Determination of PROSPECT Scintillator Proton Density for a Neutrino Flux Measurement using Quantitative Nuclear Magnetic Resonance (qNMR) Spectroscopy

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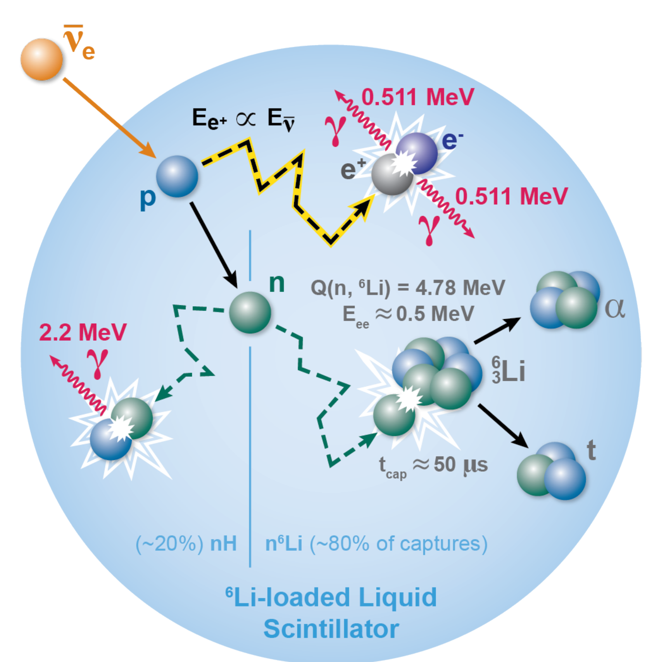
Motivation

The Precision Reactor Oscillation and SPECTrum (PROSPECT) experiment is a short-baseline reactor experiment formerly located at the High Flux Isotope Reactor (HFIR), an 85MW highly-enriched uranium reactor at Oak Ridge National Laboratory (ORNL). One of PROSPECT's goals is to measure the ***absolute antineutrino flux***, a value dependent on several variables that must all be determined to an uncertainty of ~1%:

$$\sigma_f^{obs} = \frac{R^{obs}}{\frac{P_{th}}{\langle E_f \rangle} \cdot \frac{N_p}{4\pi L^2} \cdot \varepsilon_{det}}$$

VALUE	RELATIVE UNCERTAINTY	
R^{obs}	0.9%	✓
P_{th}	1.4%	✓
$\langle E_f \rangle$	0.1%	✓
L	(pending)	⏱
ε_{det}	(pending)	⏱
N_p	**GOAL: ≤ 1%**	**?**



$$\bar{\nu}_e + p \rightarrow e^+ + n$$

Fig. 1: Inverse Beta Decay in the ^{6}Li-doped PROSPECT scintillator.

An improved measurement of the absolute antineutrino flux would improve our knowledge of reactor fission yield, which directly correlates to the total number of neutrinos produced from ^{235}U sources (like HFIR!)

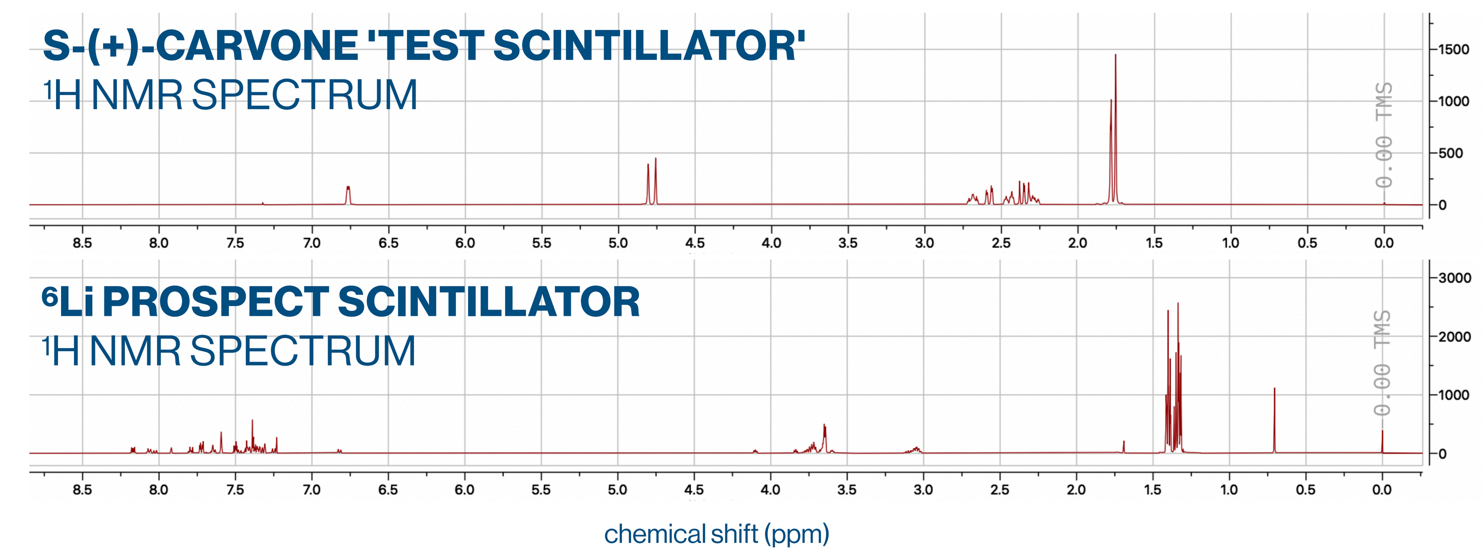
Proton Density Measurement

Elemental combustion (CHN) analysis is the standard method for determining the proton density of a compound. While effective, combustion analysis is not reliably able to produce measurements within the required uncertainty threshold for an absolute measurement.

Traditional NMR is able to identify compounds by their bonds to active nuclei (in this case ^{1}H, or protium), but is unable to provide any *quantitative* information on the active nuclei concentration. By combining the unknown material with a known reference chemical (a 'standard'), the hydrogen density of the material can be comparatively determined via integration.

Methods

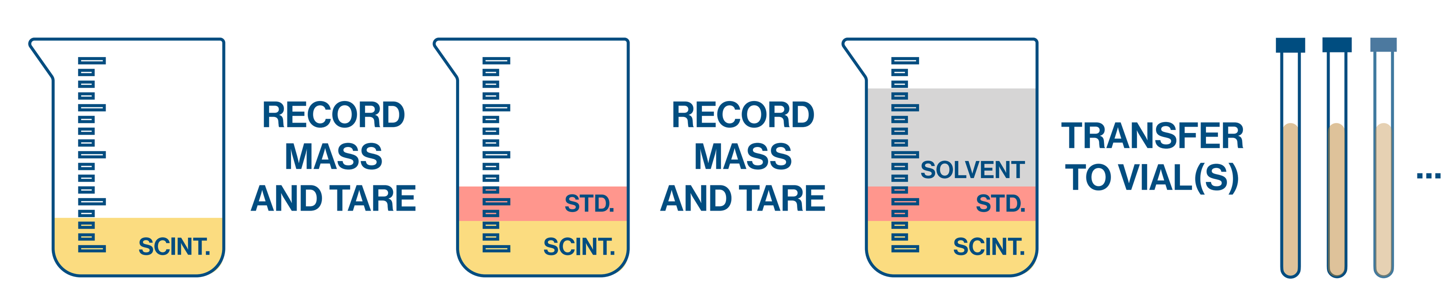
In refining the qNMR procedure, a suitable analogue for the scintillator was chosen: a compound with a similarly-complex ^{1}H NMR spectrum, but a known chemical formula (and thus proton density):



Three chemical standards, all soluble in the deuterated chloroform solvent, were chosen for their sharp, well-defined, and distinct peaks. These standards are all highly-pure (≥ 99.8% assay) and have a known chemical structure (number of hydrogen atoms per molecule, $n_{H_{std.}}$):

STANDARD	FORMULA	T_1	CHEM. SHIFT	MOLAR MASS
duroquinone	($C_{10}H_{12}O_2$)	3.3s	δ = 2.02 ppm	164.20 ± 0.02 g/mol
dimethyl sulfone	($(CH_3)_2SO_2$)	2.7s	δ = 3.0 ppm	94.13 ± 0.02 g/mol
1,3,5 trimethoxybenzene	($C_6H_3(OCH_3)_3$)	2.2s 4.7s	δ = 3.75 ppm δ = 6.1 ppm	168.19 ± 0.02 g/mol

NMR samples can be prepared by mixing the test scintillator and one of the three standards into deuterated chloroform ($CDCl_3$) solvent:

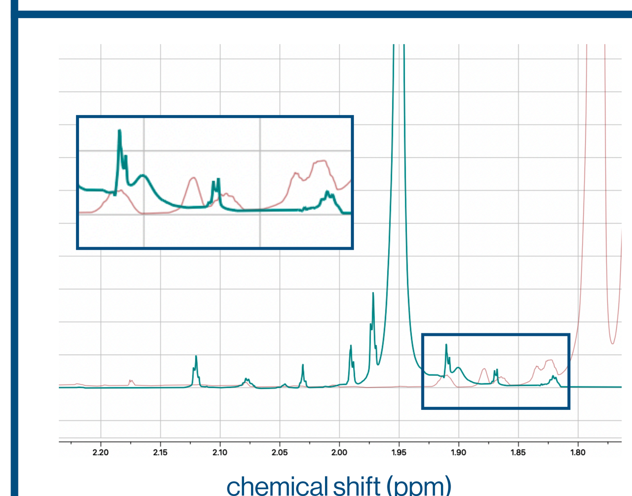
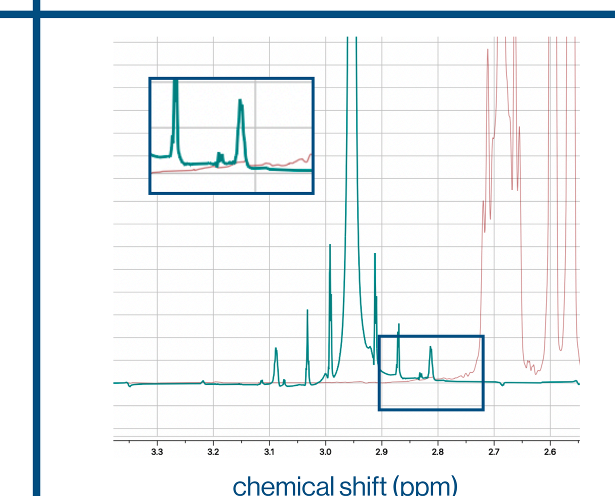


These vials are scanned in the NMR spectrometer, providing a spectrum that is then phase- and baseline-corrected. With this corrected spectrum, the peaks of the scintillator and standard are integrated. The total area under the scintillator regions ($I_{scint.}$) is directly proportional to the total number of active nuclei, so the known mass ($m_{std.}$) and structure ($n_{H_{std.}}$) of the standard can be used to find the proton density of the scintillator (in units of hydrogen molecules per gram of scintillator):

$$\rho_{H_{scint}} = \left(\frac{I_{scint.}}{I_{std.}}\right) \times \left(\frac{m_{std.}}{m_{scint.}}\right) \times \left(\frac{N_A n_{H_{std.}}}{M_{std.}}\right)$$

Results

Initial results using duroquinone and dimethyl sulfone were promising, but ultimately did not meet the 1% uncertainty threshold, largely due to overlap between the standard peak and scintillator signal. Below is the average percent error (relative to the known 'test scintillator' proton density) for each of the two mentioned standards:

duroquinone	dimethyl sulfone
$\%Err_{\rho_H} \approx -1.996\%$	$\%Err_{\rho_H} \approx -0.975\%$
	

Using 1,3,5 trimethoxybenzene (δ = 3.75 ppm, 6.1 ppm) as a standard eliminates all overlap between scintillator and standard spectrum regions, bringing the measured proton density much closer to the expected value with an average %Err of **-0.25%**:

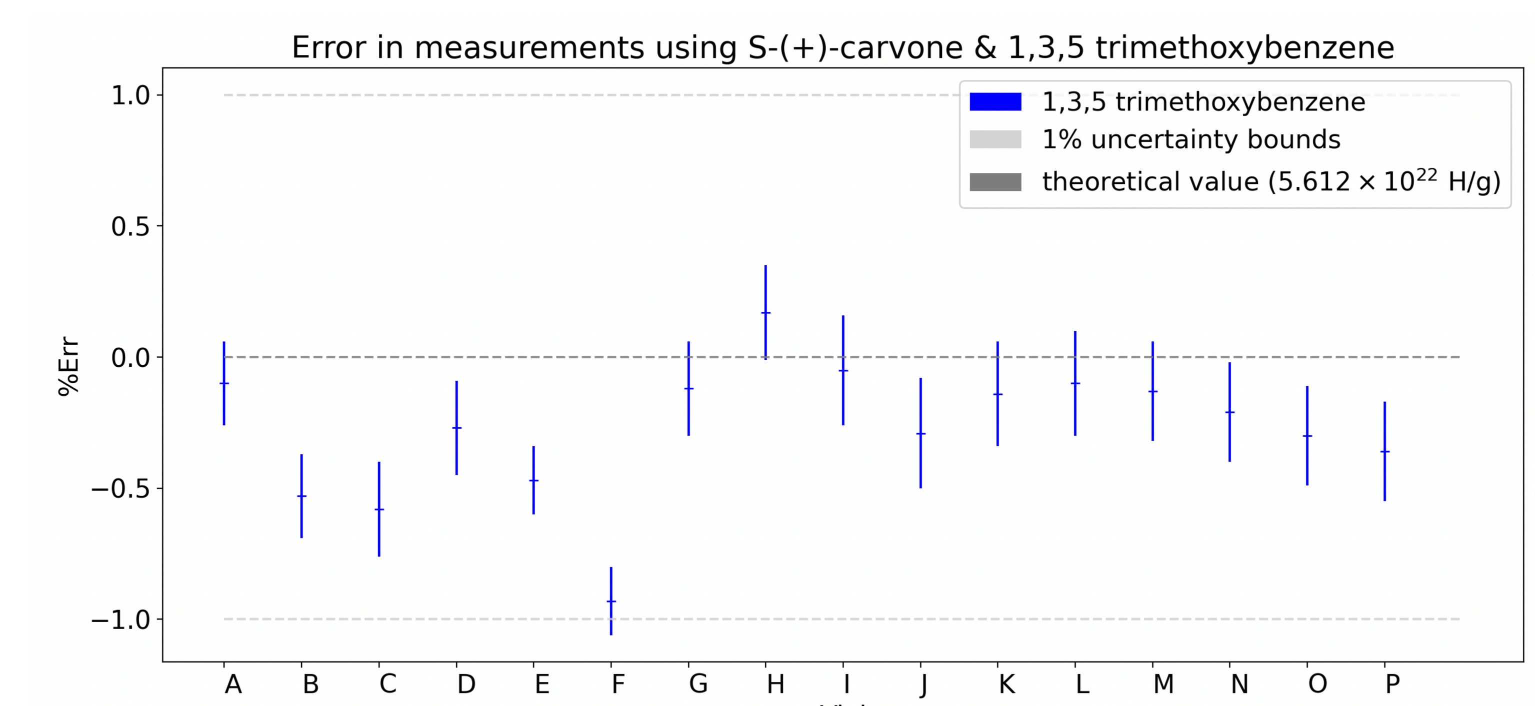


Fig. 2: Percent error in the measured proton density of S-(+)-carvone using 1,3,5 trimethoxybenzene as the standard

By avoiding scintillator-standard overlap and carefully preparing samples, the proton density of S-(+)-carvone can be reliably determined using the qNMR process. This method shows potential for use in the precise evaluation of the proton density of complex unknown solutions, specifically the PROSPECT ^{6}Li-doped liquid scintillator.

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