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# A new water-based scintillator for efficient Cherenkov and scintillation separation

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## Abstract

Neutrinos offer a unique window into the world around us, allowing us to probe otherwise unreachable regions like the interior of stars and the depths of the earth, as well as potentially offering a mechanism for monitoring nuclear activity. Both pure-water and organic liquid scintillators have been used as the detection medium of large-scale neutrino detectors. Organic liquid scintillators offer higher sensitivity at lower energies, which is desirable for many applications, but detection of the Cherenkov radiation required for directional sensitivity is very difficult. A possible solution is to use water-based liquid scintillators (WbLS), where some fraction of the water is replaced with a micellar solution of the liquid scintillator. This can enhance the detection sensitivity beyond that of pure water, without significantly affecting the ability to leverage the topological Cherenkov signature. Very specific scintillation properties are required to achieve this goal: the scintillation decay time should be significantly slower than that of the Cherenkov emission, so timing-based discrimination of Cherenkov light from scintillation can be applied. At the same time, the light yield should be high enough to enhance the overall sensitivity of the detector, but without losing too much of the Cherenkov light. In this work, we report a new water-based liquid scintillation cocktail based on a 9-methylcarbazole fluorescent dye and a linear alkylbenzene solvent. The proposed composition offers 13.8 ns scintillation decay time and 368 nm emission that matches the desired properties.

## 1 Introduction

One of the main challenges in neutrino physics is the difficulty in detecting and measuring neutrinos [1]. Neutrinos are abundant in the universe, but they are also one of the least understood particles. Because they interact so weakly with other matter, it is difficult to build instruments that are sensitive enough to detect them. In addition, because their interactions are rare even in large detectors, it can be difficult to differentiate the neutrino signals from the background noise from natural radioactivity or cosmic radiation.

Neutrinos can offer insight into a number of Nature's mysteries, including the inner workings of our Sun, the explosion mechanism of a supernova, and even the source of the

dominance of matter over antimatter in our Universe. Neutrinos are produced as a by-product of nuclear activity and, due to the extremely weak nature of their interactions, form a signature that cannot be shielded. As a result, there are several potential applications for neutrinos within the realm of nuclear security under discussion, including monitoring of reactors, and test site transparency, which refers to demonstrating the absence of nuclear testing.

There are several methods for detecting neutrinos, but most of them rely on the fact that when a neutrino interacts with matter, it can produce charged particles, such as electrons or positrons. These charged particles can be detected using a variety of instruments. In inverse  $\beta$ -decay (IBD), an electron antineutrino ( $\bar{\nu}_e$ ) interacts with a proton ( $p$ ), producing a positron ( $e^+$ ) and a neutron ( $n$ ):

$$\bar{\nu}_e + p \rightarrow e^+ + n, \quad (1)$$

and the resulting positron kinetic energy is approximately  $E_{e^+} \simeq E_\nu - 1.8$  MeV. For reactor antineutrinos with energies of 2–8 MeV, this corresponds to positron kinetic energies of about 0.2–6 MeV. Including annihilation gammas, the visible energy in the detector is  $E_{\text{vis}} \simeq E_\nu - 0.78$  MeV. Therefore, positrons from IBD are expected to have visible energies extending from just above 1 MeV up to about 7 MeV for typical reactor antineutrinos. Nuclear explosions produce mainly electron antineutrinos with energies in the 1–10 MeV range, peaking at 2–4 MeV, similar to reactor antineutrinos but released in a burst lasting only a few seconds. The positron, carrying most of the antineutrino energy, deposits its energy and annihilates with an electron producing a prompt signal with energy ranging from 1 MeV to about 8 MeV.

In water-based neutrino detectors, the positron is detected via its production of Cherenkov radiation. The production of Cherenkov light requires the charged particle to travel faster than the phase velocity of light in the target medium,  $v > c/n_r$ , where  $v$  is the velocity of the particle,  $c$  is the speed of light in vacuum, and  $n_r$  is refractive index. The refractive index of water  $n_r$  is typically  $n_r \approx 1.33$ . As a result, Cherenkov light production has a species-dependent energy threshold and doesn't result in any photon emission below it. The threshold is given by  $v = \frac{c}{n_r}$  [2], which corresponds to a minimum kinetic energy of

$$E_c = m \cdot \left( \frac{1}{\sqrt{1 - \frac{1}{n_r^2}}} - 1 \right), \quad (2)$$

where  $m$  is the particle mass. For electrons (mass  $m_e = 511$  keV), this gives the Cherenkov threshold of  $E_c \approx 0.26$  MeV in water.

However, the efficiency of Cherenkov radiation is low and limits the sensitivity for detection of low-energy neutrinos. The number of Cherenkov photons emitted per unit path length and per unit wavelength is given by the Frank–Tamm formula [3, 4]:

$$\frac{d^2 N}{dx d\lambda} = \frac{2\pi\alpha z^2}{\lambda^2} \left( 1 - \frac{1}{\beta^2 n_r^2} \right), \quad (3)$$

where  $N$  is the number of photons,  $x$  is the path length,  $\lambda$  is the wavelength,  $\alpha$  is the fine-structure constant ( $\approx 1/137$ ),  $z$  is the particle charge in units of the elementary charge,

$\beta = v/c$  is the particle velocity relative to the speed of light in vacuum (for a 1 MeV electron,  $\beta \approx 0.94$ ), and  $n_r$  is the refractive index of the medium. A relativistic track ( $\beta = 1$ ) in water ( $n \approx 1.33$ ) produces about  $N_0 \approx 250 \text{ cm}^{-1}$  optical photons in a wavelength interval between 300 nm and 500 nm [5], which is a typical sensitive spectral region of photo-detectors used in neutrino detectors. The typical range of a 1 MeV electron in water is about 4.3 mm. Assuming that  $\beta$  doesn't change significantly and ignoring Cherenkov threshold, the upper bound for the total number of Cherenkov photons produced can be estimated as:

$$N_{\text{total}} \approx 250 \times 0.43 \approx 108 \text{ photons/MeV}$$

(in the 300–500 nm range).

Liquid scintillators allow for much higher efficiency of kinetic energy conversion into light, offering a lower neutrino energy detection threshold and improved resolution. Liquid scintillators typically produce on the order of  $\approx 10,000$  photons/MeV emitted isotopically in all directions, compared to  $\approx 100$  photons/MeV for Cherenkov radiation. This large difference in photon statistics means that scintillators provide a substantially higher signal-to-noise ratio in the presence of photomultiplier tube (PMT) dark counts and other instrumental backgrounds. However, scintillation photons are emitted in response to all charged particles. As a result, other sources can mimic the coincidence signature of the IBD interaction, for example an atmospheric neutrino can collide with a nucleus in the target material, and liberate a neutron. The recoiling nucleus produces scintillation that can mimic the prompt positron and, if the neutron then is captured, the interaction can be difficult to distinguish from an IBD signal. The use of Cherenkov light provides a tool to reject such background, since the nucleus will not produce the Cherenkov signature expected from the positron.

Water-based liquid scintillators (WbLSs) are a class of materials that attempts to find a synergy between pure water and organic liquid scintillators for the detection of neutrinos. Normally, liquid scintillators do not mix with water. However, the use of a surfactant allows the creation of a microemulsion of a liquid scintillator by encapsulating hydrophobic liquid scintillator in surfactant aggregates called micelles. Surfactants typically consist of molecules that contain both hydrophilic (water-attracting) and hydrophobic (water-repelling) parts. A typical micelle has a spherical shape with the hydrophilic regions in contact with the water and the hydrophobic regions in the center of the micelle. The hydrophobic center of the micelle confines the organic liquid scintillator inside.

When a neutrino interacts in WbLS, it produces secondary charged particles such as electrons or positrons that travel several centimeters through the medium. Because the scintillator is dispersed in nanometer-scale micelles throughout the water, these particles inevitably pass through and deposit energy in both phases along their tracks. Energy deposited in the scintillator micelles produces scintillation light. Any portion of the track where the particle moves faster than the Cherenkov threshold in water produces Cherenkov photons. Water itself is non-luminescent, so energy deposited outside the scintillator micelles does not generate scintillation. The presence of scintillator increases the total light yield and improves sensitivity to low-energy neutrino interactions, while the predominantly aqueous environment preserves a measurable Cherenkov component. Although scintillator micelles absorb strongly in the UV, the Cherenkov spectrum extends into the visible range. Cherenkov photons between approximately 350 and 550 nm fall within the transparency window of the scintillator phase and can reach the photodetectors without significant absorption,

Table 1: Major liquid scintillator neutrino detectors, their scintillator material formulations, target mass/volume,  $\tau$  fast scintillation decay component, and references. Abbreviations: **DPA** – 9,10-diphenylanthracene; **PC** – pseudocumene (1,2,4-trimethylbenzene); Norpar-15 – normal paraffins with 14 to 17 carbon atoms; **LAB** – linear alkyl benzene; **p-TP** – para-terphenyl (primary fluor); **Hex** – hexanol; **IPB** – cumene (isopropylbenzene); **PPO** – 2,5-diphenyloxazole (primary fluor); **bis-MSB** – 1,4-bis(2-methylstyryl)benzene (wavelength shifter); **Gd** – gadolinium compound (neutron capture agent); **n-C12** – normal-dodecane; **b-PBD** – butyl-phenyl-bipheny-oxydiazole; **TeBD** – tellurium butanediol; **DDA** – N,N-Dimethyldodecylamine; **BHT** – butylated hydroxytoluene

| Detector   | Scintillator                                       | Mass (tons)       | $\tau$ (ns)      | Ref.    |
|------------|----------------------------------------------------|-------------------|------------------|---------|
| KamLAND    | n-C12 + PC + PPO                                   | ~1000             | 6–8              | [6]     |
| Borexino   | PC + PPO                                           | ~280              | 3.3–3.6          | [7, 8]  |
| Daya Bay   | LAB + PPO + bis-MSB (+ Gd)                         | 200 + 185 (Gd-LS) | N/A              | [9, 10] |
| SNO+       | LAB + PPO                                          | 780               | 5                | [11]    |
|            | LAB + PPO + TeBD + DDA + BHT + bis-MSB             |                   |                  |         |
| LSND       | Mineral oil <sup>1</sup> + b-PBD                   | 167               | 2                | [12]    |
| CHOOZ      | Norpar-15 + IPB + Hex + Gd + p-TP + bis-MSB        | 5                 | ~7               | [13]    |
|            | Norpar-15 + IPB + Hex + PPO + DPA                  | 107               | ~7               |         |
| Palo Verde | Mineral oil + PC + Gd + PPO + bis-MSB <sup>2</sup> | 11.3              | <10 <sup>3</sup> | [14–17] |

enabling direct detection of Cherenkov light. The simultaneous collection of scintillation and Cherenkov photons supports improved event reconstruction and thereby enhances the precision of neutrino measurements [18].

One of the main advantages of WbLSs is that they allow the combination of some Cherenkov sensitivity of water-based detectors with a high light yield of liquid scintillators, allowing the detection of low-energy neutrinos. Future neutrino experiments may use multiple technologies for the separate detection of scintillation and Cherenkov photons. Cherenkov light is emitted essentially instantaneously (tens of picoseconds), whereas the scintillation signal exhibits nanosecond-scale kinetics. Slowing down the scintillation of the WbLS cocktail would allow for improved pulse-shape discrimination when prompt photons can be classified as mostly due to Cherenkov radiation, while delayed photons are mostly due to scintillation [19–22]. Cherenkov photons would fall within an early time window of order 0-1 ns, depending on detector timing resolution, while scintillation photons dominate later times. Tab. 1 lists major liquid scintillator neutrino detectors together with their scintillator material formulations and fast scintillation decay component. Most of these compositions are dominated by PPO and bis-MSB fluorescent dyes with decay times ranging from 2 ns (LSND) to 6-8 ns (KamLAND). The Palo Verde experiment has not reported scintillation decay times but upper limit of 10 ns could be estimated from historical data. This highlights the need to develop WbLSs with decay times significantly slower than those of most research and commercially available materials, see also Tab. 2. This time sorting of the detected photons works only if some of Cherenkov light can travel essentially unaffected by the absorption of the organic scintillator. The Cherenkov radiation spectrum is very wide and extends into the visible region. By selecting the appropriate organic dye in the scintillator, it is possible to have an UV ( $<400$  nm) scintillation emission, leaving the Visible region ( $>420$  nm) clear for the Cherenkov light. Furthermore, while Cherenkov radiation is broadband, only its long-wavelength component ( $>420$  nm) propagates efficiently in WbLS without being reabsorbed. For this reason, the WbLS cocktail has to be formulated so that the scintillation emission is confined predominantly to the near-UV ( $<400$  nm), where absorption and re-emission by the fluor are strong but Cherenkov production is comparatively weak. This intentional spectral separation enables “spectral sorting”: photons with wavelengths above  $\sim 400$  nm form an essentially pure Cherenkov sample, whereas photons in the UV–blue region contain the scintillation signal and only a small prompt Cherenkov component. Such a wavelength-based division can be implemented using dichroic filters or wavelength-selective optics, providing an additional practical method to distinguish scintillation from Cherenkov light in hybrid detectors [23]. Ideally, WbLSs would also allow for a tunable decay time and light yield that enables different modes of operation of the neutrino detector, depending on the need for higher detection sensitivity or directional resolution. This could open a new opportunity for a broad range of applications of a single neutrino detector that could be tuned to the desired detection requirements.

Table 2 summarizes representative liquid scintillators, water-miscible cocktails (WmC), and WbLS research formulations together with their main characteristics. EJ-309, produced by Eljen Technology, is a fast organic liquid scintillator with excellent pulse-shape discrimination capability, widely used in neutron–gamma separation studies. BC-501A, produced by Luxium Solutions, is a classical commercial formulation delivered by a different supplier, offers similar properties as EJ-309. EJ-351 (Eljen Technology) represents a water-miscible

cocktail, providing moderate light output while tolerating limited aqueous content. Ultima Gold, produced by Revvity, is a family of cocktails optimized for liquid scintillation counting of aqueous solutions. To the best of the authors’ knowledge, there are currently no commercial WbLS formulations available; therefore, we reference a research study for comparison. To date, only a single WbLS formulation, based on LAB with PPO, has reported both scintillation decay times and scintillation emission spectra. Despite the diversity of commercial and experimental materials, none of these formulations exhibit scintillation decay times in the intermediate range of 10–20 ns combined with emission below 400 nm, which are the target properties motivating the present study.

Table 2: Summary of basic properties of commercially available liquid scintillators, water-miscible cocktails, and previously researched WbLS formulations.  $\lambda_{em}$  – emission peak,  $\tau$  – scintillation decay time of a fast component

| Name / Formulation    | Group | Commercial       | $\lambda_{em}$ (nm) | $\tau$ ( ns) | Reference |
|-----------------------|-------|------------------|---------------------|--------------|-----------|
| EJ-309 (Eljen)        | LS    | ✓                | 424                 | 3.5          | [24]      |
| BC-501A (Luxium)      | LS    | (✓) <sup>4</sup> | 425                 | 3.2          | [25]      |
| EJ-351 (Eljen)        | WmC   | ✓                | 425                 | 3.8          | [26]      |
| Ultima Gold (Revvity) | WmC   | ✓                | 428                 | 3.1          | [27–29]   |
| LAB + PPO             | WbLS  | ✗                | 360–380             | 2.0–2.7      | [21, 30]  |

LS – Liquid Scintillator, WmC – Water-miscible Cocktail, WbLS – Water-based Liquid Scintillator

To deliberately develop Water-based Liquid Scintillators (WbLS) for future neutrino detectors, it is necessary to articulate a set of performance targets, even though the exact requirements remain under active discussion within the community. In general, next-generation experiments demand optical transparency with attenuation lengths exceeding 10 m at the scintillation emission wavelength and similarly long scattering lengths to preserve directional information. One approach is for the scintillation timing profile to be significantly slower than in previous experiments, with no fast scintillation component and a tunable slow component in the 10-100 ns range that enables separation of Cherenkov and scintillation light. A light yield on the order of 100 photons/MeV is sufficient to achieve calorimetric performance for neutrino beam events (GeV-scale energies) while maintaining a large early-time Cherenkov window. For low-energy physics, such as neutrino less double beta decay, a much higher light yield is critical (10,000 photons/MeV or higher). The scintillation emission spectrum should be narrowly peaked below 400 nm (ideally around 320–390 nm with  $\leq 40$  nm FWHM), ensuring minimal spectral overlap with the visible Cherenkov region and within the acrylic vessel transparency. These values provide a practical framework for assessing WbLS formulations, high transparency, controlled timing, moderate light yield, and UV-weighted emission, while acknowledging that the precise optimization will depend on the specific physics goals of forthcoming neutrino experiments.

Our previous attempts at slowing down scintillation process of WbLSs were limited to varying the primary dye concentration [30]. In this work, we propose to slow down the scintillation process by replacing the primary dye with a slower fluorophore, while using a

<sup>4</sup>Recently discontinued.



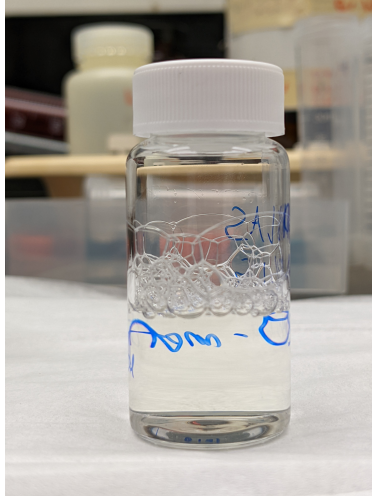


Figure 2: A photograph of the studied WbLS cocktail showing the typical appearance of these scintillating microemulsions.

cuvettes and subtracted from steady-state and pulse X-ray data. Details of the procedure has been described in the Appendix. No attempts were made to degas the samples due to the tendency for foaming.

Steady-state X-ray excited luminescence was measured using a Bruker 50 kV, 50 mA rotating copper anode X-ray generator, directed into the sample perpendicular to the collection optics. The sample emission was dispersed using a SpectraPro-2150i spectrometer and detected with a PIXIS:100B charge-coupled device (CCD) camera. Emission spectra were corrected for spectrometer transmission, CCD camera sensitivity, and dark current. An exposure time of 10 minutes was used for both the radioluminescence measurement and dark frames. The CCD dark current was estimated from 10 dark frames.

Scintillation time decays were measured using time-correlated single-photon counting (TCSPC) with a Hamamatsu N5084 light-excited X-ray tube, operated at 40 kV, driven by 200 fs, 400 nm Ti:Sapphire Coherent Mira 900 laser pulses. A Hamamatsu R3809U microchannel photomultiplier tube (PMT) was used to detect scintillation photons and generate the stop signal. No wavelength discrimination was used to select the light emitted by the samples. Start pulses from the Ti:Sapphire laser and stop pulses from the microchannel PMT were processed through an Ortec 9308 picosecond analyzer in a single-hit mode. The ratio of stop-to-start pulse rates was kept below 1.2% to minimize pile-up and distortion of the scintillation profile. The instrument response function (IRF) was determined using a  $\sim 3 \times 3 \times 3 \text{ mm}^3$  single crystal of  $\text{PbF}_2$ , chosen for its prompt Bremsstrahlung emission under X-ray excitation. To suppress internal reflections and minimize photon trapping, all crystal faces except the one facing the photodetector were coated with black paint. The measured temporal profile of the Bremsstrahlung signal was fitted with a Gaussian function, yielding an IRF full width at half maximum (FWHM) of 197 ps. The scintillation decay profiles were fitted using a double-exponential rise time and a single-exponential decay time function:

$$I(t) = A \left( 1 - e^{-t/\tau_{r1}} - e^{-t/\tau_{r2}} \right) e^{-t/\tau_d}, \quad (4)$$

where  $\tau_{r1}$  and  $\tau_{r2}$  are the prompt and delayed rise time constants, and  $\tau_d$  is the decay time

constant. As the measured exponential rise times were slower than the IRF they were not deconvolved.

Photoluminescence emission and excitation spectra were collected using a Fluorolog 3 (Horiba Jobin Yvon) spectrophotometer. Absorbance measurements were performed using an Agilent 8453 UV-Vis spectrometer with a 10-second integration time.

### 3 Results

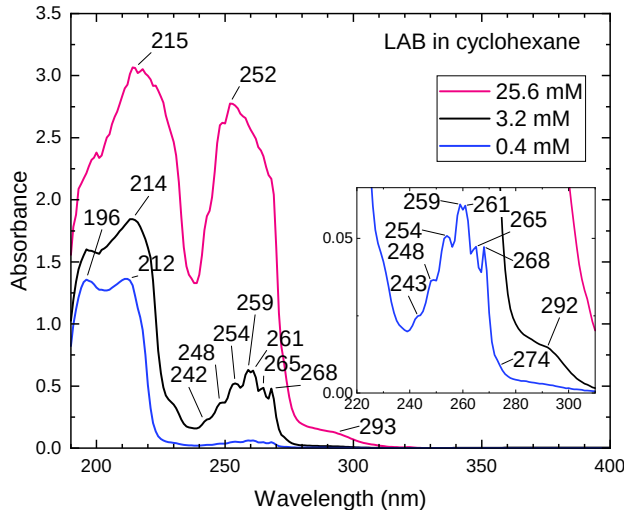


Figure 3: Absorption spectrum of LAB in cyclohexane measured as a function of concentration. Inset shows details of the 220-310 nm absorption range of 0.4 mM solution.

Fig. 3 shows absorption spectra of LAB in cyclohexane for three different concentrations. The highest concentration sample 25.6 mM has two major absorption peaks: 215 nm and 252 nm. A shoulder between 280 nm and 310 nm is observed with a local maximum at around 293 nm. A vibrational structure is not clear for any peak at 25.6 mM. Following the naming convention of Perimeter Free Electron Orbital (PFE0) model [32], we interpreted the 252 nm peak as  $^1A \rightarrow ^1L_b$  transition of the phenyl ring, while the peak at 215 nm is interpreted as  $^1A \rightarrow ^1L_a$  transition. The decrease in the concentration to 3.2 and 0.4 mM reveals the vibration structure of the  $^1L_b$  transitions. The change of absorbance is not proportional to the concentration due to non-linear response of the spectrometer for optical densities larger than 2.

The excitation and emission spectra of the 3.2 mM LAB solution diluted in cyclohexane are shown in Fig. 4, together with an absorption spectrum expressed as molar extinction coefficient  $\epsilon$ . The emission spectrum has a maximum at 289 nm when excited at  $\lambda_{exc} = 250$  nm; a weak vibrational structure is visible. The excitation spectrum has a peak at 259 nm. The vibrational structure of the excitation peak is less obvious than that in the absorbance spectrum. The excitation peak at 259 nm can be assigned to the  $^1A \rightarrow ^1L_b$  transition as previously seen in the absorption spectrum. Conversely, the 289-nm peak is the related reverse transition  $^1L_b \rightarrow ^1A$ , as suggested by the reflection symmetry between excitation

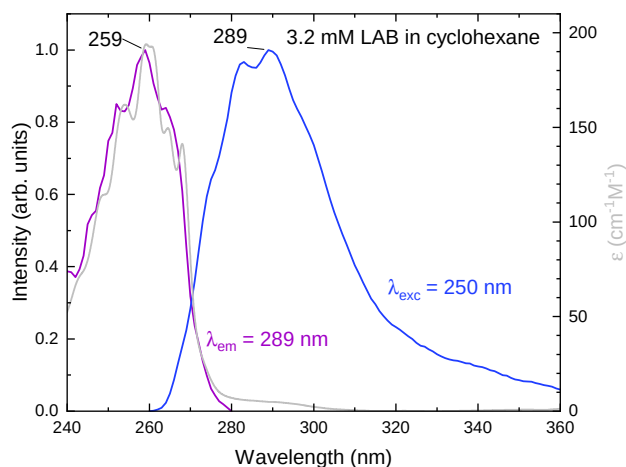


Figure 4: Photoluminescence excitation (purple), emission (blue), and molar extinction coefficient (gray) spectra of a 3.2 mM LAB solution in cyclohexane. The photoluminescence spectra were acquired using a front-face measurement geometry.

and emission spectra. The 290 nm shoulder in the absorbance spectrum does not contribute to the excitation of peak 289 nm and seems to have a different origin.

The surfactant used in the proposed cocktail, LAS, has a chemical structure similar to that of the solvent, LAB, see Fig. 1. Both compounds have a phenyl ring attached to an alkyl chain. The main difference is the presence of the polar  $\text{SO}_3^-$  group in the surfactant. This polar group can affect the electron density in the phenyl group and consequently affect the emission spectrum. Fig. 5 shows photoluminescence emission excited at 250 nm (orange) and excitation spectrum of the emission wavelength of 296 nm in a 101.6  $\mu\text{M}$  LAS solution in cyclohexane. The absorbance of 26.0 mM LAS solution expressed in units of molar extinction coefficient  $\epsilon$  (gray) is provided for reference. The observed emission spectrum has a maximum at around 302 nm, which is similar to the emission spectrum of LAB, see Fig. 4. The excitation spectrum of LAS coincides with the onset of absorption at  $\sim 270$  nm. The maximum of the LAS excitation spectrum at 254 nm is located at an energy very similar to that of the maximum excitation intensity of LAB at 259 nm. It appears that the emission in both the LAS and LAB originates from the phenyl group, resulting in similar emission and excitation spectra.

Fig. 6 shows emission, excitation, and absorption spectra of 0.31 mM 9-methylcarbazole in cyclohexane solution. The mirror symmetry relation between excitation and emission spectra is very clear and indicates little differences in the nuclear configurations of the excited and ground states. The maximum emission intensity is located at 361 nm, with an additional peak at 345 nm and a shoulder at  $\sim 380$  nm. The excitation of 360-nm emission (green) coincides with the absorption spectrum (gray).

Fig. 7 shows the optical properties of the new WbLS cocktail. The blue and red curves correspond to photoluminescence emission spectra excited at 280 nm and measured in Front Face (FF) and Right Angle (RA) configurations, respectively. The FF measurement has a significant tail in the range of 290-335 nm and a peak at 352 nm. RA measurement lacks these features. Both spectra are nearly identical above 360 nm sharing the maximum at 367

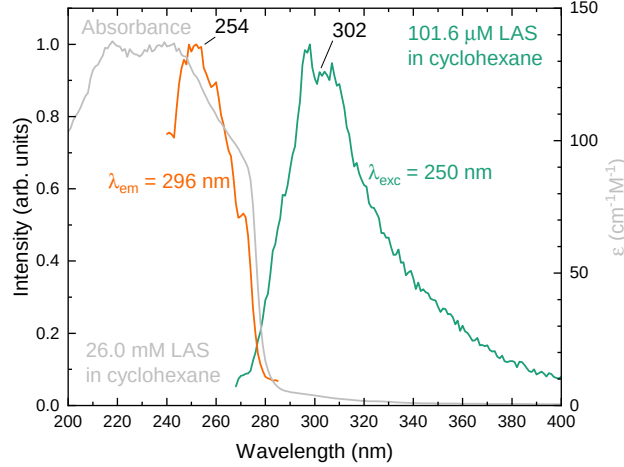


Figure 5: Photoluminescence excitation (orange) and emission (green) spectra of a 101.6  $\mu\text{M}$  LAS solution in cyclohexane, and molar extinction coefficient  $\epsilon$  of a 26.0 mM LAS in cyclohexane (gray). The photoluminescence spectra were acquired using a right-angle measurement geometry.

nm and a shoulder peak at 387 nm. This difference can be explained by self-absorption of the sample, as the absorption band at the 300-350 nm range is reaching 3 OD at 330 nm (gold curve) and is strongly overlapping with the sample emission. The excitation spectrum (green line) of the 352 nm emission follows a trend similar to that of absorbance in the range 300-340 nm; however, the absorbance measurement reaches the saturation value of 4 OD below 300 nm and could not be interpreted. The observed excitation peak at 293 nm does not correspond to any of the absorption or excitation peaks observed in diluted components of the WbLS; compare Figs. 6, 4, and 5. This can be explained by the high optical density of the WbLS leading to distortions of the excitation spectrum.

Fig. 8 shows X-ray excited luminescence of the WbLS sample (purple). The spectrum has been corrected for the Suprasil cuvette scintillation as described in the appendix. A photoluminescence spectrum of the same sample excited at 280 nm RA (blue curve) and a photoluminescence emission spectrum of 0.31 mM 9-methycarbazole (9-mCz) in cyclohexane excited at 280 nm RA (green curve) were provided for reference. Both X-ray-excited and optically excited spectra at RA have a maximum at around 370 nm. Compared to a 9-mCz dilute solution in cyclohexane, the WbLS PL spectrum misses the emission peak at around 352 nm. Furthermore, the x-ray excited spectrum is shifted around 9 nm toward red in respect to the 9-mCz cyclohexane solution. The disappearance of the 352 nm peak in the X-ray excited spectrum is analogous to the disappearance of that peak in the PL spectra shown in Fig. 7 and can be explained by significant self-absorption of 9-mCz.

Fig. 9 presents the scintillation decay time profiles of the WbLS sample in a Suprasil quartz cuvette ( $\text{SiO}_2$ ). A reference spectrum (blank) was acquired using an identical empty cuvette. The background of PMT dark counts was estimated using scintillation-free data prior to the pulse and was subtracted from the data. The WbLS sample scintillation profiles exhibit two distinct rise-time components. The fast component,  $\tau_{r1} = 0.26$  ns, is observed alongside a slower component,  $\tau_{r2} = 2.32$  ns. A possible interpretation of the fast rise com-

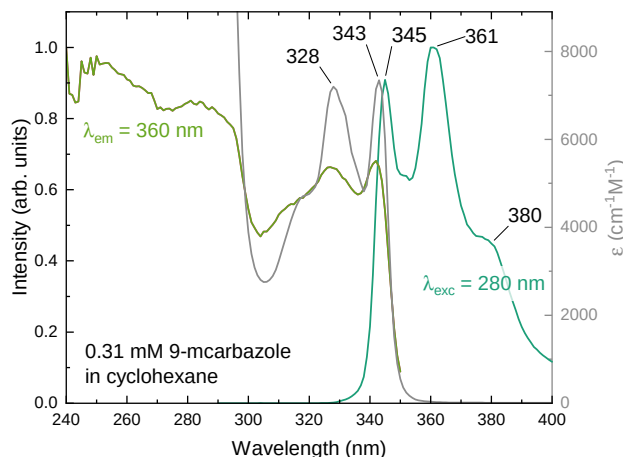


Figure 6: Photoluminescence excitation (green), emission (teal), and molar extinction coefficient  $\epsilon$  (gray) spectra of a 0.31 mM 9-methylcarbazole solution in cyclohexane. The photoluminescence spectra were acquired using a front-face measurement geometry.

ponent ( $\tau_{r1}$ ) is that it originates from rapid non-radiative energy transfer from LAB/LAS to 9-methylcarbazole, while the slow component ( $\tau_{r2}$ ) may result from radiative energy transfer, which requires photon emission followed by absorption. The measured scintillation decay time of the WbLS sample is  $\tau_d = 13.8$  ns and is significantly slower than previous compositions based on PPO (2-2.2 ns in [30] or other fluorophores reported in Tab. 2). The difference in apparent noise level before the leading edge and after the scintillation pulse is primarily due to the variable bin width employed in the histogram, which results in higher noise before the leading edge and lower noise levels in the later time intervals.

## 4 Discussion

The optical absorption spectrum of 0.4 mM LAB in cyclohexane has two strong absorption bands, a doublet at 196-212 nm and a complex vibrational structure at 242-268 nm with maximum at 259 nm, and a third weak absorption shoulder between 280 and 310 nm, see Fig. 3. Berlmán [33] has studied optical absorption of aromatic compounds in the 220-340 nm range and found a similar absorption maximum in alkyl-substituted benzene derivatives: 262 nm in toluene, 262 nm in ethyl-benzene, 261 nm in propyl-benzene, 261 nm in isopropyl-benzene, and 261 nm in *sec*-butyl benzene. These absorption maxima are very close to the 259 nm peak we observe in LAB, so we conclude that optical properties of the phenyl ring are not strongly affected by the substitution with an alkyl chain. We label the transitions responsible for the observed absorption bands using Perimeter Free Electron Orbital (PFEO) model [32]. Consequently, we interpret the 252 nm peak as the  $^1A \rightarrow ^1L_b$  transition, and the 196-212 nm doublet as the  $^1A \rightarrow ^1L_a$  transition, where  $^1A$  represents the ground state of the molecule and  $^1L_b$ ,  $^1L_a$  are excited singlet states. Both transitions are symmetry-forbidden in benzene, but become less forbidden when a substituent is added to the benzene ring and the symmetry is reduced. Additionally, vibrations of the molecule reduce symmetry temporarily and the transitions become less forbidden.

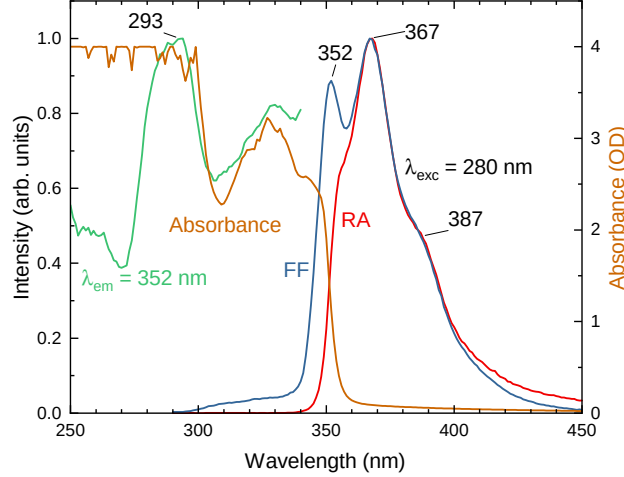


Figure 7: Optical properties of the developed WbLS cocktail based on 1%LAB of 20 g/l 9-methylcarbazole in 10% LAS water solution. Photoluminescence excitation (green), emission at right angle (red, RA), emission at front face (blue, FF), absorbance (gold) spectra.

Huang *et al.* [34] studied the LAB absorption spectrum in the limited 300-600 nm spectral range, so they were unable to detect characteristic bands of the LAB that are below 300 nm. However, they observed absorption peaks in 300-600 nm range in samples received from Jinling Petrochemical Corporation Ltd. in China. The absorption band at 330-400 nm was interpreted to be originating from impurities, possibly substituted nitro-benzene derivatives or thiocarbonyl compounds. In our work, we did not observe any characteristic absorption in that spectral range, and we concluded that our sample was not contaminated by any of these impurities. However, the featureless shoulder observed between 280 and 310 nm could have origin in other previously unidentified impurities. We conclude that high purity of LAB is extremely important for achieving the necessary optical transparency required for neutrino detection. As the 280-310 nm absorption shoulder overlaps with LAB emission at 289 nm, the presence of impurities in that spectral range may negatively affect the energy transfer process from LAB to the fluorophore. This hypothesis can be further supported by observation that the excitation spectrum of the 289 nm emission of LAB coincides with the absorption peak at 259 nm (gold and purple curves), but the excitation of 289 nm emission is not possible in the shoulder absorption range at 280-310 nm, see Fig. 4.

The optical absorption spectrum of 26.0 mM LAS in cyclohexane has a broad featureless band extending between 210 and 270 nm, and a weak shoulder between 280 and 350 nm, see Fig. 5. The lack of features could be caused by the saturation of the spectrophotometer due to the high optical density of the solution reaching 3.5 OD, which is very close to the 4.0 OD instrument maximum photometric range.

The excitation and emission spectra were measured with a further diluted solution of 101.6  $\mu$ M LAS, and a much cleaner excitation peak has been observed at 254 nm. Similarly to LAB, we interpret the 254 nm peak as the  $^1A \rightarrow ^1L_b$  transition. In contrast to the LAB, see Fig. 4, the LAS excitation peak is blue-shifted by 5 nanometers to 254 nm, while the emission peak is red-shifted by 13 nm to 302 nm. Geng *et al.* [35] studied LAS optical absorption spectra in DI water and observed two strong absorption bands, centered at  $\sim 194$  and  $\sim 225$

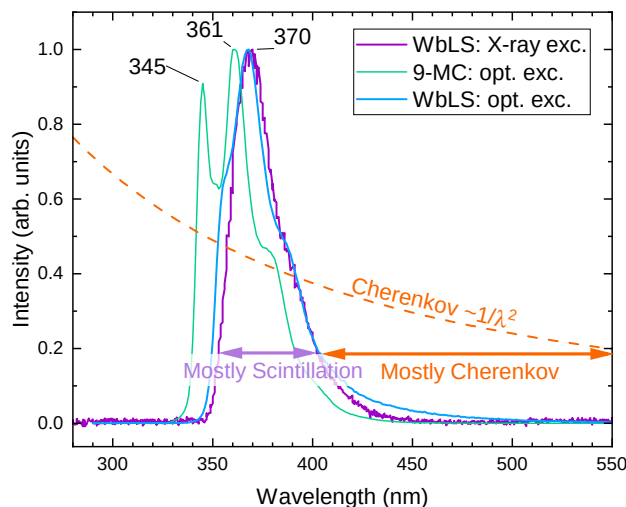


Figure 8: X-ray excited radioluminescence of the studied WbLS cocktail, a photoluminescence emission spectrum of the same sample excited at 280 nm in the right angle configuration, and a photoluminescence emission spectrum of 0.31 mM 9-methylcarbazole in cyclohexane excited at 280 nm using the front face configuration. The x-ray excited spectrum has been corrected for the quartz cuvette scintillation. The expected Cherenkov spectral dependence ( $I(\lambda) \propto 1/\lambda^2$ ) is overlaid for reference, together with an indication of spectral regions dominated primarily by scintillation photons and by Cherenkov photons.

nm, and a third but weak band at  $\sim 260$  nm. The authors assigned these bands to electronic transition of the aromatic ring in LAS. However, they have noticed that these peaks are red-shifted compared to organic compounds containing the same aromatic group, typically,  $\lambda_{max} = 184, 204, \text{ and } 255$  nm. In contrast to Gang *et al.*, we have measured the excitation peak at 254 nm, which is close to the expected 255 nm value for similar compounds, including LAB with excitation and absorption peaks coinciding at 259 nm. Geng *et al.* has interpreted the red-shift as either the result of a conjugation of the  $\text{SO}^{3-}$  group with delocalized electrons in the aromatic ring of LAS molecules, or formation of hydrogen bonding between the  $\text{SO}^{3-}$  group and  $\text{H}_2\text{O}$ . Considering that we observed excitation peak both of LAS and LAB at a similar wavelength in a nonpolar cyclohexane, we tend to interpret the difference between our work and Gang's as the result of hydrogen bonding between the  $\text{SO}^{3-}$  group and  $\text{H}_2\text{O}$ , while the difference between LAB emission at 289 nm and LAS emission at 302 nm we assign to the conjugation of the  $\text{SO}^{3-}$  group with delocalized electrons in the aromatic ring. Similarly as in the case of the LAB, we interpret the absorption shoulder between 280 nm and 350 nm as the influence of unidentified impurities.

The emission and absorption spectra of 0.31 mM 9-methylcarbazole in cyclohexane show excellent agreement with the data published by Berلمان [33]. The absorption peaks at 328 and 343 nm can be interpreted as vibronic modes of the  $^1\text{L}_b$  transition [36]. The excitation spectrum of 360 nm peak follows the absorption spectrum trends with a slight blue-shift. The mirror symmetry of the absorption in 300-350 nm range and emission spectra indicates that the geometry of the excited state is similar to that of the ground state. The absorption spectrum has a strong peak below 300 nm corresponding to the  $^1\text{L}_a$  transition but is not

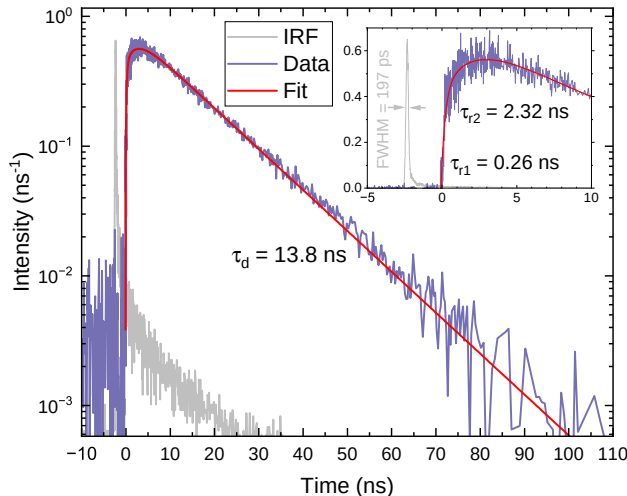


Figure 9: Scintillation decay profile of the developed WbLS cocktail (purple) and a double-exponential rise time and a single-exponential decay time fit (red). The background level was estimated using scintillation-free area before the pulse and subtracted from the data. Scintillation profile has been corrected for the quartz cuvette scintillation. The curve is normalized by its maximum. The inset shows the leading edge of the scintillation profile on a linear scale emphasizing two rise time components. The IRF has been shifted on the abscissa for clarity.

shown to emphasize the mirror symmetry of the lowest excited-state emission and absorption spectra. Such mirror image spectra are observed for 'rigid' molecules where there is no rotation around the carbon-carbon bond. This is the case of 9-methylcarbazole where two phenyl rings are fixed in a single 2D plain by a carbon-carbon bond and a carbon-nitrogen bridge.

The optical proprieties of the proposed WbLS cocktail are presented in Fig. 7. Emission spectra excited at  $\lambda_{\text{exc}} = 280$  nm were measured using two geometries (RA and FF). FF measurement (blue) has a weak emission shoulder extending from 300 nm to 340 nm, and three main peaks: 352, 367, and 387 nm. These three peaks are very similar to emission of 0.31 mM 9-methylcarbazole in cyclohexane but red-shifted: 345→352 nm, 361→367 nm, and 380→387 nm, compare Fig. 6. We interpret the 6-7-nm red shift as a result of the solvatochromic effect. The emission spectrum in Fig. 6 was measured in cyclohexane while the spectrum in Fig. 7 consists of a micellar system where 9-methylcarbazole is surrounded by LAB and LAS molecules. Similar red-shift was observed by Berlmán [33] when switching solvent from non-polar cyclohexane to ethanol. This observation indicates that 9-methylcarbazole is exposed to a much more polar environment in our WbLS cocktail compared to cyclohexane. The weak emission shoulder observed at 300-350 nm in the FF measurement we interpret as LAB and LAS emission which was not transferred to 9-methylcarbazole, see Figs. 4 and 5 where the emission of both extends between 300 and 340 nm. The FF geometry allows observation of the emitted light on the same side of the sample as the excitation, which reduces the optical path of emitted light through the sample. In the case of the incomplete radiative energy transfer between LAB/LAS and 9-methylcarbazole, it may be expected that not all

LAB/LAS emission will be reabsorbed by 9-methylcarbazole and some will escape sample unaffected.

Significant differences are observed between WbLS emission spectra  $\lambda_{\text{exc}} = 280$  nm when measured using two geometries: right angle (RA) and front face (FF), see Fig. 7. Although the FF measurement closely resembles 9-methylcarbazole in cyclohexane (Fig. 6), the RA measurement lacks one of the main peaks at 352 nm. This difference can be interpreted as the effect of self-absorption by 9-methylcarbazole. Although 9-methylcarbazole in cyclohexane was measured at a relatively low concentration and using FF geometry, Fig. 6, the WbLS concentration is much higher and the RA geometry leads to a longer optical path through the sample. In these conditions, self-absorption of the emission of 9-methylcarbazole is highly probable. This mechanism is also supported by a significant overlap in 9-methylcarbazole absorption and emission, Fig. 6, and a similar overlap of absorption and emission observed in the WbLS sample, Fig. 7.

The optical absorption spectrum of the WbLS sample in Fig. 7 has a broad band between 300 and 350 nm with intensity of 3 OD, and the spectrum is completely saturated below 300 nm. Due to the high concentration of the sample and the high optical density, only the band between 300 and 350 nm can be clearly interpreted as the absorption of 9-methylcarbazole. Comparison of Fig. 4, 5, and 6 leads to conclusion that only 9-methylcarbazole has significant absorption in that range. The excitation spectrum of 352 nm band follows the 9-methylcarbazole absorption spectrum in 300-340 nm range, and reaches maximum at 293 nm which corresponds to the direct excitation of  $^1L_b$  state of 9-methylcarbazole. The decrease in excitation intensity between 250 and 270 nm can originate from competition of the direct excitation of the 9-methylcarbazole and indirect excitation through absorption by LAB/LAS and the following energy transfer.

Fig. 9 shows the x-ray-excited scintillation decay profile of the WbLS sample. The WbLS sample exhibits a scintillation decay time of 13.8 ns, slightly faster than previously reported photoluminescence decay times of 9-methylcarbazole in organic solvents (18.3 ns in cyclohexane and 16.0 ns in ethanol) [33]. The observed decay time may also be partially influenced by oxygen-induced quenching, as no attempt was made to remove dissolved oxygen, consistent with realistic neutrino detector conditions. Oxygen is a well known photoluminescence quencher and it is reasonable to expect that it may affect the scintillation decay time. Two distinct rise-time components are observed: a fast component with  $\tau_{r1} = 0.26$  ns and a slower component with  $\tau_{r2} = 2.32$  ns. A possible interpretation is that the fast rise component arises from rapid non-radiative energy transfer from LAB/LAS to 9-methylcarbazole, while the slow rise component results from radiative energy transfer, which requires photon emission followed by re-absorption. The radiative process may involve LAB/LAS to 9-methylcarbazole or self-absorption by 9-methylcarbazole itself. While normally self-absorption is considered detrimental to scintillation process as it leads to decrease of the light yield, it may be desired for the purpose of separation of the fast Cherenkov photons by introducing a slow rise time component.

Fig. 8 shows X-ray-excited radioluminescence spectrum of the WbLS sample (purple) compared with photoluminescence emission spectrum excited at 280 nm RA and photoluminescence emission spectrum of 0.31 mM 9-methylcarbazole in cyclohexane excited at 280 nm FF. The x-ray excited emission and photoluminescence of the sample are nearly identical with maximum at around 370 nm. As previously commented, the 9-methylcarbazole spec-

trum in cyclohexane is slightly shifted compared to radioluminescence of the WbLS sample and we interpret this as a solvent effect. The similarity of x-ray excited luminescence and RA measurement of photoluminescence indicates that scintillation undergoes similar self-absorption process as discussed previously in Fig. 7. We can conclude that the scintillation of the WbLS sample originates from 9-methylcarbazole as a result of energy transfer from LAS/LAB and the final shape of the spectrum is refined by self-absorption which similarly removes the 352 nm emission peak in RA measurement shown in Fig. 7.

In addition to scintillation, charge particles can produce Cherenkov radiation in the aqueous component of the WbLS. The spectral distribution of Cherenkov light is well described by the Frank-Tamm formula (Eq. 3), predicting a photon yield proportional to  $1/\lambda^2$ . As illustrated in Fig. 8, this spectral dependence overlaps with the scintillation emission band in 350 to 410 nm range while 410 to 550 nm range is mostly scintillation-free. Using an appropriate dichroic mirror with 410 nm cutoff allows spectral separation of Cherenkov and scintillation photons.

For the majority of applications, a high light yield will also be a critical feature. The initial composition developed here has a relatively low light yield, which could not be accurately characterized using traditional method of comparing scintillation pulses with a single photoelectron spectrum of a PMT. The next step in development will focus on increasing the light yield, while preserving the time profile, emission spectrum, and transparency. Preliminary results indicated that further light yield increase is possible by increasing 9-methylcarbazole concentration, however, additional work beyond scope of this work is required to confirm that conclusion. Nevertheless, it is anticipated that a high-yield material could offer an order of magnitude more light.

## 5 Conclusions

In this article, we report a new water-based liquid scintillator cocktail with a scintillation decay time of 13.8 ns and a relatively narrow 370-nm x-ray-excited emission. The decay time is significantly slower than that of previous compositions based on PPO primary fluor, allowing for improved Cherenkov/scintillation discrimination based on the pulse shape. The emission at 370 nm matches well with modern superbi-alkali PMT sensitivity, and the absorption edge above 350 nm allows undisturbed detection of Cherenkov photons at longer wavelengths. These properties make the proposed WbLS formula a very interesting candidate for neutrino detection with Cherenkov/scintillation discrimination. However, we were not able to characterize the light yield of the sample within scope of this article, so further work is required to characterize and optimize the light yield.

## 6 Acknowledgments

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## 7 Data Availability

All data supporting the findings of this study, including optical characterization results, scintillation decay profiles, and emission spectra of the 9-methylcarbazole-based water scintillator, are publicly available in Wolszczak, W. W. (2025). *Optical and Scintillation Properties of a Water-Based Slow Scintillator with 9-Methylcarbazole as Fluor.* Zenodo. <https://doi.org/10.5281/zenodo.15485514>. The dataset includes raw and processed spectra to facilitate reproducibility and further research.

## A Appendix: quartz cuvette scintillation corrections

Hellma high performance glass (QS) cuvettes scintillate when excited with x-rays which interfered with characterization of the scintillation properties of the studied WbLS samples. Fig. 10 shows the scintillation profiles of the WbLS sample as measured (blue) and a blank measurement with a cuvette filled with DI water (green). Both measurements were performed using the same settings. The quartz cuvette has a complex decay profile consisting of a very fast prompt component and a relatively slow 116.4 ns delayed component. As can be seen from the picture, the observed scintillation both in WbLS and blank measurements comes only from delayed scintillation of the quartz cuvette ( $\text{SiO}_2$ ) after around 100 ns. The leading edge of the WbLS sample profile is obscured by prompt quartz scintillation showing a relatively "flat top" profile. A weak laser pre-pulse is observed at around -19 ns time due to inefficiency of the laser pulse picker and is believed to not affect significantly the measured scintillation profiles. As the intensity of the pre-pulse is nearly two orders of magnitude lower than the measured scintillation profiles, it is believed that it does not interfere significantly with the measurement of the decay time.

X-ray excited emission spectra were corrected for the quartz cuvette scintillation in analogue way, but additional correction was required to consider spectral filtering by the sample itself. Fig. 11 shows X-ray excited emission spectra of the WbLS cocktail (dark gray), a blank measurement of a water-filled quartz cuvette (red) and optical absorption of the WbLS sample (light gray). Scintillation emission spectrum of the quartz cuvette has three distinct peaks covering spectral range from UV to visible, with maxima at 305 nm, 571 nm, and 651 nm. By comparing WbLS and blank spectrum, we can conclude that the emission above 480 nm originates only from quartz scintillation, while the 305 nm peak is being absorbed by the WbLS sample. Following this observation, the background model of quartz scintillation

was estimated by convolution of the blank measurement with the absorption spectrum of the WbLS sample. Fig. 8 shows WbLS x-ray excited emission spectrum with the background model removed.

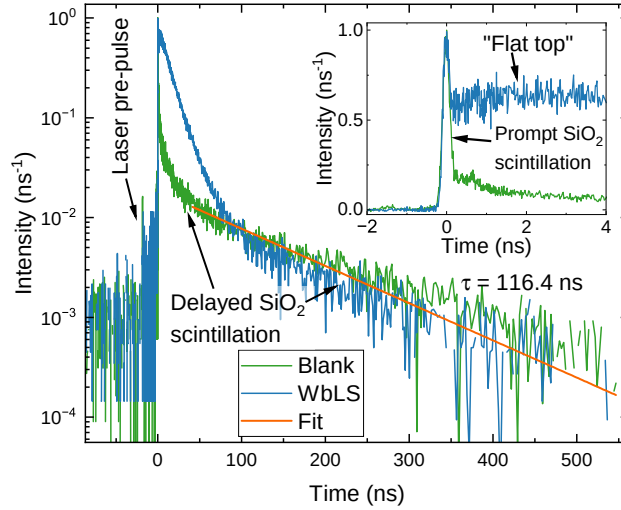


Figure 10: Uncorrected scintillation decay profiles of the developed WbLS cocktail (blue) and a blank measurement of a water-filled quartz cuvette (green). Each curve is normalized to its maximum. The orange curve shows single exponential fit of the blank measurement decay profile. The inset shows the leading edge of scintillation profiles on linear scale.

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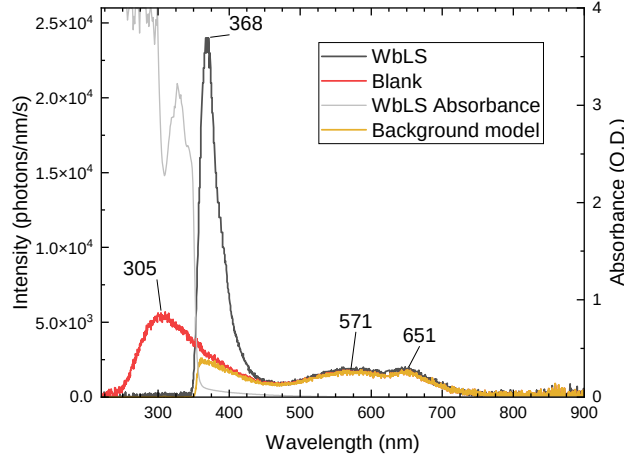


Figure 11: Uncorrected x-ray excited emission spectra of the studied WbLS cocktail (dark gray), a blank measurement of a water-filled quartz cuvette (red), optical absorption of the WbLS sample (light gray), and the background model (yellow).

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