker that significantly reduces the noise levels of the detector and preamplifier by operating at very low temperatures. These two new technologies drastically enhance the ability to obtain high-quality ^{17}O NMR data for D-glucose (see **Figure**).

This work represents the first time that a complete set of ^{17}O solid-state NMR data was recorded for any carbohydrate molecule, which paves the way for researchers to consider ^{17}O NMR as a new spectroscopic tool in glucose-related research that can range from glucose-binding proteins to glucose metabolism in live cells.

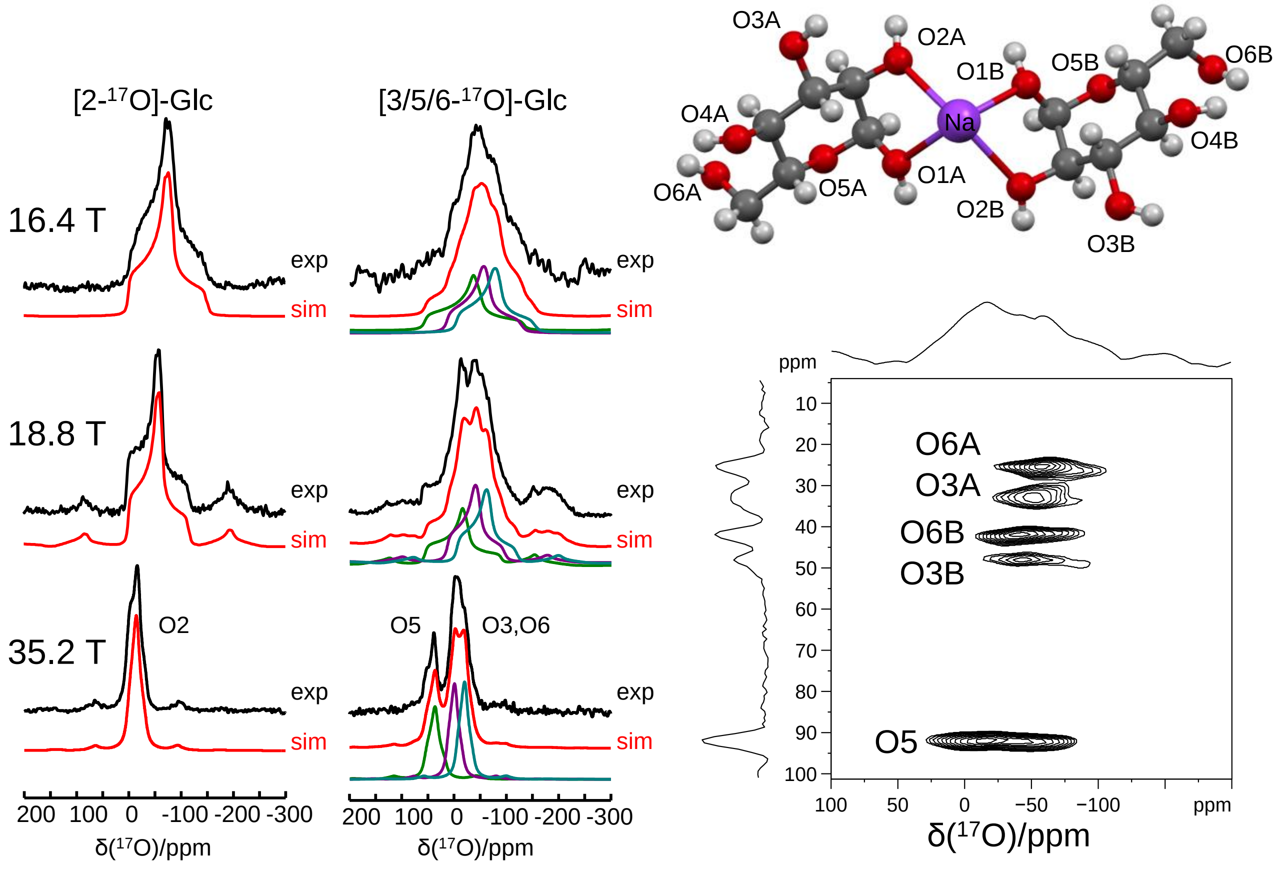

Figure: (top right) Dimer formation of α-D-glucose molecules in the crystal lattice of D-glucose/NaCl (1:1) co-crystal. **(left)** One- and two-dimensional (**bottom right**) ^{17}O NMR spectra of ^{17}O-labeled D-glucose/NaCl (1:1) cocrystal at different magnetic fields.

Facilities and instrumentation used: NMR/MRI Facility: MagLab's 18.8 T/800 MHz; DC Facility: MagLab's 36-T Series Connected Hybrid Magnet.

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