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An Efficient Approach to Pyrene-based Aggregation-induced Emission Luminogens (AIEgens)

Hongxi Guo,^[a] Xinyi Song,^[a] Xiaohui Wang,^[a] Yiwei Liu,^[a] Carl Redshaw,^[b] and Xing Feng^{[a,c]*}

Dedication ((optional))

[a]	H. Guo, X. Song, X. Wang, Y. Liu, and Dr. X. Feng
	School of Material and Exercise Guardona University of Technology.
	Guandzhou 511006, P. R. China.
	E-mail: hyxhn@sina.com (X.Feng)
[b]	Prof. Dr. C. Redshaw
	Department of Chemistry
	University of Hull
	Cottingham Road, Hull, Yorkshire HU6 7RX, U.K.
[c]	Dr. X. Feng
	Guangdong Provincial Key Laboratory of Luminescence from Molecular Aggregates (South China University of Technology)
	Guangzhou 510640, China
	Supporting information for this article is given via a link at the end of the document

Abstract: To suppress the fluorescence quenching of pyrene in the aggregation state, this article presents a facile strategy for the construction of pyrene-based aggregation-induced emission luminogens (AIEgens) via decorating the pyrene core with benzophenone units at the 1-, 2- or 2,7-positions. This set of pyrene-based compounds **1-3** displayed a weak deep blue fluorescence in solution, but an enhanced excimer emission with $\lambda_{em max}$ of 426-436 nm in the aggregation state. Interestingly, unlike reported benzophenone derivatives, this series of compounds did not exhibit thermally activated delayed fluorescence/ phosphorescent properties.

Introduction

The molecular construction of efficient solid-state emitters has attracted intensive attention because of their potential application as organic light-emitting diodes (OLEDs), [1],[2] in anticounterfeiting,^[3] as fluorescence sensors,^[4] as well as in photodynamic therapy. [5] However, the disadvantages of traditional luminescent materials are that they usually display a ubiquitous aggregation-caused quenching (ACQ) effect, which often leads to lower emission intensity in the solid state compared to in solution. [6] The most important milestone in the development of high efficiency luminescent solid state materials was when Tang and coworkers reported that silole molecules are nonemissive in solution but display bright blue emission in the solid state, which was defined as aggregation-induced emission (AIE) in 2001, [7],[8] and the proposed restriction of intramolecular motion (RIM) mechanism offer possibilities to develop a variety of AIE luminogens.^[9] The highlight of AIEgens is that they overcome the ACQ effect of conventional luminophores and expand the possible high-technological applications, both in organic electronics ^[10], and fluorescence biomedical probes.^{[9] [11]}

Pyrene (and its derivatives) is a member of the polycyclic aromatic hydrocarbons (PAHs) and possesses a large planar π -electron-enriched skeleton.^[12] Due to their excellent blue fluorescence properties, high quantum yields, enhanced carrier mobility and thermal stability, they have been widely unitized as luminescent materials for OLED devices, stimuli-response

materials and chemosensor etc.^[13],^[14] However, the planar molecular skeleton prefers to form π -stacking in highly concentrated media or in the aggregation state, resulting in a large red-shifted emission with decreased quantum yield. In order to suppress the π - π stacking of pyrene and to construct high efficiency pyrene-based solid-state materials, one strategy is to introduce bulky substituents at specific substituted positions of the pyrene core.^[15] Much effort has been exerted into exploring many approaches to functionalize the pyrene to achieve high-efficient blue emitters, not only at the active sites (1-, 3-, 6- and 8-positions), node plane (2- and 7-positions), but also at the K-region (4-, 5-, 9- and 10-positions), respectively. For example, newly prepared butterfly-shaped pyrenes was found to emit deep blue emission both (~410 nm) in solution and in the solid state with high quantum yield (\geq 0.75).^[16]

On the other hand, molecular tailoring following the RIM mechanism is a promising alternative way to enhance the luminescence efficiency of pyrene-based compounds. When the pyrene contains a tetraphenylethene (TPE)/ hexaarylbenzene (HAB) unit at the active site, node plane or K-region, intense emission is exhibited with good electroluminescence by suppressing intermolecular π -stacking. ^[17] Of course, the presence of C=C bonds linked to the pyrene framework also contributes to the enhanced fluorescence. Both the abovementioned methodologies play a significant role in realizing the transformation of pyrene-based ACQ luminogens to AIEgens. ^[18]

Benzophenone is an important component in the design of thermally activated delayed fluorescence/ phosphorescent emitters for OLED devices,^{[19],[20],[21]} due to its strong electronaccepting ability and efficient intersystem crossing. ^[22] Previously, Zhang *et al* combined triphenylamine and benzophenone to afford AIE-active room temperature phosphorescence luminophores. ^[23] More recently, Tang and coworkers reported a novel molecule, namely (4-(phenothiazin-10-yl)phenyl)(pyren-1-yl)-methanone, which possesses AIE characteristics, polymorphism and mechanochromic properties. ^[24] Such research inspires insightful strategies to prepare novel pyrene-based luminescent materials with fantastic properties. Due to the special electronic properties of pyrene, substituents at the 1-, 2- or 2,7-positions of pyrene can lead to different physical properties. For example, the electronic communication would be increased between the pyrene core and the substituent at the 1-position, leading to a red-shifted absorption and emission band. Differently, the nodal plane of pyrene passes through the C2 and C7-position of pyrene, which contributes to weakening the electronic interaction between the pyrene core and substituent. Based on this view, in this paper, we attempt to prepare a set of new pyrene-based blue emitters **1-3** via introducing the benzophenone unit at the 1-, 2- or 2,7positions of pyrene. Out of our expectation, those pyrenes exhibit deep blue emission with clear AIE characteristic, but do not display clear RTP properties. The excited state levels were calculated in order to understand the electronic transition process via theoretical calculations.

Results and Discussion

Synthesis

The target compounds **1-3** were synthesized by a facile synthetic route as shown in Scheme 1. The starting compounds **Py-2-OH** and **Py-2,7-OH** were prepared from pyrene-2,7-bis(boronate) esters and pyrene-2,7-bis(boronate) esters in high yield. ^[25]. The hydroxylpyrenes (**Py-1-OH**, **Py-2-OH** or **Py-2,7-OH**) were further involved in a substitution reaction with (4-bromophenyl)(phenyl)methanone to afford the pyrene-based light-yellow compounds **1-3**, which were characterized by ¹H/¹³C NMR spectroscopy, and high-resolution mass spectrometry (HRMS). All compounds are very soluble in common solvents (such as tetrahydrofuran (THF), dichloromethane, dimethyl sulfoxide (DMSO), and *N,N*-dimethylformamide (DMF)).



Scheme 1. The synthetic route for pyrene-based derivatives 1-3.

Theoretical calculations

To gain a deeper understanding of the molecular geometries and electronic structure of these pyrene-based AlEgens, density functional theory (DFT) was performed using Gaussian 09W at the B3LYP/ 6-311G(d,p) level. As shown in Figure 1, when the benzophenone unit(s) was connected to the pyrene core at the 1-, 2- or 2,7-positions by an oxygen atom as a bridge in compounds **1-3**, where one of phenyl ring of benzophenone is almost perpendicular to the pyrene ring with dihedral angle in range from 76-81°, the steric conformation is beneficial to adjust the distance of the π - π stacking interaction.^[26] The HOMO and LUMO levels of compounds **1-3** are mainly distributed on the pyrene ring. As the substituent position changed and the number of substituent groups increased, both the HOMO level and LUMO level increased, resulting in a broadening of the HOMO-LUMO energy gap over the range from 3.68 eV in compound 1 to 3.81 eV in compound 2 (3.80 eV in compound 3), suggesting that the substituents at the 2- or 2,7-positions can enhance the HOMO energy.



Figure 1. Optimized molecular orbital plots (B3LYP/6-311G(d,p)) of molecules 1-3; the blue and red in the molecular configuration represent electron density.

Photophysical Properties

The UV-vis absorption spectra of the three pyrene-based compounds 1-3 were recorded in THF solution and the optical data are listed in Table 1. For comparison, the absorption spectrum of pyrene is also presented. As shown in Figure 2, compounds 1-3 exhibit a pyrene-like absorption profile with wellresolved absorption bands in the range 250-450 nm, and strong absorption peaks at ~276 nm, ~335 nm and ~380 nm consistent with the $S_3 \leftarrow S_0$ excitation, $S_2 \leftarrow S_0$ excitation and $S_1 \leftarrow S_0$ excitation, respectively.^[27] For compounds 2 and 3, as the benzophenone group is introduced at the pyrene core, the absorption band is slightly bathochromic shifted (<5 nm) in the longer-wavelength direction compared to the parent pyrene, due to the node plane passing through the 2- and 7-positions, and the substituents strongly influencing the $S_2 \leftarrow S_0$ excitation. Unexpectedly, the absorption behavior of compound 1 is different from reported 1-substituted pyrene derivatives.^{[24],[28]} This may be due to the electron-rich oxygen atom directly connected to the 1carbon of pyrene, which can interfere with the electronic transition,^[29] leading to decreased molar absorption coefficients; the value of molar absorption coefficients follows the order 3>2 >pyrene>1.



Wavelength (nm)

Figure 2. UV-vis absorption spectra of the pyrene-based derivatives 1-3 at a fixed concentration of 1.0×10^{-5} M in THF at room temperature.

AIE characteristics

Most pyrene derivatives are excellent fluorophores with intense fluorescence.^[15] However, pyrenes prefer to undergo an ACQ effect and this would decrease the fluorescence intensity in aggregated state. Based on our experience, groups with a twisted conformation can help to enhance the fluorescence in the aggregated state compared to in solution. To investigate their possible AIE properties, the fluorescence (FL) spectra of the pyrene-based compounds 1-3 were recorded at different water fractions (f_w) in THF/water mixtures. Compound **1** exhibits weak dual emission at 385 nm and 486 nm respectively in THF solution. Subsequently, the emission intensity remains weak and the emission peak at 486 nm almost disappeared, when the water was added into the THF solution until $f_w < 80\%$. Afterwards, the emission peak at $\lambda_{em} = 488$ nm was rapidly enhanced by ca. 8fold as the f_w increases to 99% (Figure 3A). On the other hand, the maximum emission peak of 2 is at 385 nm in THF solution, which originates from the monomer emission of the pyrene units.^{[3],[26],[30],} As f_w increases to 80%, the emission intensity at 385 nm decreased with an enhanced emission at 487 nm with an enhanced emission intensity of 2-fold (Figure 3B). For compound 3. the fluorescence spectra revealed similar emission behavior in THF/H₂O mixtures to compound 2. Compound 3 emits weaker deep blue fluorescence (FL) in THF solution with a maximum emission peak at 398 nm. As water is added, the emission peak at 398 nm decreased and a new emission peak at 436 nm gradually increased (Figure 3C)



Figure 3. (A-C) PL spectra of compounds 1-3 in THF/water mixtures with different water fractions (f_w). (D) Plot of relative PL intensity (II_0) *versus* the composition of a THF/water mixture of 1-3, respectively. I is the fluorescence intensity in different THF/water mixtures with different f_w , and I_0 is the fluorescence intensity in pure THF solution ($\lambda_{ex} = 343$ nm for 1, λ_{ex} 339 nm for 2 and λ_{ex} 341 nm for 3, respectively).

Furthermore, the concentration-dependent PL spectra of compounds **1-3** were measured. As the concentration increases, compound **1** exhibits an enhanced long-wavelength emission peak at 485 nm, which originates from the excimer emission via a J-aggregation. while the emission of compound **3** was red-shifted from 398 to 427 nm, and the emission of compound **2** exhibits a slight change when the concentration was increased from 10^{-7} M to 10^{-3} M, indicated that compound **1** adopts a different molecular

arrangement from compounds 2 and 3. (Figure S13) In addition, the 2- and 2,7-substituted pyrenes 2 and 3 possessed a narrower full width at half maxima of 29-31 nm. The red-shifted emission in the aggregated state indicated that the compounds 1-3 prefer to form dimers, leading to a highly excimer emission; the corresponding absolute FL quantum yields (ϕ_{FL}) are 0.87%, 0.60% and 2.30% respectively, which may be due to the free rotation of the benzophenone unit consuming the energy by a non-radiation decay pathway.^[31] Although the ${\cal P}_{\sf FL}$ was enhanced by 8.18% for 1, 6.02% for 2 and 8.70% for 3 in the solid state respectively, these compounds still display a relative low Φ_{FL} compared to the previous reports,[32] indicating that these compounds undergo a strong intermolecular interaction, such as π - π stacking and H-bonding interaction.^[33] It seems that the compounds 1-3 are in according with the AIE characteristics, with an α_{AIE} (Φ_{solid}/Φ_{soln}) order of 2 > 1 > 3, via the introduction of benzophenone units at the pyrene core.

Furthermore, the fluorescence lifetimes of the compounds 1-3 were measured in THF solution and in the solid state and are listed in Table 1 and Figures S15-S17. The calculated radiative decay rate (k_r) of the compounds 1-3 increased by about 3.0-7.5fold in the solid state compared with those in solution, and the nonradiative decay rate (k_{nr}) of compound **1** decreased 9.35 x 10⁸ to 2.70 x 10⁸, while the k_{nr} of compounds 2 and 3 slightly increased (ca. ~1.50) in the solid state compared to in solution. Thus, both the results of the calculated fluorescent radiation transition rates and the plots of relative PL intensity (I/I₀) versus the f_w (Figure 3D) suggest that these pyrene-based compounds 1-3 are indeed AIE-active fluorophores. In addition, the solvatochromic effect of these pyrene-based AIE luminogens (AlEgens) were measured in different polarity solvents. Compounds 2 and 3 display a slight bathochromic shift both in their absorption and emission spectra, indicating that the solvent polarity has a limited effect on the optical behavior (Figures S11-S12). This maybe due to the similar dipole moments in the ground state and in the Franck-Condon excited-state (LE state).^{[34] [35]} While compound 1 exhibits a dual emission in polarity solvents, the long-wavelength emission is red-shifted from 486 nm (in THF) to 575 nm (in acetonitrile), which maybe due to the formation of a dimer which is sensitive to the polarity of the solvents (Figure S10). In addition, the long-wavelength emission intensity at 486 nm became stronger as the concentration increased from 10⁻⁷ to 10⁻³ M, indicating that the compounds tend to form a strong dimer at high concentration (Figure S13).

Mechanical Stimuli Properties

The AIEgens with a twisted conformation usually show a clear tunable-emission color under external mechanical stimuli, As shown in Figure 4A, 4C and 4E, the emission spectra of this series of pyrene-based compounds 1-3 exhibit blue emission with the maximum λ_{em} at 436 nm, 426 nm and 434 nm in the solid state, respectively, which has a slightly red-shift compared to in THF solution. Moreover, the compounds 2 and 3 (with benzophenone groups at the 2- or 2,7-positions of pyrene) show a

Table 1. The photophysical properties of three pyrene-based AIEgens 1-3.

Compd.	$\epsilon (\lambda_{max abs})$ $(M^{-1} cm^{-1})^a$	<u>λ_{maxPL}</u> (nm)	$\underline{\varPhi}_{f}$ solns ^a / solid ^b	<u>τ (ns)</u> solns ^a / solid ^b	α_{AIE}^{c}	${f K}_r ~~(imes 10^8~{f S}^-)^d$ solns ^a / solid ^b	$K_{nr} \xrightarrow{(\times 10^8 \text{ S}^-)^e}$ solns ^a / solid ^b	LUMO (eV)	HOMO (eV)	Eg (eV)
1	343 (34966)	385, 486 (0%) 472 (99%) 436 (solid)	0.87/8.18	1.26/3.45	9.40	0.08/0.24	9.35/2.70	-1.72	-5.40	3.68
2	339 (48062)	385 (0%) 473 (99%) 426 (solid)	0.60/6.02	11.68/5.30	10.02	0.02/0.15	1.17/1.76	-2.03	-5.84	3.81
3	341 (50144)	398 (0%) 436 (99%) 434 (solid)	2.30/8.70	1.59/0.98	3.78	0.13/0.72	5.46/7.61	-2.28	-6.08	3.80

^{a)} Maximum absorption wavelength measured in THF solution at room temperature. ^b Measured in solid. ^c $\alpha = \Phi_{\text{solid}}/\Phi_{\text{soln.}} dk_r = \text{radiative decay rate } (\Phi/\tau)$. ^ek_{nr} = nonradiative decay rate $(1/\tau - k_r)$. ^f Calculated by DFT (B3LYP/6-311G(d,p)).

narrower full width at half maximum (FWHM) emission compared to compound **1** (benzophenone group at the 1-position of pyrene). Upon exposure to an external force, the emission of the compounds displays a slightly red-shifted emission to 448 nm for **1**, 444 nm for **2** and 437 nm for **3**, with a decreased PL intensity, respectively. This may be due to the planarization between the pyrene ring and the benzophenone unit leading to a stronger intramolecular interaction.



Figure 4. The PL spectrum of (A) **1**, (C) **2**, (E) **3** before and after grinding, Insert: The images of **2** in the crystal state and after grinding taken under 365 nm UV light. Wide angle XRD diffractograms of (B) **1**, (D) **2**, (F) **3** in different states.

Although suitable samples for single crystal X-ray diffraction analysis were not obtained, powder X-ray diffraction (XRD) was measured to evaluate the molecular packing changes before and after grinding. As shown in Figures 4B, 4D and 4F, compounds 1-3 show sharp and intense diffraction peaks, suggesting that the compounds arrange in an well-ordered crystalline structures. Under mechanical stimulus, the XRD peaks of compounds 1 and 3 slightly changed with a weakened peak intensity, which distinctly indicated that their crystal arrangement still remained as the same organized structures. When closely examining the diffraction peak of compounds 1 and 3, the main differences is that the *d*-spacing of the ground sample decreased in the region of $2\theta = 20-30^\circ$, which is assigned to the distance of the π - π stacking interaction between pyrenes.^[36] These results indicated that the molecules 1 and 3 tend to become more planar under extremal force, leading to a strengthened intramolecular interaction. On the other hand, the XRD diffractograms of the compound 2 show clear sharp and intense reflection peaks, indicating a highly crystalline solid. In contrast, some diffraction peaks at 20 = 27.1, 32.6 and 38.6° were missing and multiple new diffraction peaks appeared in the region of $2\theta = 17-25^{\circ}$ upon grinding, which may imply that the crystal lattice has significant changed after grinding.^[37]

Conclusion

In summary, this article presents a facile approach to three pyrene-based blue emitters formed in considerable yield, where the benzophenone units were introduced at the 1-, 2- or 2,7-positions of pyrene. The emission spectra indicated that these pyrenes exhibit monomer emission in solution, but show excimer emission in the aggregated (solid) state. Interestingly, this series of pyrenes exhibit clear AIE characteristic. The benzophenone units are an important component to realize the ACQ-to-AIE transformation in this pyrene-based system, which may be due to the twisted molecular conformation of the pyrene-based molecules which can efficiently adjust the intermolecular interactions in the aggregation state. Thus, this study provides a new strategy to construct new pyrene-based AIEgens systems for various high-tech applications.

Experimental Section

Materials: Unless otherwise stated, all reagents used were purchased from commercial sources and were used without further purification. Tetrahydrofuran was distilled prior to use.

Characterization: ¹H and ¹³C NMR spectra (400 MHz) were recorded on a Bruker AV 400M spectrometer using chloroform-d solvent and tetramethylsilane as internal reference. J-values are given in Hz. Highresolution mass spectra (HRMS) were recorded on a LC/MS/MS, which consisted of a HPLC system (Ultimate 3000 RSLC, Thermo Scientific, USA) and a Q Exactive Orbitrap mass spectrometer. UV-vis absorption spectra and photoluminescence (PL) spectra were recorded on a Shimadzu UV-2600 and the Hitachi F-4700 spectrofluorometer. PL quantum yields were measured using absolute methods using a Hamamatsu C11347-11 Quantaurus-QY Analyzer. The lifetime was recorded on an Edinburgh FLS 980 instrument and measured using a timecorrelated single-photon counting method. Thermogravimetric analysis was carried on a Mettler Toledo TGA/DSC3+ under dry nitrogen at a heating rate of 10 °C /min. The quantum chemistry calculations were performed on the Gaussian 09 (B3LYP/6-311G (d,p) basis set) software package.

Synthesis of Methanone, [(4-(pyren-1-yloxy)phenyl)] phenyl- (1):

Under an N₂ atmosphere, a mixture of pyrene-1-OH (300 mg, 1.38 mmol, 1.0 eq.), 4-bromobenzophenone (538 mg, 2.06 mmol, 1.5 eq.), Cs₂CO₃ (896 mg, 2.75 mmol, 2 eq.) and N,N-dimethylformamide (6 mL) were stirred and heated to 130 °C in a two-necked flask for 24 h. After cooling, the reaction mixture was quenched by H_2O (50 mL) and extracted by CH_2CI_2 (50 mLx 3) three times, then the organic layer was washed successively with water and brine. The combined organic extracts were dried with anhydrous MgSO4 and evaporated. The residue was purified by column chromatography eluting with CH₂Cl₂-Hexane (1:1) to give phenyl(4-(pyren-1-yloxy)phenyl)methanone (1) as a white solid (88 mg,16%, Melting point: 108~110 °C). ¹H NMR (400 MHz, CDCl₃) δ 8.25 (d, J = 9.2 Hz, 1H), 8.19 (dd, J = 9.9, 8.0 Hz, 3H), 8.07 (d, J = 7.7 Hz, 3H), 8.03 (t, J = 7.6 Hz, 1H), 7.85 (d, J = 8.8 Hz, 2H), 7.83 - 7.78 (m, 2H), 7.74 (d, J = 8.3 Hz, 1H), 7.57 (t, J = 7.4 Hz, 1H), 7.48 (t, J = 7.5 Hz, 2H), 7.08 (d, J = 8.8 Hz, 2H) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 195.5, 162.9, 148.5, 138.0, 132.7, 132.2, 131.9, 131.3, 131.3, 129.9, 128.7, 128.3, 128.1, 127.1, 127.0, 126.5, 126.1, 125.7, 125.5, 125.3, 124.7, 123.5, 120.8, 118.4, 116.6 ppm. HRMS (FTMS+p APCI): m/z+H⁺ calcd for C₂₉H₁₈O₂ 399.1380, found 399.1373 [M+H]+.

Synthesis of Methanone, [(4-(pyren-2-yloxy)phenyl)] phenyl- (2):

Under an N₂ atmosphere, a mixture of pyrene-2-OH (200 mg, 0.917 mmol, 1.0 eq.), 4-bromobenzophenone (359 mg, 1.37 mmol, 1.5 eq.), Cs₂CO₃ (597 mg, 1.83 mmol, 2 eq.) and N,N-dimethylformamide (6 mL) were stirred and heated to 130 °C in a two-necked flask for 24 h. After cooling, the reaction mixture was quenched with H₂O (50 mL) and extracted by CH2Cl2 (50 mLx 3) three times. The organic layer was washed successively with water and brine. The combined organic extracts were dried with anhydrous MgSO4 and evaporated. The residue was purified by column chromatography eluting with CH2Cl2-Hexane (1:1) to give phenyl(4-(pyren-2-yloxy)phenyl)methanone (2) as a white solid (160 mg, 29.1%, Melting point: 158~159 °C). ¹H NMR (400 MHz, CDCI₃) δ 8.22 (d, J = 7.6 Hz, 2H), 8.12 (d, J = 8.9 Hz, 2H), 8.02 (dd, J = 8.2, 4.1 Hz, 3H), 7.91 (s, 2H), 7.87 (d, J = 8.7 Hz, 2H), 7.81 (d, J = 7.2 Hz, 2H), 7.58 (t, J = 7.3 Hz, 1H), 7.49 (t, J = 7.5 Hz, 2H), 7.15 (d, J = 8.7 Hz, 2H) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 195.6, 162.2, 153.5, 138.0, 133.0, 132.6, 132.2, 132.2, 130.6, 129.9, 128.6, 128.3, 126.8, 125.8, 125.7, 124.4, 122.1, 117.5, 116.0 ppm. HRMS (FTMS+p APCI): m/z+H⁺ calcd for C₂₉H₁₈O₂ 399.1380, found 399.1375 [M+H]+.

Synthesis Methanone, 1,1'[pyrene-2,7-diylbis(oxy-4,1-phenylene)] bis(1-phenyl-) (3):

Under an N₂ atmosphere, a mixture of pyrene-2,7-OH (200 mg, 0.854 mmol, 1 eq.), 4-bromobenzophenone (669 mg, 2.56 mmol,3 eq), Cs₂CO₃ (1.11 g, 3.41 mmol, 4 eq.), and *N*,*N*-dimethylformamide (7 mL) were stirred and heated to 130 °C in a two-necked flask for 24 h. After cooling, the mixture was quenched with H₂O (50 mL) and extracted by CH₂Cl₂ (50 mL× 3) three times. The organic layer was washed successively with water and brine. The combined organic extracts were dried with anhydrous MgSO₄ and evaporated. The residue was purified by column

chromatography eluting with CH₂Cl₂-Hexane (1:2) to give ((pyrene-2,7-diylbis(oxy))bis(4,1-phenylene))bis (phenylmethanone) **(3)** as a white solid (177 mg,16%, Melting point: 190–191 °C). ¹H NMR (400 MHz, CDCl₃) δ 8.06 (s, 4H), 7.94 (s, 4H), 7.88 (d, *J* = 8.7 Hz, 4H), 7.82 (d, *J* = 7.1 Hz, 4H), 7.59 (t, *J* = 7.4 Hz, 2H), 7.50 (t, *J* = 7.5 Hz, 4H), 7.16 (d, *J* = 8.7 Hz, 4H) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 195.5, 162.0, 153.5, 137.9, 132.6, 132.5, 132.2, 129.9, 128.3, 127.9, 121.8, 117.5, 116.7, 100.0 ppm. HRMS (FTMS+p APCl): m/z+H⁺ calcd for C₄₂H₂₆O₄ 595.1904, found 595.1901 [M+H]⁺.

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Entry for the Table of Contents

This article presents a facile strategy for the construction of pyrene-based aggregation-induced emission luminogens (AIEgens) via decorating the pyrene core with benzophenone units at the 1-, 2- or 2,7-positions.

