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REGULAR ARTICLE

Theoretical study of UV-Vis light absorption of some impurities in alkylbenzene type liquid scintillator solvents

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Abstract Special chemical impurities may greatly decrease the light transparency of liquid scintillator (LS) solvents in the wavelength region 350–450 nm, which is of great importance to the neutrino experiments. The absorption wavelengths and oscillator strengths of two types of impurities (thiocarbonyls and nitrobenzene derivatives) and some similar compounds were calculated using TD-DFT in three scintillator solvents (toluene, pseudocumene, and linear alkyl benzene). Influences of these impurity molecules on LS solvent's optical transmission in 350–450 nm were analyzed and compared with each other.

Keywords Liquid scintillator solvent · Optical transparency · UV-Vis light absorption · Chemical impurities · TD-DFT

1 Introduction

Liquid scintillator (LS) has been extensively used in neutrino experiments, including reactor, solar, and double-beta decay experiments. Generally, more than 90 wt% of LS used in a neutrino experiment is a kind of aromatic scintillator solvent. Toluene, pseudocumene, and linear alkylbenzene (LAB) are three widely used alkylbenzene type LS solvents in neutrino experiments [1].

Toluene is one of the oldest solutions for liquid scintillator in the history of neutrino and other high-energy physics experiments. Pseudocumene (1, 2, 4- trimethylbenzene) has been the most commonly used scintillator solvent in previous neutrino experiments such as Chooz [2] and Palo Verde [3]. LAB has recently been chosen as the scintillator solution in the SNO+ [4], Daya Bay [5], and Reno [6]. As the targets of neutrinos and the detection medium of the final neutrino signals (fluorescence light at ~410 nm), LS solvents must have very good optical transparency [7]. Detailed, the most important experimental requirement for large-scale (hundreds of tons) use of scintillator solvent is long light attenuation length (L_λ^{att}, defined as the distance at which the intensity of input light reduced to 1/e of the initial value) in a characteristic wavelength window 350–450 nm, e.g., greater than 10 m.

Theoretically, solvent's light transmission properties are determined by the structure of the solvent and the chemical impurities in it. Toluene, pseudocumene, and LAB with high purity do not have any UV-Vis light absorption band in 300–500 nm [8]. However, as petrochemical products, the mass-produced LS solvents also contain a lot of chemical impurities. These impurities, though in tiny concentration, may bring 350–450 nm absorption peaks to the solvents. Therefore, analyzing the detail absorption wavelengths and intensities of the impurities detected out in scintillator solvents and figuring

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out the potential influence is of vital importance to neutrino experiment.

Some LAB samples collected from the LAB plant of Jingling Petrochemical Corporation. Ltd (China) were found to have absorption bands in our characteristic window. These bands must come from the chemical impurities in samples. We selected GC × GC-MS (QP2010, Shimadzu) to analyze the composition of one failed LAB sample (NJ12-4, details of this sample can be found in Ref. [9]). GC × GC-MS is an emerging technology for chemical separations that provides an order of magnitude increase in identification capacity over traditional GC. Since different molecules have different light absorption properties in the UV-Vis region. Compounds with 350–550 nm absorption maxima usually contain some special functional groups such as nitro, nitriso, thiocarbonyl and azo [10], polycyclic aromatic molecules and systems with conjugated double bonds can have peak absorption in 350–450 nm region too. After composition analysis, three thiocarbonyls and a medium-size nitrobenzene derivative molecular were preliminarily detected out in the LAB sample NJ12-4.

Time-dependent density functional theory (TD-DFT) is well known as a powerful tool for ab initio quantum chemical studies of molecular optics and spectroscopy. TD-DFT combines the advantages of density functional theory and time-dependent formalism allowing the accurate determination of excited-state properties. The technique can deal with the same accuracy for both medium and large molecules. For some special types of organic compounds [11–14], TD-DFT with suitable hybrid functional and extended basis set can get highly accurate data of molecules' lowest-energy light absorption wavelengths.

In this paper, we calculated the wavelengths of maximum absorption (λ_{max}) and oscillator strengths (f) of the three thiocarbonyl molecules, the nitrobenzene derivative compound and some similar salts of these two types by using TD-DFT. The influence of the solvents on molecules' light absorption was considered through the polarizable continuum model (PCM). In fact, thiocarbonyl salts' light absorption has received sufficient studies in the past 50 years. More than 100 different thiocarbonyl salts' lowest-energy light absorption in cyclohexane and other solvents had been TD-DFT investigated by Fabian in 2000 and Denis Jacquemin in 2007 [15, 16]. In reference [17], Denis Jacquemin's method can obtain an excellent agreement between the theoretical and experimental λ_{max} of thiocarbonyl salts in cyclohexane, heptane, and others (mean absolute error = 9.9 nm). Therefore, we applied the same method to investigate the three thiocarbonyl molecules in solution of scintillator solvents. Auxochrome group substituted nitrobenzene derivatives (NO_2-Ph-X) are typical intramolecular charge transfer (ICT) compounds [18, 19], which are characterized by strong intensity absorption at long wavelengths. Great discrepancy was found when using PBE0 [20, 21] to evaluate the light absorption wavelengths of nitrobenzene derivatives by TD-DFT. Especially, push-pull nitrobenzene derivative compounds with donor and acceptor groups far away are problematic for TD-DFT calculations relying on conventional hybrids [22]. Therefore, we selected two different popular functionals and a series of basis sets to calculate this type compounds.

2 Impurity molecules and computational details

The four potential impurities of two types were sketched in Fig. 1. We also selected some typical thiocarbonyls and o-nitrobenzene derivative molecules (Fig. 2). In Figure 2, I and IV represent thiocarbonyls and nitrobenzene derivatives with (R_1, R_2) = (NHMe, NMe_2), (NHMe, OMe), (NHMe, Ph), and so on, X = OH, OMe, NH_2, NHMe, NMe_2. These molecules' chemical structures are similar to the thiocarbonyl and nitrobenzene derivative impurities we preliminarily detected (have the same or the similar radicals attached to the C=S group and benzene ring).

Gaussian 03 suite of programs [23] was chosen to carry out all the calculations in this article. To calculate the

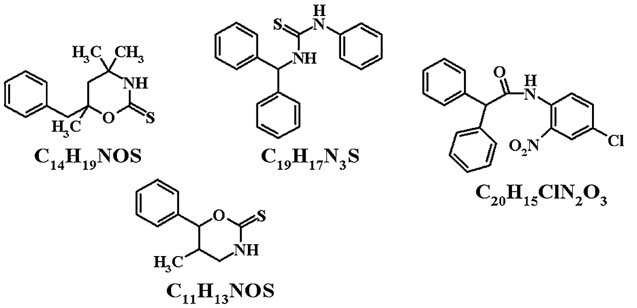

Fig. 1 Sketches of three thiocarbonyls (*left*) and a nitrobenzene derivative impurity molecules (*right*)

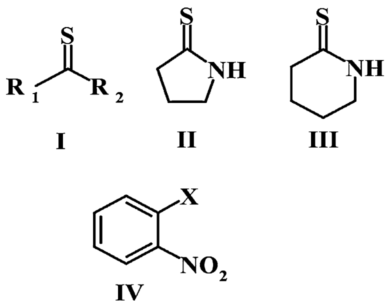

Fig. 2 Some typical thiocarbonyl salts and nitrobenzene derivatives we investigated. These molecules' chemical structures are similar to the impurities we detected

absorption wavelengths, we have used a four-step approach: (1) conformational analysis (see supplementary material); (2) the ground-state geometries have been optimized in three solvents; (3) the vibrational spectra are analytically determined to confirm that structures are actual minima (no imaginary frequencies exist); and (4) the vertical transition energies to the valence excited states are computed with TD-DFT. For thiocarbonyl molecules, the parameter-free hybrid functional PBE0 has been selected. PBE0, also referred to as PBE1PBE, includes 25% of exact exchange. The optimization and vibration spectrum (first two steps of our investigation) calculations have been carried out using the basis set 6-311g(2df, p), while the low-lying absorption spectrum of the molecules was obtained by calculation of the ground/singlet-excited-state transition energies. These TD-DFT calculations have been carried out with the basis set 6-311+g(2df,p). The statistical simple linear regression (SLR) formula [17] $\lambda_{\max,\mathrm{nm}} = -4.690 + 1.058\lambda^{\mathrm{TD-PBE0}}_{\max,\mathrm{nm}}$ was also used.

The compound ($C_{20}H_{15}ClN_2O_3$) detected in LAB sample NJ12-4 is a $(C_6H_5)_2CHCONH$ radical ortho-substituted nitrobenzene. $(C_6H_5)_2CHCONH$ has the similar auxochrome effect with CH_3CONH and NH_2 [8, 24, 25]. Therefore, we can use o-nitroaniline as the reference molecular to select the chemical model for the calculation of $C_{20}H_{15}ClN_2O_3$. PBE0 and Becke three-parameter hybrid functionals (B3LYP) [26] with different basis sets (6-31g(d), 6-311g(d,p) and 6-311g(2df,p)) were then used in o-nitroaniline's ground-state geometry optimization and vibrational frequency test, the same basis sets added with a diffuse function were used when carrying out the TD-DFT calculation. The test results in solution of toluene are shown in Table 1.

Table 1 Functional and basis set study for the $\lambda_{\max}$ of o-nitroaniline in toluene, $\lambda^{\exp}_{\max} = 395\,\mathrm{nm}$

Model	$\lambda^{\mathrm{TD}}_{\max}$ (f)
B3LYP/6-31+g(d)//B3LYP/6-31g(d)	397 (0.128)
B3LYP/6-311+g(d,p)//B3LYP/6-311g(d,p)	395 (0.128)
B3LYP/6-311+g(2df, p)//B3LYP/6-311g(2df,p)	391 (0.126)
B3LYP/6-31+g(d)//PBE0/6-31g(d)	390 (0.130)
B3LYP/6-311+g(d,p)//PBE0/6-311g(d,p)	388 (0.130)
B3LYP/6-311+g(2df,p)//PBE0/6-311g(2df,p)	385 (0.127)
PBE0/6-31+g(d)//B3LYP/6-31g(d)	382 (0.141)
PBE0/6-311+g(d,p)//B3LYP/6-311g(d,p)	380 (0.141)
PBE0/6-31+g(d)//PBE0/6-31g(d)	375 (0.143)
PBE0/6-311+g(2df,p)//B3LYP/6-311g(2df,p)	376 (0.138)
PBE0/6-311+g(d,p)//PBE0/6-311g(d,p)	373 (0.142)
PBE0/6-311+g(2df,p)//PBE0/6-311g(2df,p)	370 (0.139)

λ are reported in nm with oscillator strengths given between *brackets*

Table 2 The macroscopic parameters of the three scintillator solvents needed for PCM calculation

Solvent	Eps	Density in g/cm^3	Rsolv in Å
Toluene	2.385	0.867	2.82
Pseudocumene	2.38	0.876	3.055
LAB	2.16	0.856	3.888

In Table 1, B3LYP with the combination of basis sets [6-311+(d,p)//6-311G(d,p)] get the same value of o-nitroanline's lowest-energy $\lambda_{\max}$ with the experimental measured UV-Vis spectra ($\lambda^{\mathrm{TD}}_{\max} = \lambda^{\exp}_{\max} = 395$ nm in toluene). Therefore, we can use this method to calculate $C_{20}H_{15}ClN_2O_3$ and the similar o-nitrobenzene derivative molecules.

In our calculation, the influence of the scintillation solvents is evaluated by means of the polarizable continuum model (PCM, default IEF-PCM approach in Gaussian 03 suite of programs) [27–29]. In PCM, the solution is treated as a structure-less material, characterized by its macroscopic parameters (dielectric constant: eps, density of the solvent, solvent radius: rsolv and so on). We have carried out calculations in toluene using the parameters implemented in Gaussian 03. Since LAB is not a default solvent listed in the Gaussian 03's solvent table, we experimentally measured the dielectric constant and the density of LAB ourselves, the relevant parameters of pseudocumene can be found in Lange's Chemistry Handbook [30]. PCM parameters of the three scintillator solvents are listed in Table 2.

3 Results and discussion

3.1 Thiocarbonyl impurities and some similar thiocarbonyl molecules

Calculation results (absorption wavelengths $\lambda_{\max}$ and intensities, evaluated by oscillator strengths, f) of the three thiocarbonyl impurity molecules and some similar thiocarbonyl molecules in scintillator solvents are shown in Table 3. $C_{19}H_{17}N_3S$ is found to have absorption peak at 358 nm, the corresponding oscillator strength is about 0.02. It is a medium-intensity $n \rightarrow \pi^*$ electron transition. The other two impurity molecules ($C_{14}H_{19}NOS$, $C_{11}H_{13}NOS$) are found to have absorption maxima around 310 nm. As for the small-size thiocarbonyls, most of the molecules we investigated have absorption maxima in the characteristic window 350–450 nm, except for molecules I1, I3, I4 and I6. The two cyclic thiocarbonyl molecules (II and III) and compound I8 all have $\lambda_{\max}$ above 355 nm, but the corresponding oscillator strengths f is 0 or 0.0001. Hence, these are forbidden transitions. From Table 3, we

Table 3 Absorption wavelengths (nm) and oscillator strengths of the thiocarbonyl molecules in toluene, pseudocumene, and LAB

Molecules	(R_1, R_2)	λ_{max} (f) in three LS solvents		
		Toluene	Pseudocumene	LAB
$C_{14}H_{19}NOS$	–	312 (0.0011)	312 (0.0011)	312 (0.0012)
$C_{11}H_{13}NOS$	–	312 (0.0001)	311 (0.0001)	311 (0.0001)
$C_{19}H_{17}N_3S$	–	358 (0.0194)	353 (0.0270)	358 (0.0185)
I1	(NHMe, Me_2)	316 (0.0052)	316 (0.0053)	317 (0.0050)
I2	(NHMe, Ph)	409 (0.0092)	409 (0.0092)	411 (0.0089)
I3	(NHMe, OMe)	293 (0)	292 (0)	293 (0)
I4	(NHMe, Me)	345 (0)	345 (0)	346 (0)
I5	(NHCOMe, NMe_2)	352 (0.0013)	352 (0.0013)	351 (0.0012)
I6	(NHCOMe, OMe)	340 (0)	340 (0)	341 (0)
I7	(NHCOMe, Me)	432 (0.0002)	432 (0.0002)	432 (0.0002)
I8	(NHPh, Me)	387 (0.0001)	387 (0.0001)	388 (0.0001)
I9	(NH_2, Ph)	422 (0.0085)	422 (0.0085)	424 (0.0083)
I10	(NMe_2, Ph)	395 (0.0147)	396 (0.0146)	398 (0.0145)
I11	(t-Bu, Ph)	559 (0.0048)	559 (0.0047)	560 (0.0047)
I12	(Ph, Ph)	600 (0.0044)	600 (0.0044)	602 (0.0042)
II	–	352 (0.0001)	352 (0.0001)	353 (0.0001)
III	–	357 (0)	357 (0)	359 (0)

Table 4 λ_{max} in nm and f of $C_{20}H_{15}ClN_2O_3$ and similar o-nitrobenzene derivatives

Molecules	λ_{max} (f) in three LS solvents			λ_{max}^{exp}, solvent
	Toluene	Pseudocumene	LAB	
$C_{20}H_{15}ClN_2O_3$	413 (0.0922)	413 (0.0910)	412 (0.0867)	–
IV, $X = NH_2$	395 (0.128)	395 (0.128)	393 (0.126)	395, toluene
$X = NHMe$	412 (0.156)	412 (0.156)	410 (0.154)	429, ethanol
$X = NMe_2$	441 (0.0899)	442 (0.894)	439 (0.879)	415, ethanol
$X = OH$	339 (0.0870)	339 (0.865)	337 (0.0857)	356, toluene, 347, ethanol
$X = OMe$	349 (0.0919)	348 (0.922)	347 (0.0917)	320, toluene, 323, ethanol

can also find that the absorption intensities of most thiocarbonyl compounds are very weak ($f < 0.01$) in LS solvents except $C_{19}H_{17}N_3S$. Therefore, the influences of thiocarbonyl compounds on LS solvents are very limited.

3.2 Nitrobenzene derivative impurity and some similar molecules

Lowest-energy absorption wavelengths and oscillator strengths of $C_{20}H_{15}ClN_2O_3$ and other o-nitrobenzene derivative molecules were listed in Table 4. A strong light absorption maximum around 412 nm with $f \approx 0.09$ was figured out in $C_{20}H_{15}ClN_2O_3$. The molecular orbitals involved in the electronic transition corresponding to the lowest-energy λ_{max} are sketched in Fig. 3.

The approach TD-B3LYP/6-311+g(d,p)//B3LYP/6-311g(d,p) can get reliable absorption wavelengths of small-size nitrobenzene derivatives. The biggest variation occurs in NO_2-Ph-OMe (29 nm). After considering the error factor, all the five o-nitrobenzene derivative compounds may influence the light absorption of LS solvents in 350–450 nm region. From Tables 3 and 4, o-nitrobenzene derivative compounds' absorption intensities ($f \sim 0.1$) are an order of magnitude greater than thiocarbonyl molecules . Hence LS solvents are more sensitive to o-nitrobenzene type molecules than thiocarbonyl compounds.

3.3 Discussion

According to Lambert-Beer theory [31], mixed solvents' light attenuation length can be written as

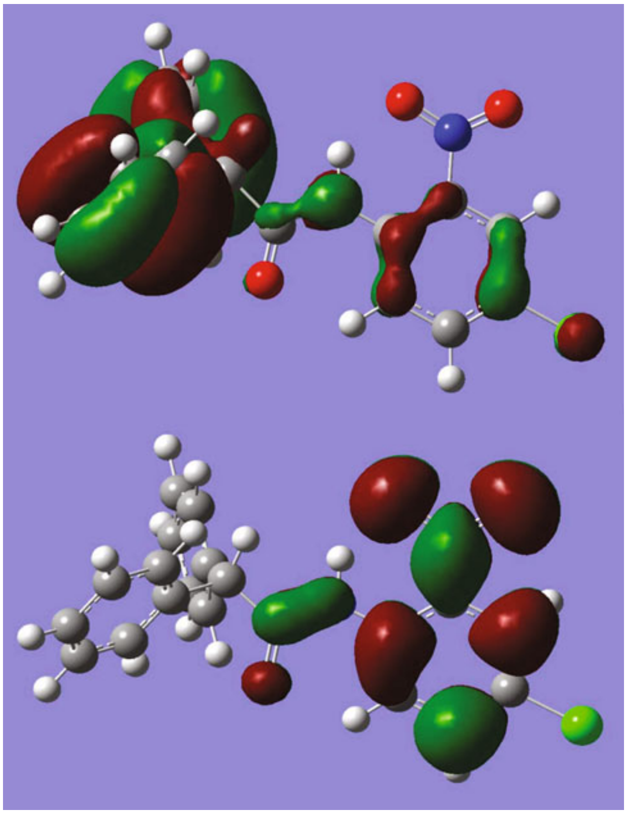

Fig. 3 HOMO (*top*) and LUMO (*bottom*) of $C_{20}H_{15}ClN_2O_3$ in linear alkyl benzene. These orbitals have been obtained with B3LYP/6-311+g(d,p)

$$L_\lambda^{att} = \frac{0.4343}{abs_\lambda/b} = \frac{0.4343}{\sum c_i\varepsilon_i(\lambda)}, \quad (1)$$

where λ, abs_λ, b, c_i and ε_i are wavelengths, the value of absorbance, width of sample, concentrations of absorbers in mol/L, and molar extinction coefficient in $L \cdot mol/L^{-1} \cdot cm^{-1}$. Theoretically, a quantitative comparison between the experimental molar extinction coefficient (ε) and calculated oscillator strength (*f*) for a given transition band is difficult due to the overlap with neighboring electronic or vibration bands. However, we can treat the excited electron as a 1D oscillator, the approximative equation [32] of oscillator strength and molar extinction coefficient then can be writen as

$$f = 4.32 \times 10^{-9} \int \varepsilon(v)dv, \quad (2)$$

where $\varepsilon(v)$ are the molar extinction coefficients corresponding to different wavelengths (in cm^{-1}). So, in a small area, the peak molar extinction can be estimated by $\varepsilon_{max} \approx f/(4.32 \times 10^{-9} v_{1/2})$ with $v_{1/2}$ the half width of peak absorption band (around 1,000 cm^{-1} level). This is a crude approximation that simply means that ε_{max} has a linear relation with oscillator strength *f*. According to Eq. (1), $L_\lambda^{att} = 10\,m$ equals to $\sum c_i\varepsilon_i$ or $abs_\lambda/b = 0.0434$. Therefore, for weak 350–450 nm absorbers (e.g., thiocarbonyl salts, $\varepsilon < 100, f < 0.001$) the influence of the impurities on LS solvents is limited, while for the medium- and strong intensity 350–450 nm absorbers (e.g., o-nitrobenzene derivatives, $\varepsilon > 1,000, f \geq 0.01$), even tiny concentration ($\sim$0.001 mol/L, $\sim$100 ppm level) of these impurities will greatly decrease the attenuation length of the alkylbenzene type LS solvents.

4 Conclusions

Three thiocarbonyl impurities and some similar thiocarbonyl molecules were investigated by TD-PBE0/6-311+g(2df,p)//PBE0/6-311g(2df,p) in three alkylbenzene type scintillator solvents. One of the three impurities was found to have absorption maximum in our characteristic window ($\lambda_{max} = 358$ nm, $f \approx 0.02$). The influences of other thiocarbonyl molecules on scintillator solvents are weak and varied with the different radicals substituted to the C=S bond.

O-nitroaniline was selected as the reference molecular to calculate the nitrobenzene derivative impurity. TD-B3LYP/6-311+g(d,p)//B3LYP/6-311g(d,p) was selected to compute the λ_{max} of $C_{20}H_{15}ClN_2O_3$. An absorption peak with strong oscillator strength around 412 nm was figured out. This method can get acceptable λ_{max}^{TD} of other small-size o-nitrobenzene derivatives too. O-nitrobenzene derivative with auxochrome group substituted can have stronger light absorption than those of thiocarbonyls. Special methods aim to remove these two types of impurities should be applied before these liquid scintillator solvents can be used.

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