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N-(2-ethylhexyl)carbazole: a new fluorophore highly suitable as a monomolecular liquid scintillator

Eva Montbarbon,^[a,b,c] Fabien Sguerra,^[a] Guillaume H. V. Bertrand,^[a] Élodie Magnier,^[a] Romain Coulon,^[a] Robert B. Pansu,^[b] and Matthieu Hamel^{*,[a]}

Abstract: In this work we report the synthesis, the photophysical properties and the applications in scintillation counting of *N*-(2-ethylhexyl)carbazole (EHCz). This molecule displays all required characteristics for an efficient liquid scintillator (emission wavelength, scintillation yield), and can be used without any extra fluorophores. Thus, its scintillation properties are discussed, as well as its fast neutron/gamma discrimination. For the latter application, the material is compared with traditional liquid scintillator BC-501A, and other liquid fluorescent molecules classically used as scintillation solvents such as xylene, pseudocumene (PC), linear alkyl benzene (LAB), diisopropylnaphthalene (DIN), 1-methylnaphthalene (1-MeNapht) and 4-isopropylbiphenyl (iPrBiph). For the first time, an excimeric form of a molecule is advantageously used in scintillation counting. A moderate discrimination between fast neutrons from gamma rays was observed in bulk EHCz, with an apparent neutron/gamma discrimination potential that is one half of BC-501A.

Introduction

Liquid scintillators are mostly ternary mixtures of two different fluorophores dissolved in an aromatic solvent. When a radiation impinges the material, it deposits part (Compton scattering) or totality (photoelectric effect) of its energy. At the end of the ensuing ionisation cascade and *via* Förster energy transfer the scintillator gives a luminescent response preferentially in the visible spectrum, ideally centered around 420 nm, where most of the commercial photomultiplier tubes have an optimal quantum efficiency. Such sensors find various applications, from nuclear research to high energy physics. The most known liquid scintillator is perhaps Saint-Gobain's BC-501A (and its EJ-301 analogue from Eljen Technology), which is a xylene-based liquid scintillator, characterized by a 425 nm emission, a fast photoluminescence decay time, a high light yield (78% of anthracene, i.e. $\approx 12,000$ ph.MeV⁻¹) and an efficient Pulse Shape Discrimination (PSD) capability

between fast neutrons and gamma rays.

The last decade has seen many efforts in the chemical improvement of organic scintillators, both in the liquid^[1] or the plastic^[2] states. To the physicist concern, liquid scintillators present several drawbacks, as they are prepared from hazardous solvents with low flashpoint and must be sealed under inert atmosphere to retain their properties. Most of the recent improvements are therefore performed in the frame of better liquid scintillators for PSD purpose, but also for a reduced toxicity, biodegradation and not-flammability.

As early as 1958, scientists were already concerned about flammability and volatility of liquid scintillators, and *meta*- and *para*-isopropylbiphenyl's isomers were the first molecules considered as a decent alternative.^[3] But it was only in the 2000's that chemical tuning provided EJ-309 liquid scintillator, designed for PSD, and composed of an almost not-flammable solvent (most probably phenylxylylethane, PXE). Pseudocumene is the base of Pico-Fluor 40, and LAB and DIN are found now in many liquid scintillators. In the frame of n/γ pulse shape discrimination, it was recently reported, for the first time, a moderate PSD in non-aromatic solvents, such as ethanol or heptane.^[4] Non-hydrocarbon solvents are also extensively studied.^[5] Ultimately, scintillating systems were also almost reached in water.^[6]

In this context, we wish to present herein our most recent work concerning new liquid scintillators. More precisely, we would like to introduce the use of *N*-(2-ethylhexyl)carbazole (EHCz), a liquid fluorescent molecule, that can act as a whole liquid scintillator. It does not need indeed to be loaded with UV and violet-emitting fluorophores for scintillation purpose.

To the best of our knowledge, there is no example in the literature of liquid scintillator made of a unique compound acting as both solvent and emitter, unless traditional solvents used to prepare liquid scintillators (e.g. xylene, toluene, benzene) were considered as such. We wish to introduce herein *N*-(2-ethylhexyl)carbazole (hereafter designated as EHCz) as a potent one component liquid scintillator, moreover being used at its excimer form. This molecule is already known in the field of liquid dye laser,^[7] as very recently EHCz was used as solvent-free liquid organic laser for Distributed Feedback application.^[8] A multi-gram synthesis affords an easy access to the molecule, which we fully describe in terms of photophysical properties. Then the main characteristics of scintillation counting are given and the pulse shape discrimination

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Supporting information for this article is given via a link at the end of the document.

between fast neutrons and gamma rays is ultimately evaluated.

Table 1. Main characteristics of suitable solvents for the preparation of liquid scintillators.

Solvent	<i>p</i> -xylene	PC	DIN	LAB	4- <i>i</i> PrBiph	1-MeNapht	EHCz
CAS number	1330-20-7	95-63-6	38640-62-9	67774-74-7	7116-95-2	90-12-0	187148-77-2
Flash point (°C) ^a	25	48	130	140	133	82	170
λ_{abs} (nm) – S ₀ → S ₁ main transition ^b	273	273	285	265	257	287	231, 262
λ_{em} (nm)	301, 350 ^c	362	351	340	328	380, 426 ^c	368, 420 ^c
Stokes shift (cm ⁻¹)	3400	9005	6600	8300	8420	8520	5720
Radioluminescence (nm)	308	378	364	348	370	394	430
TCSPC (ns) ^d	8.2	2.15	30.6	34.7	4.1 (26)	27.6	20.6
					9.7 (74)		
Density (g cm ⁻³)	0.86	0.88	0.96	0.86	1.46	1.02	1.00
Refractive index (n ₂₀ /D)	1.50	1.50	1.56	1.48	1.58	1.62	1.58

^a closed cup; ^b concentration 10⁻² – 10⁻⁴ mol L⁻¹ in spectroscopic cyclohexane; ^c emission wavelength of the excimer; ^d considered as a monoexponential decay, unless otherwise stated; data relative to the bulk liquid.

Results and Discussion

State of the art

Table 1 resumes relevant characteristics of regular solvents used in liquid scintillation: xylene(s) – mainly its *para* isomer, pseudocumene (PC), diisopropylnaphthalene (in the form of multiple isomers, DIN), linear alkyl benzene (a complex mixture of organic compounds with formula C₆H₅C_nH_{2n+1}, with *n* in the range 10 to 16, LAB), 4-isopropylbiphenyl (4-*i*PrBiph) and 1-methylnaphthalene (1-MeNapht). These solvent usually are methylated derivatives of benzene, naphthalene or biphenyl (Figure 1). Density, flash point and refractive index are from the literature, when available, or from experiments performed in our institute.

Unfortunately, most of these solvents have major drawbacks and cannot be used without addition of one or many fluorophores: (1) they have a rather low flashpoint; (2) can be hazardous when handled; or (3) the radioluminescence maximum is under 400 nm (photomultiplier tubes used for scintillation purpose have a maximal quantum efficiency between 400 and 450 nm and thus radiation detection is less efficient for fluorophores emitting below 400 nm).

Probably the main drawback associated with liquid scintillators is their low flash points, which prevent them from several applications, at the benefit for plastic scintillators. For instance, these last years have seen several developments for replacing

liquid scintillators by plastics in the field of neutron/gamma discrimination.^[9] Table 1 references data from the literature (usually the MSDSs), except the value for EHCz which was experimentally determined. It shows that only 4 out of 7 common solvents have a flash point in the range 100 – 150°C, and xylene(s) and pseudocumene have a very limited flash point (25 and 48°C, respectively). In this context, only liquid siloxanes are competitive, but still need the loading of primary and secondary fluorophores,^[5] thus leading to probable loss of light if the Förster energy transfer is not sufficient enough. In that context EHCz could be an alternative because of its high flashpoint (170°C) and an intense radioluminescence centered at 420 nm, all these advantages being obtained with this single molecule, at its excimer form.

Synthesis

A thorough literature survey reveals that a carbazole substituted at the *N* position with a hydrocarbon, alkyl moiety always almost leads to a solid molecule at room temperature. The two known exceptions are EHCz, whose melting point is close to 0°C, and a poly(ethylene oxide) with carbazole moiety.^[10] The latter compound displays a slightly lower photoluminescence quantum yield (0.28) compared with EHCz (0.31). Although EHCz is a commercial product, it is rather expensive when large volumes are needed. We therefore turned our attention into a straightforward synthesis, involving the reaction between carbazole and 2-ethylhexyl bromide in the presence of sodium hydride (Scheme 1). The titled compound was isolated as a colourless, viscous liquid after chromatography on silica gel and/or

distillation. The optimized sequence allowed us preparing the titled compound on a multi-gram scale. As expected for scale up the yield was decreased, also minimally, from 82% for a 5 g synthesis down to 73% for a 25 g preparation. Purification by flash chromatography on silica gel gave us a purity suitable enough for scintillation application (scintillation grade).

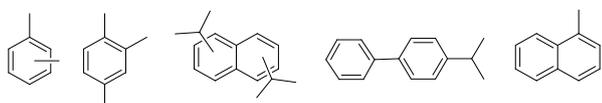
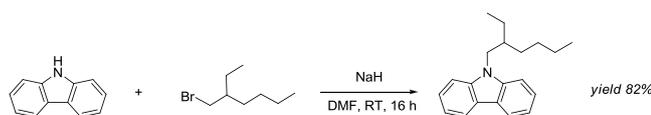


Figure 1. Topological representation of xylene(s), pseudocumene, diisopropylnaphthalene (mixture of isomers), 4-isopropylbiphenyl, and 1-methylnaphthalene (from left to right). LAB is not shown due to the complex composition. BC-501A is a xylene-based liquid scintillator containing various fluorophores.



Scheme 1. Synthesis of *N*-(2-ethylhexyl)carbazole.

Photophysical characterization

Fluorescence spectra, radioluminescence, Time Correlated Single Photon Counting (TCSPC) and quantum yields were recorded in our facility (see Electronic supplementary information for experimental details). Density and refractive indexes could be found in the literature. However, we recorded EHCz refractive index and found a value of 1.58 at 589 nm, and a higher value of 1.64 at 404 nm. The refractive indexes from 404 to 706 nm are given in the supplementary material, with a relative standard uncertainty of ± 0.001 .

Pure EHCz displays a structured emission with two peaks at 417 and 434 nm (Figure 2, top). Fluorescence lifetime was acquired by time correlated single photon counting (TCSPC) and was found to be 20 ns. Once diluted in dichloromethane (10^{-2} to 10^{-4} mol L $^{-1}$) the emission is still structured and blue-shifted to 367 and 351 nm, respectively, and the emission lifetime is shortened to 10.2, then 6.3 ns. The hypsochromic shifts, accentuated by the dilution, are consistent with a decrease in the number of molecules participating in the excimer. At low concentration the shift stops and the emission bands present a thinner structure, characteristic of mono-molecular excited species. This behavior is typical of carbazole emitting as a single species, and emission wavelength dependence with the concentration of EHCz was already reported by Kubota and coworkers.^[10] The same conclusion can be drawn from the time resolved experiments (Figure 2, bottom). The slower time response from pure EHCz can be attributed to high order excimer, where excited states delocalization increases its stability, whereas high dilution provides faster decay time corresponding to less delocalized excited state and ultimately monomolecular exciton. These photophysical properties are characteristics of carbazole derivatives excimers that can be seen for instance in polyvinylcarbazole (lifetime of about 42 ns at 420 nm^[11]). Time measurements of other solvents reported in the Table 1 are also given in the Supporting Information (Figure SI1).

When diluted, the Stokes shift of EHCz is close to 5,700 cm $^{-1}$ (based on the third shoulder at 293 nm at the concentration 10^{-4} M, see Table 2). Compared with other solvents, this is not the highest Stokes shift ever recorded, as Pseudocumene (PC) presents a 9,000 cm $^{-1}$ value. To determine the Stokes shift of the neat form, the absorption spectrum was recorded using a 0.05 mm long optical cell. The last absorption shoulder was seen at 386 nm, giving therefore a reduced Stokes shift of about 3,900 cm $^{-1}$ (for both calculations the radioluminescence maximum was taken into account). However the transparency of the liquid was good enough at its emission wavelength, with a 78% value at 420 nm.

Fluorescence quantum yield of EHCz was calculated in three dichloromethane-based solutions (ranging from 0.2 to 0.9 10^{-4} mol L $^{-1}$) and was evaluated to be 0.70 ± 0.02 which is way higher than the other scintillation solvents cited above (see Table 1). The main photophysical characteristics of EHCz diluted in dichloromethane or in neat form are given in Table 2.

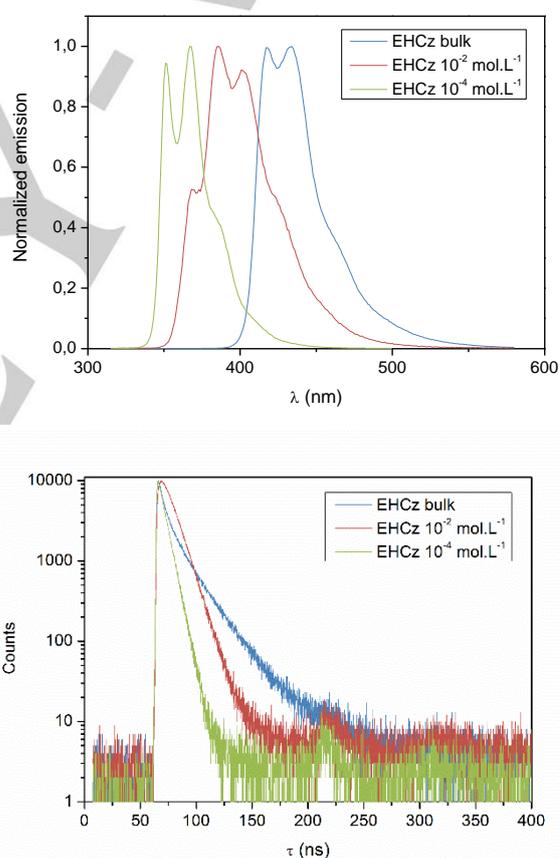


Figure 2. Influence of the EHCz concentration on fluorescence spectra (top) and fluorescence decay times (bottom). For the TCSPC experiment: $\lambda_{\text{ex}} = 274$ nm; $\lambda_{\text{monitoring}}$ at their respective maximum of emission.

Radioluminescence

Using the Fluoromax-4P spectrofluorimeter with the excitation light shut down, and a highly active ^{90}Sr - ^{90}Y beta emitting radioactive source ($E_{\text{mean}} = 933$ keV, $E_{\text{max}} = 2280$ keV), we were able to record the optical response of liquid

scintillators. To this, the emission slit was opened at its maximum available on this device, which presents the drawback to enlarge the emission response, leading therefore to pseudo-Gaussian shapes instead of well-defined luminescence spectra. Under ionizing radiation, EHCz displays a broad emission spectrum centered on 430 nm (Figure 3) and a FWHM of 57 nm which is similar to BC-501A (emission at 428 nm and FWHM of 60 nm). It is also noteworthy that EHCz is, after BC-501A, the best emitter of scintillation photons. The number of scintillation photons emitted during the time experiment is indexed for each liquid scintillator in Table 3.

Table 2. Photophysical properties of *N*-(2-ethylhexyl)carbazole at various concentrations.

[EHCz] (mol L ⁻¹)	Absorption ϵ (L mol ⁻¹ cm ⁻¹)	Emission (nm)	TCSPC (ns)	χ^2	Φ_{PL}
neat	-	417, 434	30	1.57	0.3*
10 ⁻²	-	386, 401	11	1.92	-
10 ⁻⁴	231 (139,000), 262 (98,000), 293 (55,100), 344 (24,600)	351, 367	7	1.09	0.7±0.02

* ref [10].

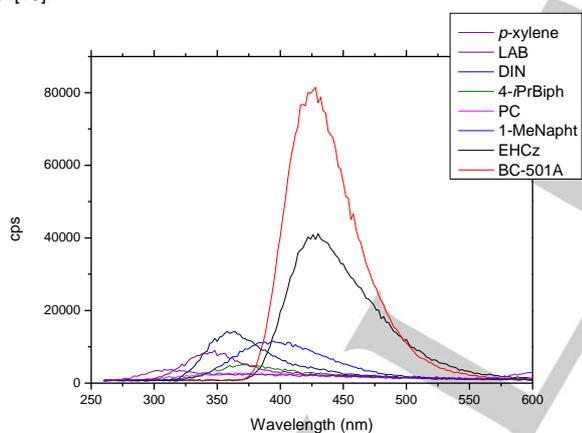


Figure 3. Radioluminescence spectra of pure liquids under β irradiation (^{90}Sr - ^{90}Y – 36 MBq): *p*-xylene, LAB, DIN, 4-isopropylbiphenyl, pseudocumene, 1-methylnaphthalene, BC-501A, and EHCz (from lower to higher wavelengths of maximum emission).

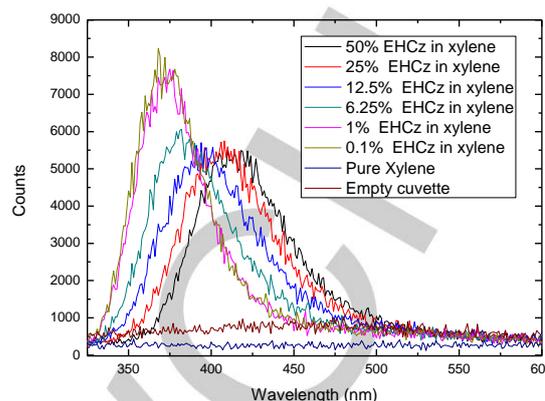


Figure 4. Radioluminescence spectra under β irradiation (^{90}Sr - ^{90}Y – 25 MBq) for 0 – 50 vol% EHCz in xylene. No emission of xylene is visible in this experiment.

In order to understand the possible effect of excimer formation on the scintillation process, the luminescent response to the ^{90}Sr - ^{90}Y radioactive source was then recorded with the concentration of EHCz in xylene, from 0.1 up to 50 vol% (Figure 4). *P*-xylene was used to promote the energy deposition of ionizing particles at high dilution. Upon dilution of EHCz, the radioluminescence is blue shifted from 430 to 370 nm. This hypsochromic shift correlated with the dilution is consistent with results from fluorescence measurements. At high concentration the broad radio-emission band is due to an excimer or, less likely, an exciplex with the xylene, lower concentration gave a thinner band, once again characteristic of a low order excimer, or even monomolecular exciton. Integral beneath the radioluminescence curves shows that the concentration does not impact photon intensity, which means that excimer formation does not affect the scintillation process (see Figure S12 in the supporting information). This result confirms that it is favorable to use pure EHCz as its emission wavelength is better suited for standard photomultiplier tubes and its efficiency is not affected by excimer formation. The dilution effect is also confirmed to be harmful when recording the energy spectra of a 37 MBq, ^{137}Cs radioactive source emitting 662 keV gamma rays. Relative to pure EHCz, 50 and 25 vol% xylene solutions emitted 93 and 89% photons, with a total number of counts of 72 and 64 %, respectively. This is shown in the Figure S13 in the supporting information.

EHCz has a strong stability towards irradiation. Radioluminescence monitored at 420 nm and performed during 30 min with a highly active 36 MBq ^{90}Sr - ^{90}Y beta source in close contact with the quartz cuvette did not display any kind of signal loss, as well as for BC-501A (see Figure S14 in the supporting information).

Effective quantum efficiency for the detection of EHCz

EHCz was fully described in terms of its photophysical properties, this means for its intrinsic properties.

The intended application, which is neutron/gamma discrimination, involves a detection system, made of a photodetector and an electronic digitizer. The photodetector used at the laboratory is a Hamamatsu H1949-51 photomultiplier tube (PMT), designed from a standard alkali photocathode but slightly shifted to the UV region compared with other standard PMTs.

In order to characterize the coupling between the scintillator and the photodetector, the quantum efficiency criterion is introduced. Effective quantum efficiency is the probability that a scintillation photon (created by interaction of radiation with matter) arriving at the photocathode of the PMT produces a photoelectron.^[12] Equation 1 gives the definition of effective quantum efficiency η_Q of a given scintillator.

$$\eta_Q = \frac{\int_0^\infty I(\lambda)Q(\lambda)d\lambda}{\int_0^\infty I(\lambda)d\lambda} \quad \text{Equation 1}$$

Where λ is the wavelength and Q is the distribution of the photocathode efficiency (given by the PMT manufacturer, herein Hamamatsu).

Effective quantum efficiency values for tested solvents and BC-501A are listed in Table 3. According to Table 3, the coupling between EHCz and H1949-51 PMT is not the best, but its value is similar to that one of BC-501A. In fact, the weak difference between them is certainly due to the slight shift of the photocathode efficiency in the UV region.

Table 3. Quantum efficiency of various liquid dyes and BC-501A.

Solvent	N_{ph}	η_Q (%)
<i>p</i> -xylene	339480	18.38
Pseudocumene	274360	19.30
DIN	612870	22.49
LAB	439320	21.11
4-isopropylbiphenyl	340130	20.65
1-methylnaphthalene	631930	22.34
EHCz	1746140	20.99
BC-501A	2837630	22.26

Radiation detection

Despite all the above mentioned qualities of EHCz, the most important part to our eyes is the possibility to detect radiations. To this, 5 cm long quartz cuvettes were exposed

to gamma rays. One of the edges of the cuvette is optically coupled with Rhodorsil optical grease to a standard photomultiplier tube (see experimental section for details). With a digital oscilloscope, each scintillating pulse is digitalized and then recorded. Then a histogram is built from the integration of the pulse area.

The spectra represented in Figure 5 are typical from a Compton interaction between the incident gamma ray and the scintillator; no full energy peak is thus observed. However, with the same experimental conditions, it is possible to evaluate the scintillation yield (expressed in photons per deposited MeV), based on a rule of thumb with a known scintillator. In our case, it is BC-501A, with a 12,000 ph MeV⁻¹. Assuming that the EHCz Compton edge is located at 50% of BC501-A's Compton edge, we can therefore determine that EHCz gives 6,000 ph MeV⁻¹. From the radioluminescence spectra, EHCz liberates approximately 60% of photons relative to BC-501A, and it is the same percentage when comparing the Compton edges of EHCz and BC-501A.

Neutron/gamma pulse shape discrimination

One of the main advantages of liquid scintillators is their ability to perform a very good discrimination between fast neutrons and gamma rays. Again, appropriate solutions towards flammable scintillators are very welcome in this field.^[4,13,14] In this context, a 3 cm³ quartz cuvette was exposed to a 1MBq, ²⁵²Cf neutron/gamma radioactive source, and its response was compared to a BC-501A sample of same dimension. Both results are presented in Figure 6. It shows that EHCz displays a moderate pulse shape discrimination in neat form, with a naked eye lecture giving neutrons and gamma lobes (in the top and bottom parts of the Figure, respectively). The separation is two times better for BC-501A, despite non-optimized digitizer parameters for the latter. Indeed, due to the large decay time difference between EHCz and BC-501A liquid scintillators (20 and 3.2 ns, respectively) and for the sake of a better comparison, digitizer parameters were kept equivalent for both experiments. It is noteworthy that a special care must be taken in the removal of any residual oxygen in the medium, which can preclude any PSD. In addition, 1-Methylnaphthalene and 4-*t*-PrBiphenyl in their pure forms were also confronted to an AmBe source as well as with BC-501A, with another setup; they did not display any kind of discrimination as such (see Figures S15-7 in the supporting information).

Discussion

To the best of our knowledge, this is the first time that excimers are advantageously used for the production of efficient liquid scintillators. The production of such excimers dissipates energy: typically 0.42 eV in our case. But this

loss of energy is at the benefit of both the Stokes shift and the suitability with photomultiplier tube quantum efficiency. This explains why EHCz does not require any extra fluorophore to be efficient enough. Compared with xylene and 1-methylnaphthalene which are also able to produce excimers when undiluted, at 349 and 428 nm wavelengths, respectively, EHCz is the best excimer liquid scintillator. Ultimately, it is always assumed that the energy occurring from radiation/matter interaction is transferred from the matrix to the fluorophore *via* Förster interaction. As herein this liquid scintillator is composed of only one molecule, this is therefore the first example of liquid scintillation counting without Förster interaction.

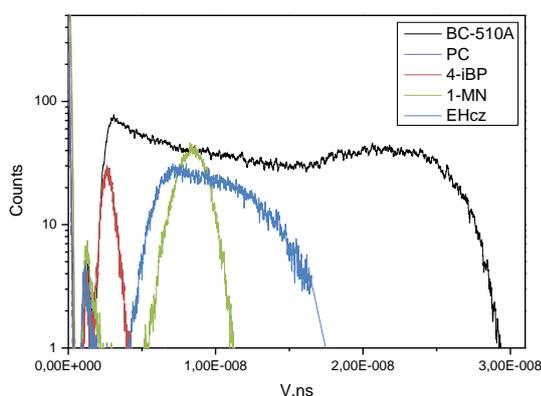


Figure 5. Comparison of the ^{137}Cs scintillation gamma spectra obtained for BC-501A (black), *N*-(2-ethylhexyl)carbazole (blue), 1-methylnaphthalene (green), 4-isopropylbiphenyl (red), where the background residual signal has been discarded. Data were obtained for 3 mL liquid samples.

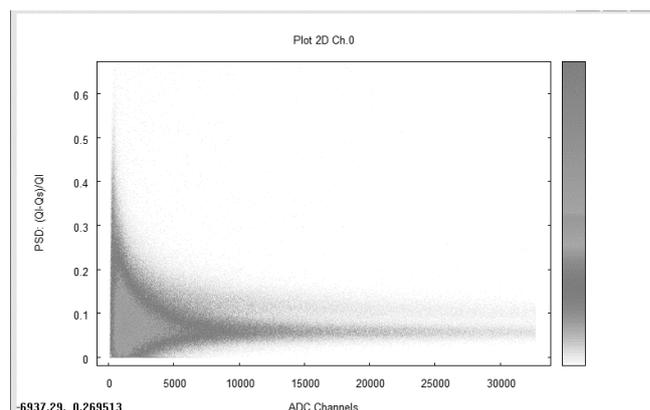
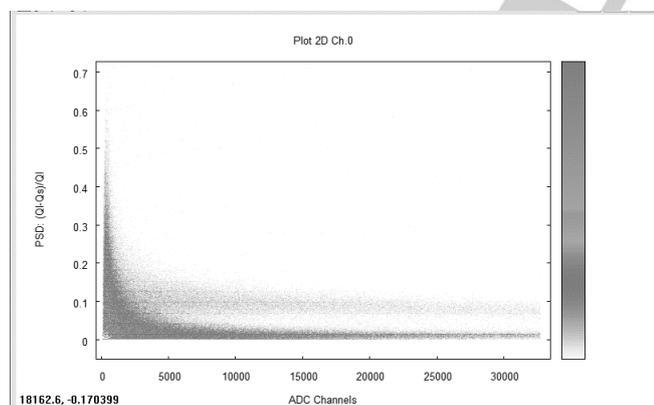


Figure 6. PSD plots for a ^{252}Cf radioactive source measurement with BC-501A (top) and EHCz (bottom). The same parameters for both samples were applied.

Conclusions

We report herein the use of *N*-(2-ethylhexyl)carbazole, a colourless, fluorescent liquid molecule which can act as a liquid scintillator medium just by itself. It was prepared in high yield by deprotonation of carbazole followed by nucleophilic substitution with 2-ethylhexyl bromide. It is noteworthy that this reaction sequence can be extended to a 0.1 mole scale. No additive is required as the photophysical properties satisfy scintillation criteria. This compound was evaluated in terms of absorption and emission spectra, TCSPC, quantum yield and scintillation properties: decay time, energy spectra, and fast neutron/gamma pulse shape discrimination. As such, it respects all the criteria of a liquid scintillating system. It is optically transparent to its own light with a wavelength cut of the absorption around 402 nm for 1 cm optical path and absorbance 1. Both photoluminescence and scintillation wavelength maxima are located around 420 nm, with the main emission driven by the excimers when used in bulk. The decay time is fast enough for scintillation application, and good scintillation yield was observed. Ultimately, we were glad to observe a visible pulse shape discrimination between fast neutrons and gamma rays.

At this stage we do not have any feedback regarding neither the chemical stability, nor its behaviour under high ionizing radiation flux, but it will be studied in future experiments.

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French Direction Générale de l'Armement and Secrétariat Général de la Défense et de la Sécurité Nationale for their funding (G.H.V.B., F.S.).

Experimental Section

Xylene was obtained from VWR. 1-methylnaphthalene was obtained from Merck. These two solvents were used without purification. Pseudocumene was obtained from Sigma-Aldrich and was distilled prior to use. 4-isopropylbiphenyl was obtained from Alfa Aesar and was purified on a silica gel pad prior to use. BC-501A was obtained from Saint-Gobain Crystals and Detectors. Sodium hydride and 2-ethylhexylbromide were obtained from Sigma Aldrich. Carbazole was purchased from Labosi or from Sigma-Aldrich.

^1H spectrum was recorded at 400 MHz on a Bruker AVANCE 400 spectrometer. Chemical shifts (δ) are given in ppm, referenced to the residual proton resonance of CDCl_3 (7.26 ppm). Coupling constants (J) are given in Hertz (Hz). The terms m, d, t, sept, refer to multiplet, doublet, triplet, septuplet.

EHCz was synthesized according to a previously published procedure.^[15] Carbazole (4 g, 23.9 mmol, 1 equiv.) and NaH (1.32 g, 55 mmol, 2.3 equiv., previously washed with pentane to get rid of mineral oil) were stirred under argon in DMF (100 mL) for 30 min. 2-Ethylhexylbromide (5.2 mL, 29.3 mmol, 1.2 equiv.) was added dropwise and the mixture was stirred overnight. Water was added (50 mL) and the product was extracted with diethyl ether (3 × 100 mL). The organic layer was concentrated to 50 mL and washed with brine (3 × 50 mL). The organic layer was dried with anhydrous magnesium sulfate, filtered and evaporated. The product was purified by column chromatography (SiO_2 , cyclohexane) to afford the product as colorless oil (5.5 g, 19.7 mmol, 82%, Lit.^[15] 49%).

The same reaction was performed on a 20 g scale of carbazole, leading to *N*-(2-ethylhexyl)carbazole with a 73% yield.

^1H NMR: δ 0.86 (t, 3H, 3J 7.3); 0.91 (t, 3H, 3J 7.3); 1.21 – 1.43 (m, 8H); 2.07 (sept, 1H, 3J 6.7); 4.10 – 4.21 (m, 2H); 7.39 (d, 4H, 3J 8.2); 7.45 (dt, 4H, 3J 6.9, 4J 1.1).

All photophysical experiments were conducted in Suprasil Quartz cuvettes.

UV-visible spectra were measured at room temperature in cyclohexane on a Jenway 6715 UV/Vis spectrometer, wavelengths are given in nm and extinction coefficients ϵ are presented in $\text{L mol}^{-1} \text{cm}^{-1}$.

Fluorescence, radioluminescence and Time-Correlated Single Photon Counting (TCSPC) experiments were performed with a Horiba Jobin Yvon Fluoromax 4P spectrofluorometer. Radioluminescence spectra were acquired by using the following procedure. In the Fluoromax

4P spectrofluorometer, the excitation light was shut down. In the centre of the experimenter chamber, the ^{90}Sr - ^{90}Y β emitting source (25 or 37 MBq) placed close to the scintillator cell. Spectra were acquired with an integration time of 0.5 s nm^{-1} . TCSPC experiments were performed by illuminating the liquid scintillator with a laser diode operating at 274 nm.

Gamma spectra were recorded as follows: the sample was optically coupled to a Hamamatsu H1949-51 photomultiplier tube operating at negative voltage. A 387 kBq ^{60}Co radioactive source was used to excite the material. 100,000 pulses were recorded with a Lecroy HDO6054-MS digital oscilloscope, were integrated and sorted as an energy histogram. Dilution experiments were performed with a 37 MBq ^{137}Cs radioactive source and pulses were sorted and treated with a custom-made electronic board.^[16]

A Schmidt + Haensch DSR λ refractometer was used for the determination of the EHCz refractive index.

Determination of the EHCz flash point was performed at Filab (www.filab.com).

Pulse shape discrimination leading to the separation of fast neutrons vs. gamma rays was performed using a CAEN DT5730B digitizer, monitored with the DPP-PSD software. An unshielded, ≈ 1 MBq ^{252}Cf source was placed 2 cm close to 3 cm^3 samples. Experiments with other solvents were performed at CEA DAM/DIF using the FASTER module.^[17] 3 cm^3 samples were coupled to a Hamamatsu H10580 PMT with optical grease, then exposed to an unshielded 370 MBq AmBe source.

Keywords: Carbazole • Scintillation • Fluorescence • Excimer

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FULL PAPER

We report herein the synthesis of *N*-(2-ethylhexyl)carbazole and its use as a monomolecular liquid scintillator.

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