

Using monochromatic light to measure attenuation length of liquid scintillator solvent LAB

Rui Zhang¹ · De-Wen Cao¹ · Chang-Wei Loh¹ · You-Hang Liu¹ · Fang-Liang Wu¹ · Jia-Liang Zhang¹ · Ming Qi¹

Received: 5 July 2018 / Revised: 20 August 2018 / Accepted: 23 August 2018 / Published online: 24 January 2019

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Abstract Linear alkylbenzene (LAB) will be used as solvent for the liquid scintillator in the central detector of Jiangmen Underground Neutrino Observatory. The sheer size of the detector imposes significant challenges and the necessity to further improve the optical transparency of high-quality LAB. In order to study high optical transparencies, we continuously improve our measurement setup and use monochromatic light to measure the attenuation lengths of LAB samples. Moreover, the effects of organic impurities on LAB samples are studied to understand their interaction mechanisms and further improve the optical transparency of LAB.

Keywords Neutrino detector · Linear alkylbenzene · Light absorption

1 Introduction

The neutrino observatory Jiangmen Underground Neutrino Observatory (JUNO) is designed to precisely measure the energy spectrum of reactor antineutrinos to determine the neutrino mass hierarchy and measure the oscillation

parameters [1–4]. Neutrino oscillation is an indicator for their nonzero mass and the only experimental discovery beyond the Standard Model. By investigating the mass hierarchy, we can gain a better understanding of the origin of neutrino mass.

The JUNO is located in Guangdong, China, approximately 53 km away from the Yangjiang and Taishan nuclear power plants. It consists of a spherical antineutrino detector (diameter of 35.4 m) as central detector, which will be filled with 20 kilotons of liquid scintillator (LS) surrounded by 18,500 new 20-inch broad photomultiplier tubes (PMTs). To reach its scientific goals, the energy resolution has to be above 3% at 1 MeV, corresponding to 1200 photon electrons per MeV. Apart from the required high-efficiency PMTs, a highly transparent LS is also crucial.

To achieve excellent optical properties—i.e., high transparency and light yield, long-term chemical stability, and low toxicity—linear alkylbenzene (LAB) is chosen as organic solvent for the LS. It is doped with 2,5-diphenylloxazole (PPO) as fluor and p-bis-(o-methylstyryl)-benzene (bis-MSB) as wavelength shifter. Besides JUNO, Daya Bay [5–8], SNO⁺ [9], RENO [10], and Double Chooz [11] have also used LAB as LS solvent. The optical transparency of LAB is quantified by its attenuation length. In the JUNO experiment, the attenuation length of the LAB samples should be comparable to the size of the central detector.

In collaboration with the Jinling Petrochemical Corporation (hereafter called “Jinling”), we have successfully improved the LAB attenuation lengths from 10 m for the Daya Bay experiment to 25.8 m for the JUNO experiment. Some LAB samples are potentially scalable for a mass production of 20 kilotons [12]. To obtain LAB samples with longer light attenuation lengths, the impurities in the

This work was supported by the National 973 Project Foundation of the Ministry of Science and Technology of China (No. 2013CB834300) and Strategic Pilot Science and Technology Project of the CAS (No. XDA10010000), and the National Natural Science Foundation of China (No. 116201 004).

✉ Ming Qi
qming@nju.edu.cn

¹ National Laboratory of Solid State Microstructures and School of Physics, Nanjing University, Nanjing 210093, China

LAB must be identified and then reduced as much as possible, in particular, impurities with strong absorption within the 350–450 nm scintillation spectrum. Preliminary studies on organic impurities [13, 14] have been performed to discover which impurities can reduce the attenuation length of LAB. In our latest analysis, three suspicious impurities with characteristic absorptions in the range of 350–450 nm were found via high-precision gas chromatography–mass spectrometry (GC–MS) (Thermo Scientific, Q Exactive GC–MS, Trace 1310). Their reduction or elimination might enable an increase in the LAB attenuation length to a larger value than the current maximum of 25.8 m. Therefore, it is promising to experimentally measure how long the attenuation length can become when impurities are eliminated.

To meet the stringent requirements for a LAB light attenuation length of 30 m, a further improvement of the measurement device and an optimization of the stability and reliability of the measurement method are essential. In this paper, we introduce recent progress on measurement methods and specifically describe the use of monochromatic light to accurately measure the attenuation lengths of LAB samples. Simultaneously, related topics such as the estimation of the effect of suspicious impurities on the attenuation length are discussed.

2 Experimental preparation

2.1 Attenuation length and Beer–Lambert law

The attenuation length L_λ is the distance at which the intensity of the incident light with wavelength λ has dropped by a factor of $1/e$. It can be expressed as follows [15]:

$$I = I_0 e^{-x/L_\lambda}, \quad (1)$$

where I is the intensity of the light after it has travelled the distance x in the sample and I_0 the initial intensity.

According to the Beer–Lambert law, the absorbance of the sample is proportional to the concentration c of the attenuation species and length l of the light path [16]:

$$A = \epsilon c l, \quad (2)$$

where A is the absorbance with $A = \log(\frac{I_0}{I})$ and ϵ the molar extinction coefficient.

The main components of LAB exhibit no absorption peaks in the 350–450 nm range. However, there are hundreds of impurities in LAB samples, some of which can exhibit absorption in this light range. For N attenuation species in the sample:

$$A = l \sum_i^N \epsilon_i c_i. \quad (3)$$

Together with Eq. (1), we obtain:

$$L_\lambda = \frac{1}{\sum_i^N \epsilon_i c_i}. \quad (4)$$

The Beer–Lambert law is only valid for ideal monochromatic waves. If the spectrum of the incident light is not monochromatic, the light intensity should be the weighted average of the LED spectrum $f(\lambda)$:

$$I = I_0 \int f(\lambda) e^{-x/L(\lambda)} d\lambda. \quad (5)$$

The LED used in our experiments has a wide spectrum. Thus, the measurement results should be an averaged effect of multi-wavelength light. We used an optical filter to obtain more monochromatic light and thereby as accurate measurements of the attenuation length as possible.

2.2 Sample preparation

A series of LAB samples were prepared and tagged as NJ42#, NJ46-R#, NJ48#, NJ49#, and NJ50#. All samples except NJ42# are commercial products. However, they were produced in different batches, and the qualities are therefore slightly different. As commercial LAB productions could not meet the requirements in our previous work, we produced high-quality LAB samples [12] with an improved production process by adjusting a set of technological parameters. The NJ42# sample is one of the high-quality LAB samples. The NJ46-R# sample was prepared from LAB sample NJ46#, which was mildly contaminated. Hence, its light attenuation length is much lower than those of other samples. Further, an LS sample based on LAB with 0.07 g/L PPO and 13 mg/L bis-MSB doping was prepared.

3 Experiments

3.1 Experimental setup

The optical measurement apparatus is shown in Fig. 1. Three LEDs with 400 nm, 430 nm, and 470 nm wavelengths are mounted as light sources to the top of the setup. The attenuation length can be measured at different LED wavelengths by moving the translation station. Usually, a wavelength of 430 nm is selected to match the response of the PMT in the JUNO experiment. The signal generator (AFG3102) drives the LED to emit pulsed light, which is then parallelly collimated by the lens. Monochromatic light is obtained with a bandpass filter. The beam passes through

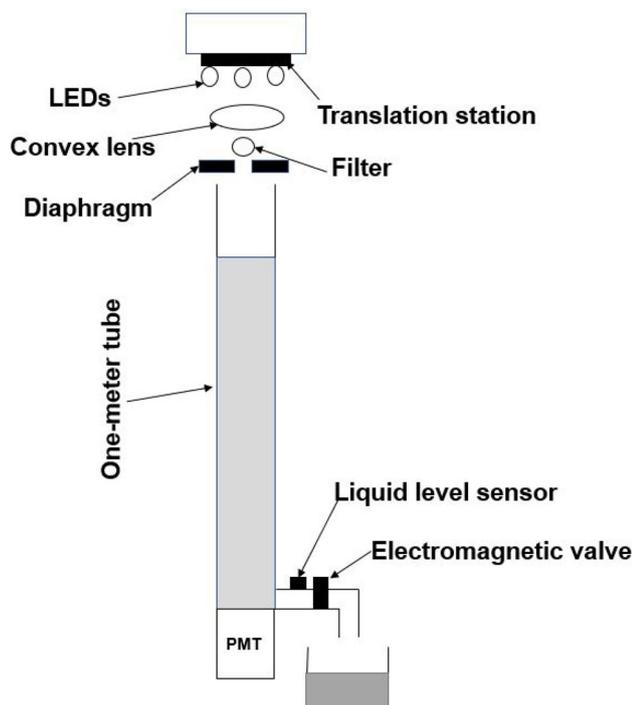


Fig. 1 Schematic of experimental setup

a diaphragm with an adjustable aperture and a 1-m stainless steel tube with Teflon-covered inner wall. The LAB sample is filled into the 1-m tube, and the height of the liquid level is controlled via an electromagnetic valve located at the bottom of the tube.

A PMT (Hamamatsu R7724; 51 mm diameter) is installed at the bottom of the equipment to receive the attenuated light. The signal coming from the PMT is then transmitted to the data acquisition (DAQ) system [17] and converted to an ADC channel value proportional to the signal intensity with a charge-to-amplitude converter (QADC) (CAEN V965). With the ADC channel value, Eq. (1) can be expressed as:

$$ADC_x = ADC_0 e^{-\frac{x}{L}}, \quad (6)$$

where ADC_x is the ADC value at height x of the liquid level and ADC_0 the ADC value when the 1-m tube is empty. After measuring the ADC channels of different liquid levels, we obtain the light attenuation length by fitting the data with Eq. (6).

The lens and aperture of the diaphragm are adjusted to achieve a parallelly collimated light beam propagating toward the central spot of the PMT. In this study, some measurement parameters were optimized to obtain accurate and stable results. To reduce the fluctuations in the output of the electronic equipment, the ambient temperature was stabilized to approximately 0.2 °C. Before the actual

measurement of the LAB samples, we used high-purity water to test our device and ensure optimal conditions.

3.2 Light spectra of LEDs

The light spectra of the three LEDs were detected with an FX2000-RD fiber optic spectrometer. The results are shown in Fig. 2 and Table 1. The attenuation length of the LAB changes with the wavelength [18]. It is often measured at 430 nm for reference because the spectrum of the scintillator light peaks at 430 nm, which is also the region in which the PMTs reach maximal quantum efficiency.

3.3 Selection of filters

In this work, we used bandpass filters to obtain more monochromatic light at 430 nm for more accurate measurement results. The specifications of the filters are given in Table 2. Figure 3 presents the spectrum of the LED light for different filters. The light transmittance of the Thorlabs filter is only 45%, resulting in a very weak light intensity, which requires the adjustment of other measurement parameters. Hence, the filter cannot meet our experiment requirements. Although the FWHM of the Thorlabs filter is smaller, our experiments were mainly carried out with a Semrock filter.

4 Results and discussion

4.1 Attenuation length measurement of LAB

We measured a series of different LAB samples with and without filter, respectively. The results are shown in Figs. 4, 5, and Table 3. We discovered that the attenuation lengths are improved to various degrees under monochromatic light. Besides, the filter effects on different LAB samples are not equal, which suggests that the LAB samples have complicated mixtures of impurities with diverse sensitivities to distinct wavelengths.

4.2 Attenuation length measurement of LS

Figure 6 shows the results for the LS sample measured with and without filter. The data of the setup without filter are not well fitted with the Beer–Lambert law owing to the various impurities in PPO and bis-MSB, whereas more accurate attenuation lengths for LS with filter were obtained, as shown in Fig. 6b.

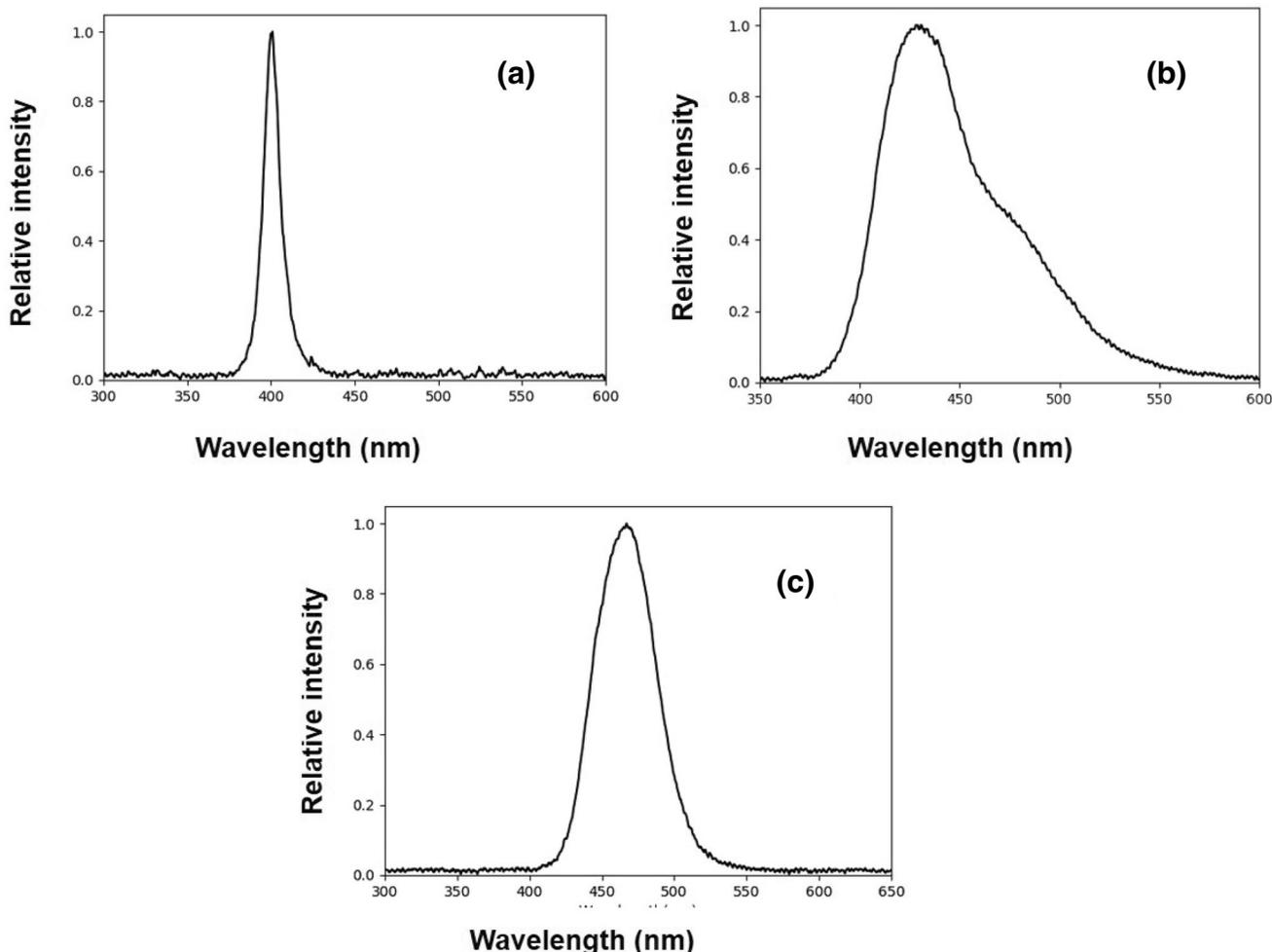


Fig. 2 Spectra of three LEDs used in our experiment. The wavelengths of the LEDs are **a** 400 nm, **b** 430 nm, and **c** 470 nm, respectively

Table 1 Specifications of three LEDs used in our experiment

	Central peak (nm)	FWHM (nm)
LED1	401	12
LED2	430.5	58
LED3	469.5	60

4.3 Estimation of effect of organic impurities

We focused on analyzing the organic impurities in LAB samples to identify the ones influencing the optical transparency of LAB samples. With a LAB light attenuation

length of more than 20 m, the impurity concentration is already very low and close to the resolution limit of GC-MS. We are facing the conundrum of whether to further accurately measure the impurity concentrations without knowing their degree of influence on the transparencies of LAB samples. However, according to Eq. (3), it might be possible to use the Beer-Lambert law to estimate the effect of a certain impurity on the optical transparencies of LAB samples. The absorption peak of the impurity is at a single wavelength. Hence, analyzing the influence of a certain impurity on the LAB is only possible using a filter to obtain monochromatic incident light.

In Ref. [12], we calculated suspicious impurity compounds that exhibit absorptions in the 350–500 nm range.

Table 2 Specifications of bandpass filters used in experiment

Filter type	Central wavelength (nm)	FWHM (nm)	Transmittance (%)
Thorlabs FB430-10	430	10	> 45
Semrock FF01-427/10-25	427	14	> 93

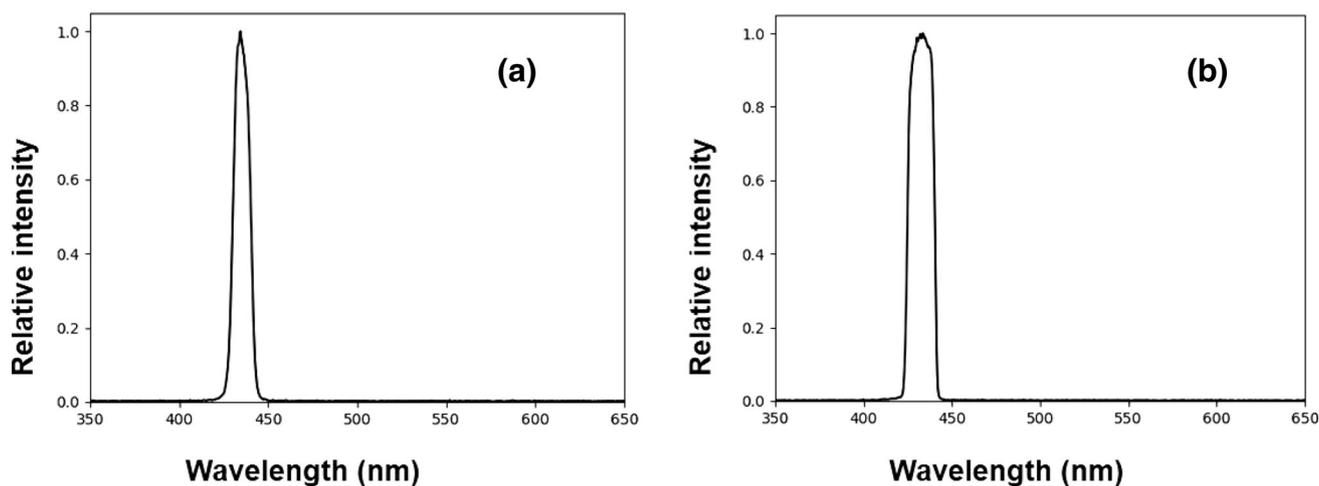


Fig. 3 Spectrum of light source after use of **a** Thorlabs and **b** Semrock filters

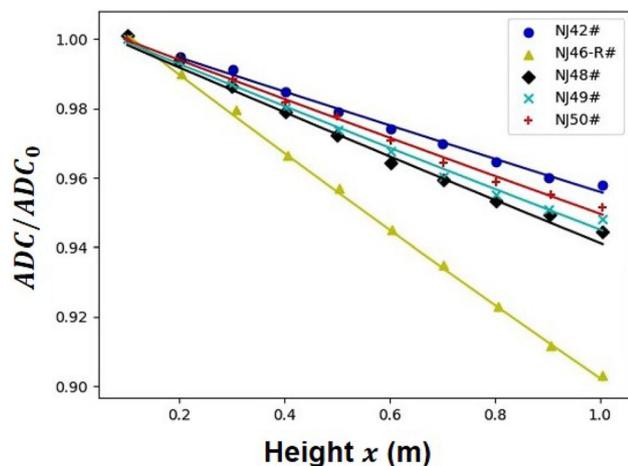


Fig. 4 (Color online) ADC/ADC₀ of NJ42#, NJ46-R#, NJ48#, NJ49#, and NJ50# for various LAB liquid heights x , where ADC/ADC₀ refers to the ADC value at height x normalized to the ADC value at height x_0 , which is the maximal value obtained from the data

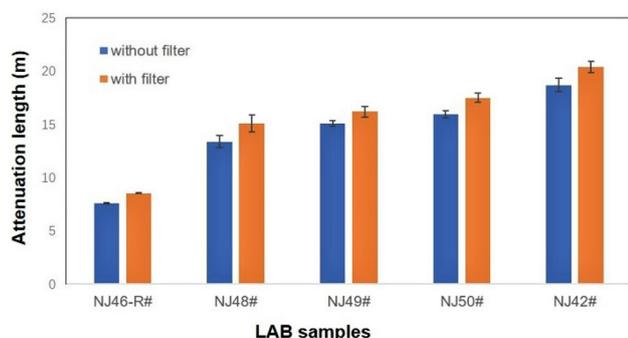


Fig. 5 (Color online) Comparison of attenuation lengths of NJ46-R#, NJ48#, NJ49#, NJ50#, and NJ42# measured with and without filter

The impurity $C_{34}H_{36}N_2O_4$ was found in all three samples. Hence, it was chosen as an example. Our goal is to estimate

Table 3 Comparison of attenuation lengths of different LAB samples measured with and without filter

LAB samples	No filter	With filter
NJ42#	18.71 ± 0.61	20.41 ± 0.56
NJ50#	15.94 ± 0.34	17.50 ± 0.42
NJ49#	15.10 ± 0.26	16.20 ± 0.50
NJ48#	13.38 ± 0.56	15.10 ± 0.78
NJ46-R#	7.59 ± 0.06	8.56 ± 0.05

the effect of the impurity concentration on the LAB attenuation length. To this end, we applied Eqs. (1) to (4):

$$I = I_0 e^{\frac{-x \times (\epsilon_1 \epsilon_1 + \epsilon_2 \epsilon_2 + \dots)}{0.4343}} \quad (7)$$

The molar extinction coefficient ϵ can be estimated via [14]:

$$\epsilon = \frac{f}{4.32 \times 10^{-9} \times \Delta\nu} \quad (8)$$

where f is the oscillator strength and $\Delta\nu$ the width of the peak absorption band in cm^{-1} .

We divided the impurities into two parts: the impurity to be determined and the part, which contains all other yet unknown impurities.

$$I = I_0 e^{\frac{-x \times (c^* \epsilon^* + \sum \epsilon_i \epsilon_i)}{0.4343}} \quad (9)$$

where c^* and ϵ^* are the concentration and molar extinction coefficient of the single impurity of interest, respectively.

Figure 7 shows the attenuation length measurements of LAB NJ50#. By using Eq. (9) to fit the data and upper limits of the fitting parameter of c^* , we obtained different hypothetical concentrations for this impurity.

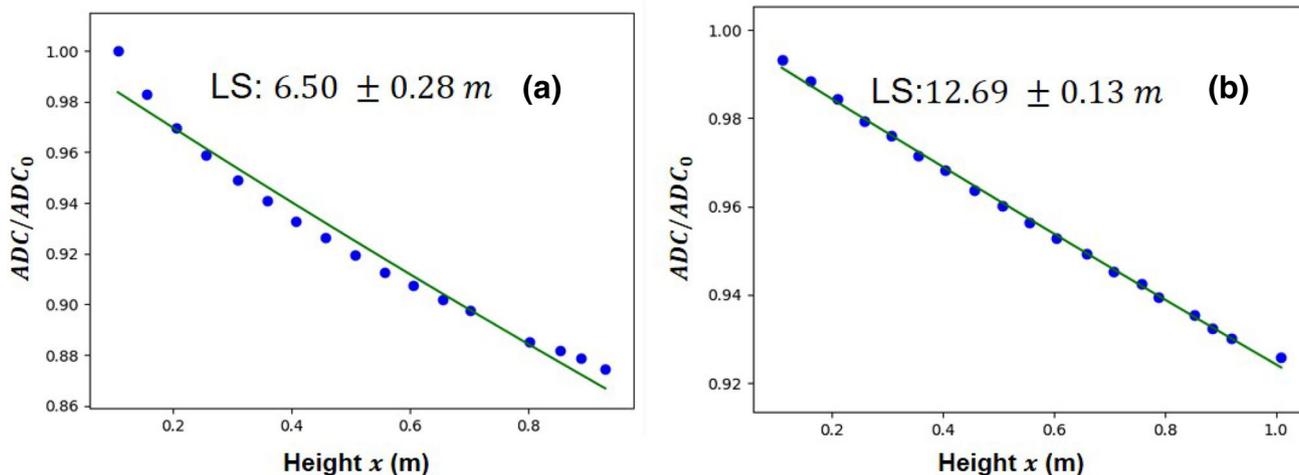


Fig. 6 Measurement results for LS samples **a** without filter and **b** with filter. The attenuation lengths obtained from an exponential fit are 6.5 m and 12.69 m, respectively

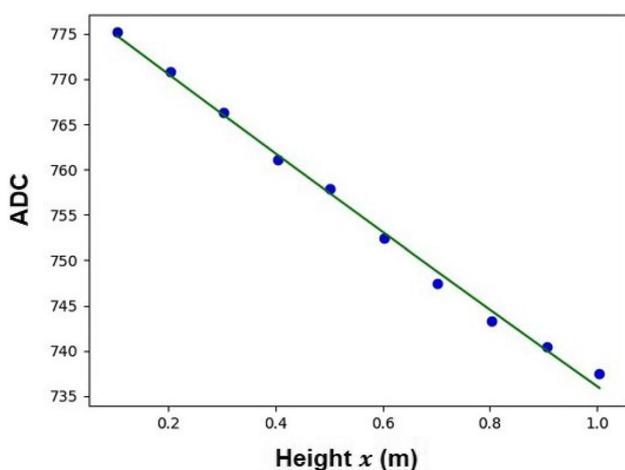


Fig. 7 Measurement results of LAB NJ50# with filter for various LAB liquid heights x

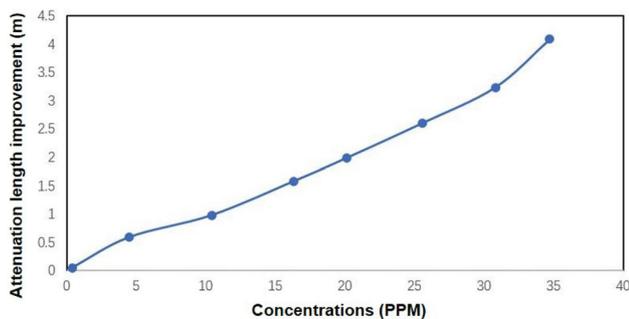


Fig. 8 Effects of different hypothetical concentrations of impurity $C_{34}H_{36}N_2O_4$ on attenuation length of LAB NJ50#. If we can remove the impurity, the attenuation length will improve. The improvement is significant for high impurity concentrations

Figure 8 shows the effect of the impurity with different hypothetical concentrations. If the concentration of the

impurity $C_{34}H_{36}N_2O_4$ in LAB NJ50# sample is below several ppm, it has no high impact on the attenuation length of the sample. The proposed method could provide us a fast and simple way to identify suspicious impurities with absorption peaks near 430 nm and the upper limit of impurity concentrations that are still tolerable while achieving a specific attenuation length. In the case presented in Fig. 8, the value was set to 30 m.

4.4 Considerations

In order to accurately measure the light attenuation length of the LAB sample, we will continue to improve our experimental measurement devices and methods including upgrades of our current DAQ system and better filters. As shown in Fig. 9, we plan to apply preparative high-performance liquid chromatography to separate impurities from LAB samples and determine high impurity concentrations, which will be analyzed via GC-MS. This would help us to make a more detailed study on the chemical structure of impurities and the light absorption properties of LAB samples.

5 Conclusion

The attenuation lengths of LAB samples with and without filter were measured, respectively. After filtering, a more accurate attenuation length at 430 nm was measured. The attenuation lengths of different LAB samples exhibited various degrees of improvements, which gives us a hint on how to increase the optical transparency of LAB. Moreover, the effects of impurity concentrations were analyzed, and a method to estimate the possible effect of different

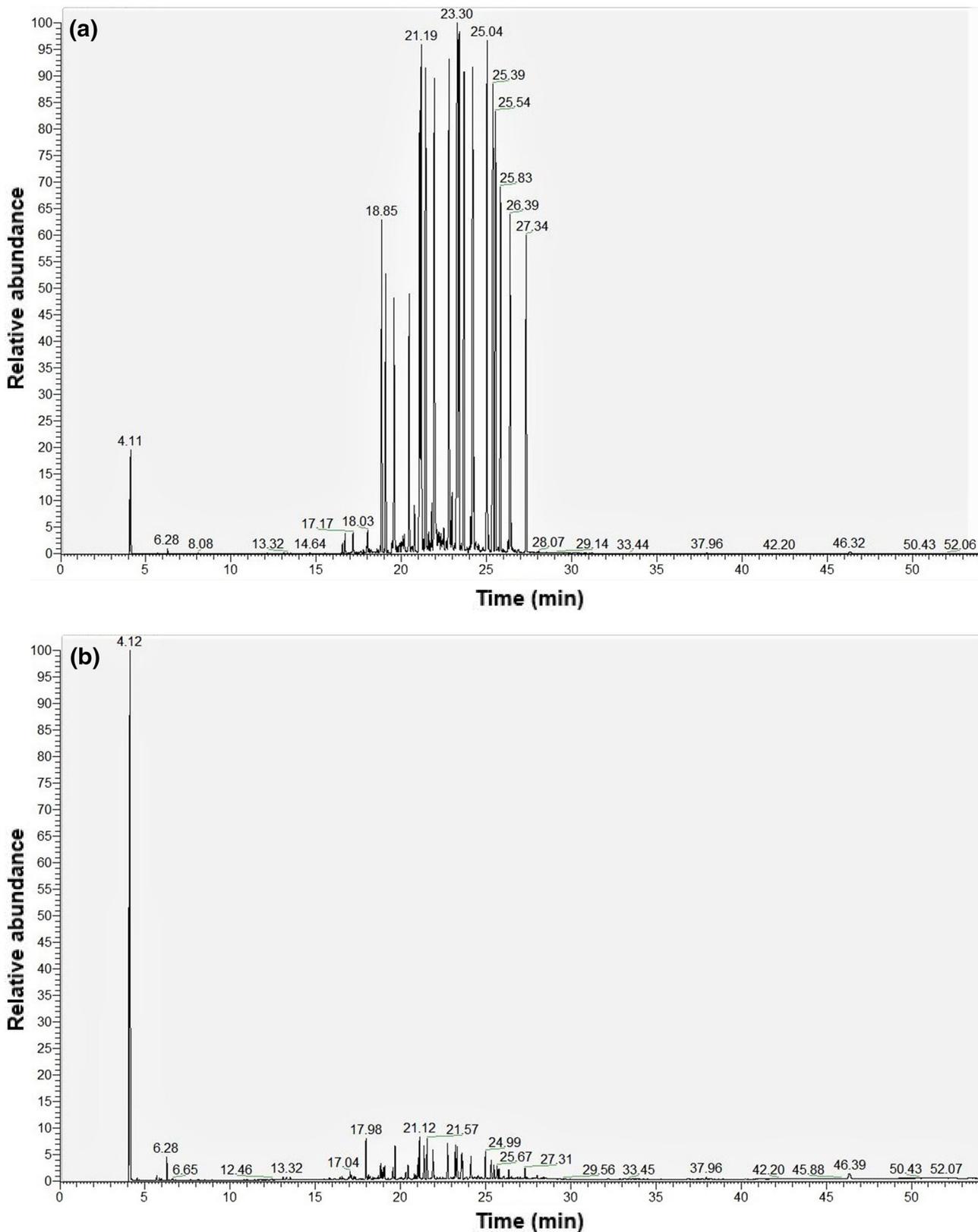


Fig. 9 Gas chromatogram of LAB samples: **a** initial LAB sample, **b** impurity LAB data without main LAB components

certain hypothetical impurity concentrations was proposed. This method can promote an efficient determination and elimination of suspicious impurities, thereby eventually improving the attenuation length to values higher than those of present LAB samples.

Acknowledgements We are grateful for the warm help and enlightening insights from Yi-Fang Wang, Jun Cao, Sen Qian, Li Zhou, Tao Hu, Ya-Yun Ding, Zhe Ning, Na Zhu, Guang-You Yu, Hai-Bo Yang, and Ai-Zhong Huang.

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