

Electronic Supplementary Information

Visible room-temperature phosphorescence of pure organic crystals via a radical-ion-pair mechanism

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General experimental details

Fluorescence and phosphorescence spectra and phosphorescence lifetime were measured on JASCO FP-8500 fluorospectrometer with a 150-W xenon lamp as an excitation light source. A disk cell (ϕ 5.5 mm, thickness 1–3 mm) was used for solid samples (4–20 mg). All the measurements, unless otherwise stated, were carried out by a photomultiplier voltage of 175 V (248 V for 3Cl), excitation and emission band widths of 5 nm, a response of 0.5 s, a data acquisition interval of 0.5 nm for fluorescence or 0.2 nm for phosphorescence, and a scan speed of 500 nm/min. The chopper rotation for phosphorescence excitation and emission measurements was adjusted as follows: a shutter open-close cycle of 100 ms, an acquisition delay time of 50 ms, an acquisition period of 25 ms, and an acquisition repeat of two cycles. The background corrections of all the emission and excitation spectra were performed with a combination of a D₂ lamp (JASCO ESC-843, 30 W, 200–360 nm) and a halogen lamp (JASCO ESC-842, 20 W, 350–750 nm). For the measurement of luminescence properties, all the samples were purified by recrystallization: IPA (Sigma-Aldrich, 99%) and **IPAd₄** (CDN Isotopes Inc., 99.4 atom%D) were recrystallized from methanol (LC/MS grade, Wako Pure Chemical Industries, Ltd.); **IPAd₂** was recrystallized from methanol-*d*₄ (NMR solvent, 99.8% D, Kanto Chemical Co., Inc.); TPA (Tokyo Chemical Industry Co., Ltd., >99.0%), 4-fluorobenzoic acid (4FBz, Tokyo Chemical Industry Co., Ltd., >98.0%), 4-chlorobenzoic acid (4ClBz, Tokyo Chemical Industry Co., Ltd., >99.0%), 4-bromobenzoic acid (4BrBz, Tokyo Chemical Industry Co., Ltd., >98.0%), and 4-iodobenzoic acid (4IBz, Tokyo Chemical Industry Co., Ltd., >98.0%) were recrystallized from ethanol (spectroscopy grade, Wako Pure Chemical Industries, Ltd.; for TPA, special grade, Kanto Chemical Co., Inc.); PMA (Tokyo Chemical Industry Co., Ltd., >98.0%), benzoic acid (Bz, Kanto Chemical Co., Inc., >99.5%), benzoic acid-*d*₅ (Bzd₅, Cambridge Isotope Laboratories Inc., 98%), and 2- and 3-halogenated benzoic acids (2FBz, 2ClBz, 2BrBz, 2IBz, 3FBz, 3ClBz, 3BrBz, 3IBz, Tokyo Chemical Industry Co., Ltd., >98.0%; for 3ClBz, >99.0%) were recrystallized from water (Millipore Milli-Q Integral-3); benzoic acid-*d*₁ (Bzd₁) was recrystallized from D₂O (NMR solvent, 99.8% D, Kanto Chemical Co., Inc.).

Lifetime measurement

For all the compounds except 2IBz and 4IBz, the temporal change in emission intensity after 1-s irradiation was measured consecutively for 10 times. For 2IBz and 4IBz, the chopper rotation mode was used with a “shutter cycle”–“delay time”–“acquisition period” combination of 25–11–7, 50–20–15, or 100–40–30 (ms), and an acquisition repeat of 10. The decay curve thus obtained was accumulated and analyzed by a data analysis software, Igor Pro (ver 6.2.2.0, WaveMetrics, Inc.).

For a multiexponential decay curve, the rightmost part of its semilog curve was fitted to a straight line, the semilog curve subtracted by the fitted line, and the residual semilog curve again subjected to a linear regression analysis at the rightmost part; these operations were repeated until the residual semilog curve became linear or a further repeat was statistically insignificant due to a small data points number. Lifetime τ_n and a contribution coefficient A_n were obtained for each regression analysis using equation (1) (emission intensity $I(t)$ vs elapsed time t).

$$I(t) = A_1 e^{-t/\tau_1} + A_2 e^{-t/\tau_2} + A_3 e^{-t/\tau_3} + \dots \quad (1)$$

Quantum yield measurement

Quantum yields were measured with an integrating sphere unit (JASCO ILF-835, 100 mm ϕ) on FP-8500. A sample was put in an all-quartz cell (10 \times 3 \times 10 mm), and the excitation and emission band widths were adjusted at 10 nm. The photomultiplier voltage was adjusted so that the irradiation peak intensity was settled between 4000 and 8000 arb. units. The quantum yield Φ and absorbance A were calculated by equations (2) and (3):

$$\Phi = \frac{N_{em}}{N_{abs}} = \frac{E_1 - E_2 \times L_2/L_3}{L_1 \times A} \quad (2), \quad A = \frac{L_3 - L_2}{L_3} \quad (3)$$

N_{em} and N_{abs} are the numbers of photons emitted from and absorbed by the sample, respectively. The emission strength parameters, L_n and E_n , were determined by the integrated intensity of the corresponding band in the emission spectra. The incident light strength (L_1) was obtained with the empty integrating sphere. The sample-scattered light strength (L_2) and the gross emission strength of the sample (E_1) were measured by using the directly irradiated sample. The wall-scattered light strength (L_3) and the indirect emission strength (E_2), where the sample was unintendedly irradiated by the wall-scattered light, were obtained with the sample placed away from the incident light path in the integrating sphere.

Absorption spectra of solids

Absorption spectra of solids were measured by using the same setting, as for the quantum yield measurement with the preinstalled program. Substantial absorption spectra were obtained in the range between 220 and 700 nm. The shorter wavelength gave spike-like noises. Low-temperature phosphorescence measurements were performed with a Jasco PMU-830 liq. N₂ cooling unit and an NMR-tube (ϕ 5 \times h 10 mm) or a Jasco PPH-150 disk cell (ϕ 7 \times d 0.5 mm).

Purification of IPA

Commercial isophthalic acid (IPA, Sigma-Aldrich, 99%, 5.00 g) was purified through a silica gel column chromatography (Silica Gel 60N, 40-100 μm , Kanto Chemical, Co., Inc.) with CHCl_3 /methanol/acetic acid (9/1/0.01) as an eluent. The chromatography-purified IPA (1.74 g) was sublimed using a Buchi GKR-50 glass tube oven at 170 $^\circ\text{C}$ under 2 mmHg. The sublimed IPA (1.00 g) was dissolved into an analytical-grade ethanol (Wako Chemical Ltd.) by sonication and filtered through a filter paper. To the filtrate was added 300 mL of ultrapure water (Merck Millipore Milli-Q Integral-3), and the solution was left overnight. The precipitated crystals (605 mg) were collected by filtration. This recrystallization process was repeated three times.

Measurement of luminescence intensity change by irradiation power

The sensor unit of a power meter (Thorlabs PM100A), which has a light-passing hole of the same diameter as the sample disk (5.5 mm), was set in the spectrometer compartment of FP-8500. The excitation light power (350 nm) was modulated by a combination of two light-shielding cards and an excitation bandwidth (2.5-20 nm); the each irradiation power (μJs^{-1}) was recorded prior to luminescence measurements.

Measurement of luminescence intensity change by external magnetic field

Modulation of magnetic flux density was carried out with an electromagnet (Fujita FSGP-90, ϕ 90 \times h 60 mm) connected to a constant voltage source (Kikusui Model 7354) and a power meter (Keithly 2400 Source Meter). A standard curve of voltage vs magnetic flux density was made with a gauss meter (FW Bell 5180), whose probe tip was put on the center of the electromagnet. The magnetic flux density varied linearly from 1.8 to 80 mT with a voltage variation from 0 to 90 V. A sample was placed on the center of the electromagnet and covered with a crystal glass (ϕ 20 \times h 1.0 mm). Irradiation and detection were conducted with a fiber unit (JASCO OBF-832) attached with optical fibers, whose tips were adjusted at 4.5 mm above the sample so that the incident and emitting light courses made a right angle. The phosphorescence intensity was defined as the integrated phosphorescence intensity at 500 nm from 0.1 to 3.0 s after 1-s irradiation at 308 nm.

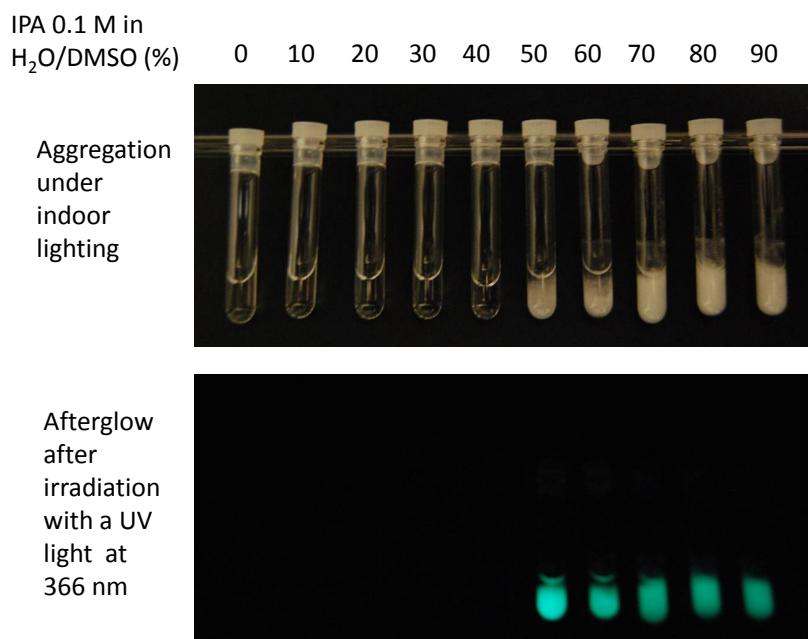


Fig. S1 Aggregation-induced phosphorescence of IPA. To a solution of IPA in DMSO was added water so that the final concentration is 0.1 M. IPA was precipitated at the water concentration of no less than 50% (top). Afterglow was observed for only the precipitated samples (bottom).

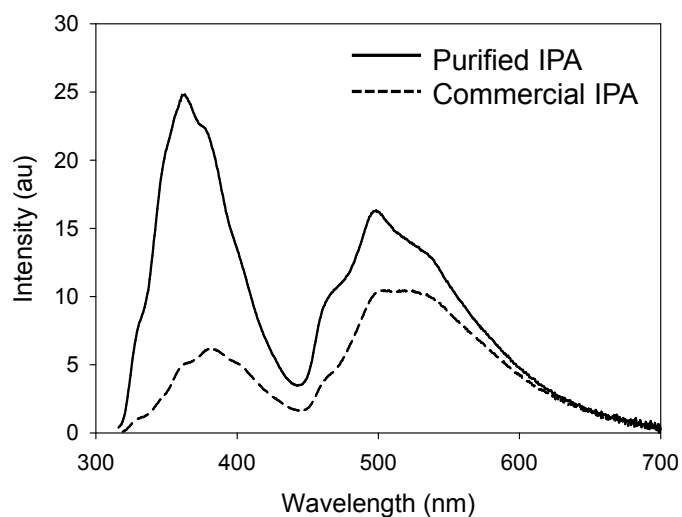


Fig. S2 Phosphorescence spectra of purified and commercial IPAs at 296 K excited at 306 nm and 309 nm, respectively. The commercial IPA was purchased from Sigma-Aldrich and it was purified by the method in the main text. For the time-resolved spectrum, afterglows of 50–75 ms were measured. Excitation wavelengths with the maximum emission intensities were employed.

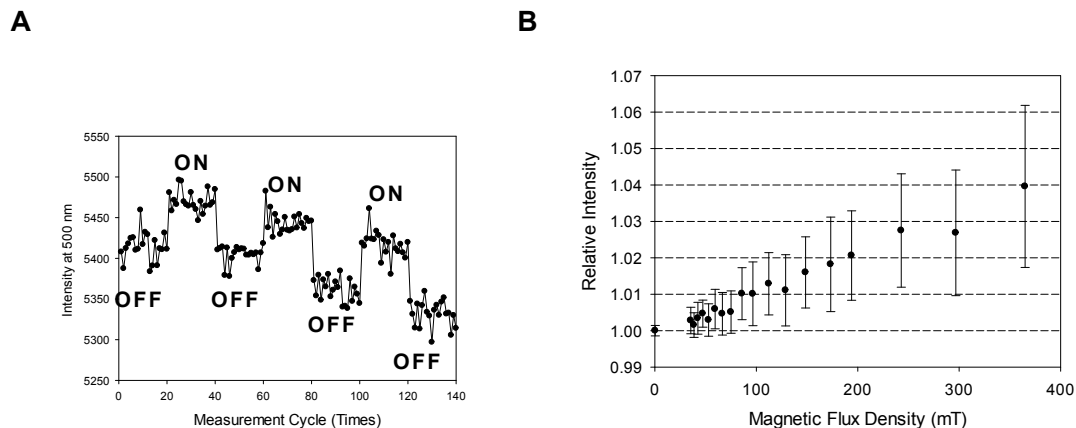


Fig. S3 .Extended data for the magnetic field effect on the phosphorescence of IPA. (A) On-off magnetic-field (0.4 T) effects on the phosphorescence intensity at 500 nm of IPA. (B) The magnetic field effect at a higher region (up to 0.4 T). IPA was excited at 308 nm under an external magnetic field from a neodymium permanent magnet. Magnetic flux density was varied by changing the distance between IPA and the magnet. The data represent the mean value from four experiments and the error bars are \pm s.e.m.

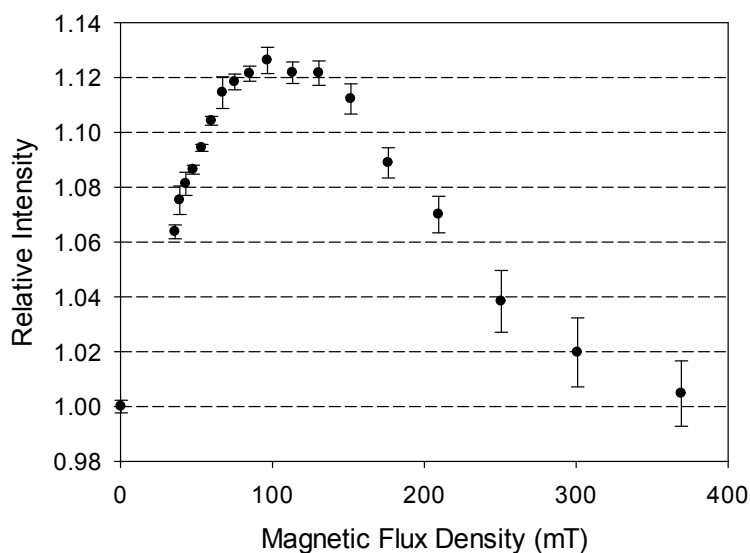


Fig. S4 Magnetic field effect on the delayed fluorescence of IPA at 390 nm. IPA was excited at 308 nm under an external magnetic field from a neodymium permanent magnet. Magnetic flux density was varied up to 0.4 T by changing the distance between IPA and the magnet. The data represent the mean

value from six experiments and the error bars are \pm s.e.m.

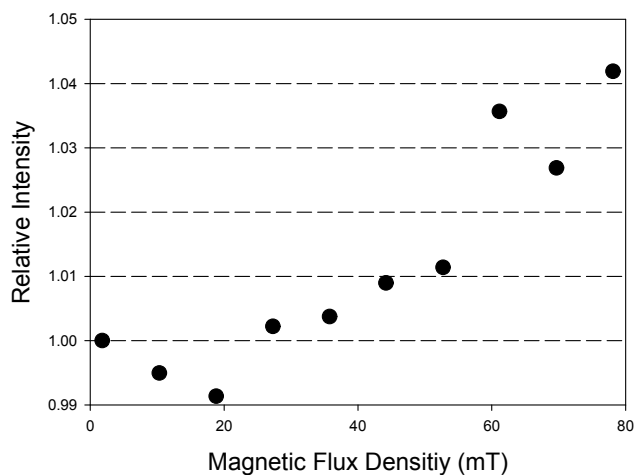


Fig. S5 Magnetic field effect on the phosphorescence intensity at 525 nm of sodium 2-naphthate on a filtering paper. A solution of 2-naphthoic acid (10 mg) in 1 M NaOH (1 mL) was spotted on a filtering paper (NRK, No.704×22 m/m) and the spot was dried with a heat gun. The filtering paper was excited at 290 nm under an external magnetic field from an electromagnet connected to a constant voltage supply with the voltage variation between 0 and 90 V.

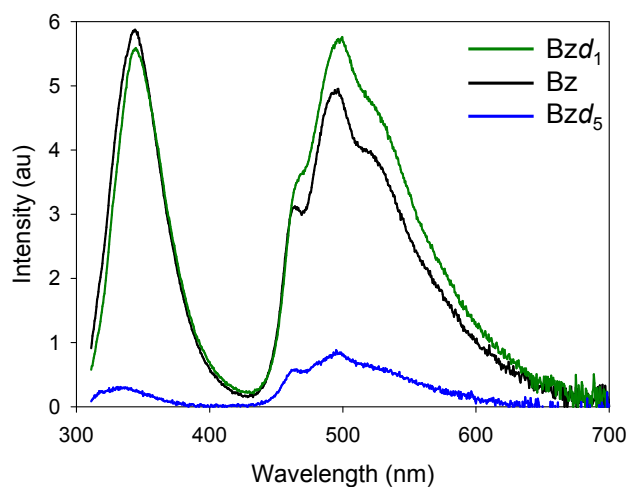


Fig. S6 Magnetic isotope effects on the phosphorescence spectra of benzoic acid (Bz), Bzd₁, and Bzd₅. The excitation wavelength was 301 nm. For the time-resolved spectrum, afterglows of 50–75 ms were measured.

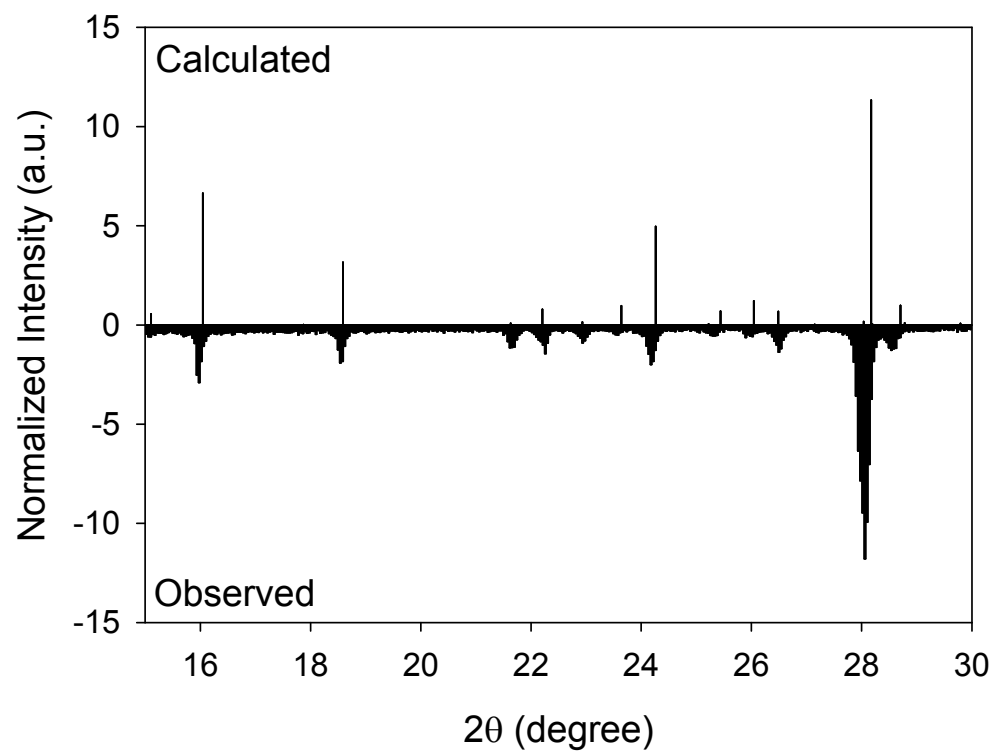


Fig. S7 Simulated (positive) and observed (negative) XRD patterns of IPA. Powder X-ray diffraction (XRD) measurements were performed on an X-ray diffractometer for a pole point figure measurement, X'Pert-MPD-OEC, in the 2θ range between 15° and 100° . There was no significant peak above 30° . The peak intensities and signs are normalized so that they can be compared easily. The simulated XRD measurement was calculated for BENZDC10¹ with a Crystal Maker software, CrystalDiffract ver 1.4.5. BENZDC10 was taken from the Cambridge Structural DS 2013 data base.

Fig. S8 CT-like photoexcitation of a Bz dimer. The Bz dimer structure (top left) was taken from the BENZAC01² file provided in Cambridge Structural DS 2013. The transitions at 213.3 nm and 213.7 nm with oscillator strengths (*f*) of 0.209 and 0.173, respectively were calculated by TD-DFT on CAM-B3LY at the 631Gd level with Gaussian 09³.

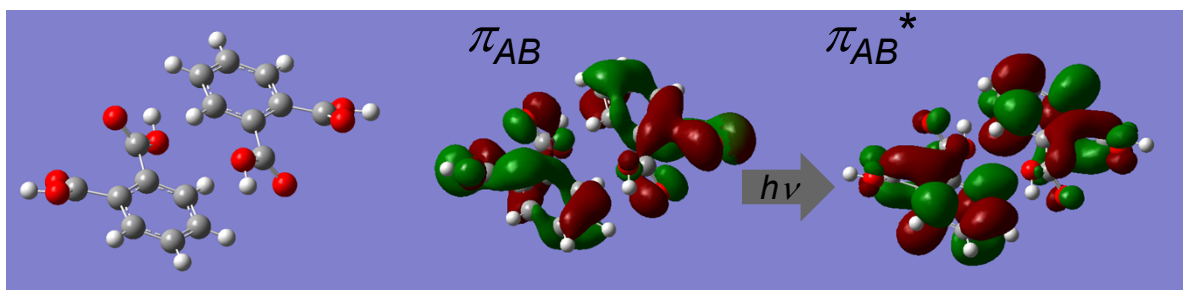


Fig. S9 TD-DFT calculation for an OPA dimer. The OPA dimer structure (left) was taken from the PHTTHAC01 file provided in Cambridge Structural DS 2013; the molecular orbitals for the dimers were π_{AB} (middle) and π_{AB}^* (right). The distance between the two benzene rings is 4.85 Å. The π_{AB} - π_{AB}^* transition at 198 nm with an oscillator strength of 0.50 was calculated by TD-DFT on CAM-B3LY at the 631Gd level with Gaussian 09³.

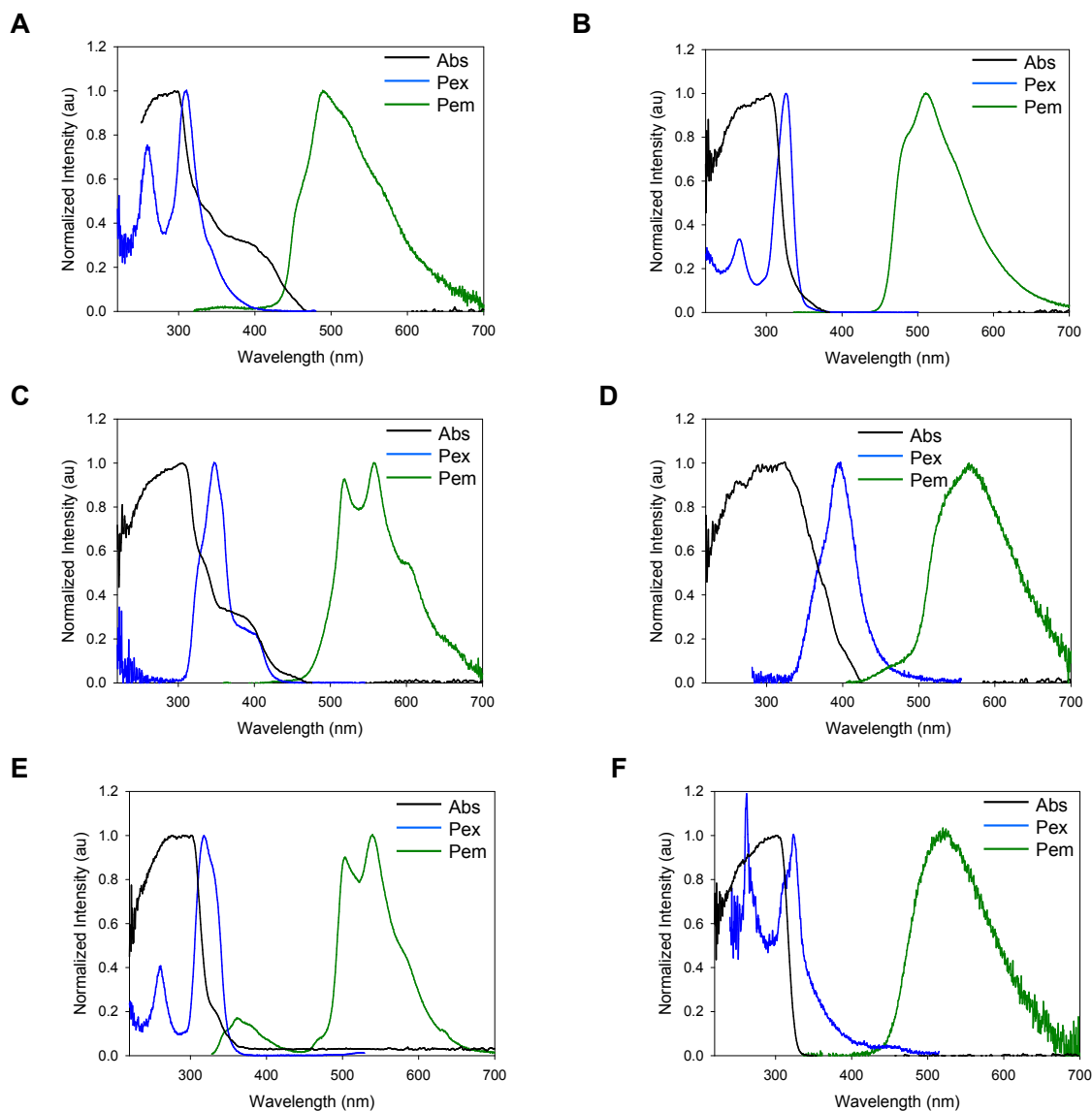


Fig. S10 Absorption spectra (Abs) and phosphorescence excitation (P_{ex}) and emission (P_{em}) spectra at 296 K of the compounds stated in the main text. For the time-resolved spectra, afterglows of 50–75 ms (2FBz, 2ClBz, 2BrBz, 3FBz) or 11–18 ms (2IBz, 3ClBz) were measured. (A) 2FBz: excitation at 310 nm for P_{em} and emission at 490 nm for P_{ex}. (B) 2ClBz: excitation at 326 nm for P_{em} and emission at 511 nm for P_{ex}. (C) 2BrBz: excitation at 348 nm for P_{em} and emission at 557 nm for P_{ex}. (D) 2IBz: excitation at 395 nm for P_{em} and emission at 566 nm for P_{ex}. (E) 3FBz: excitation at 318 nm for P_{em} and emission at 539 nm for P_{ex}. (F) 3ClBz: excitation at 324 nm for P_{em} and emission at 525 nm for P_{ex}.

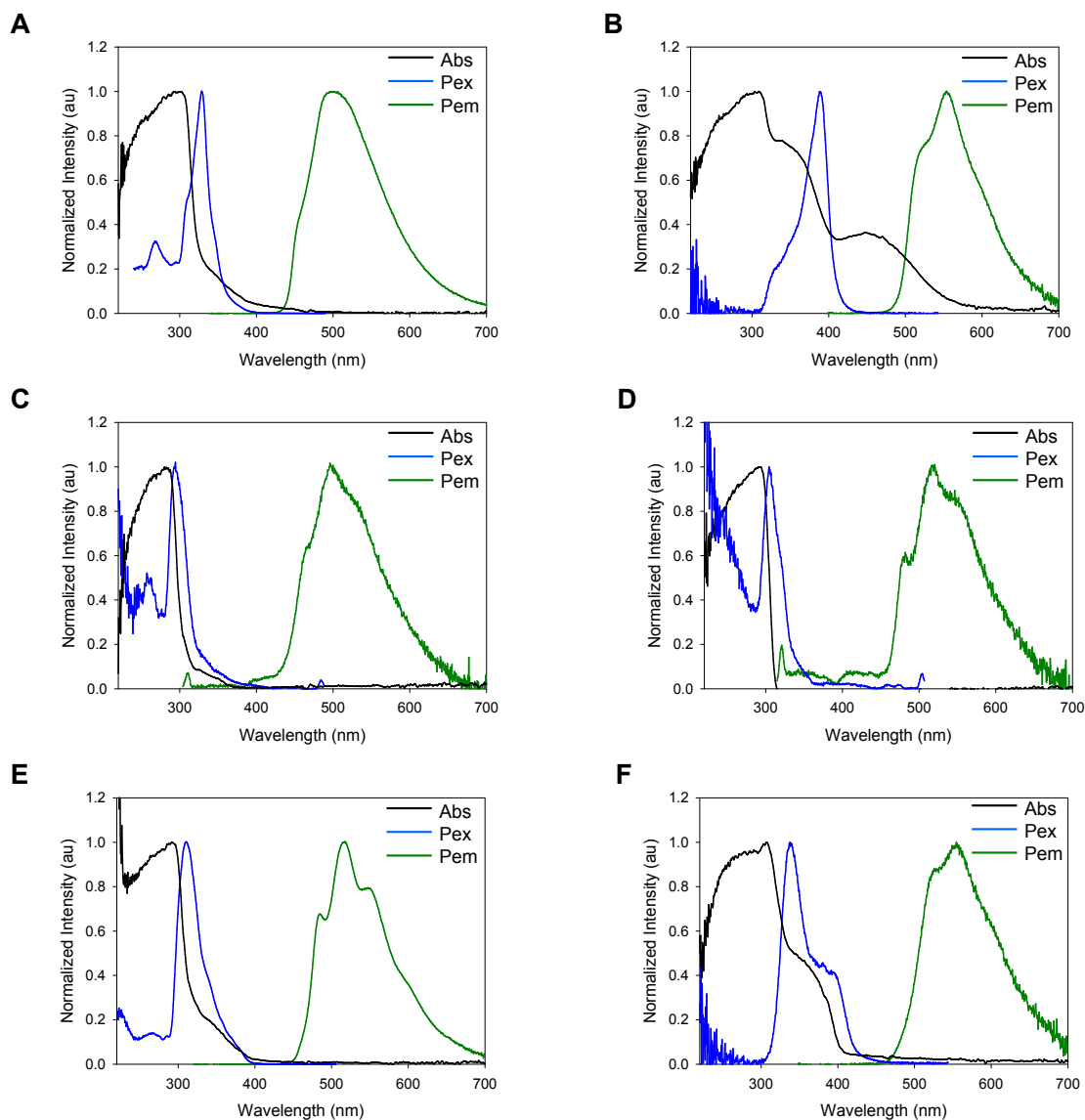


Fig. S11 Absorption spectra (Abs) and phosphorescence excitation (P_{ex}) and emission (P_{em}) spectra at 296 K of the compounds stated in the main text. For the time-resolved spectra, afterglows of 50–75 ms (3IBz, 4FBz, 4ClBz, 4BrBz) or 11–18 ms (3BrBz, 4IBz) were measured. (A) 3BrBz: excitation at 329 nm for P_{em} and emission at 500 nm for P_{ex} . (B) 3IBz: excitation at 388 nm for P_{em} and emission at 553 nm for P_{ex} . (C) 4FBz: excitation at 294 nm for P_{em} and emission at 498 nm for P_{ex} . (D) 4ClBz: excitation at 305 nm for P_{em} and emission at 517 nm for P_{ex} . (E) 4BrBz: excitation at 310 nm for P_{em} and emission at 515 nm for P_{ex} . (F) 4IBz: excitation at 338 nm for P_{em} and emission at 554 nm for P_{ex} .

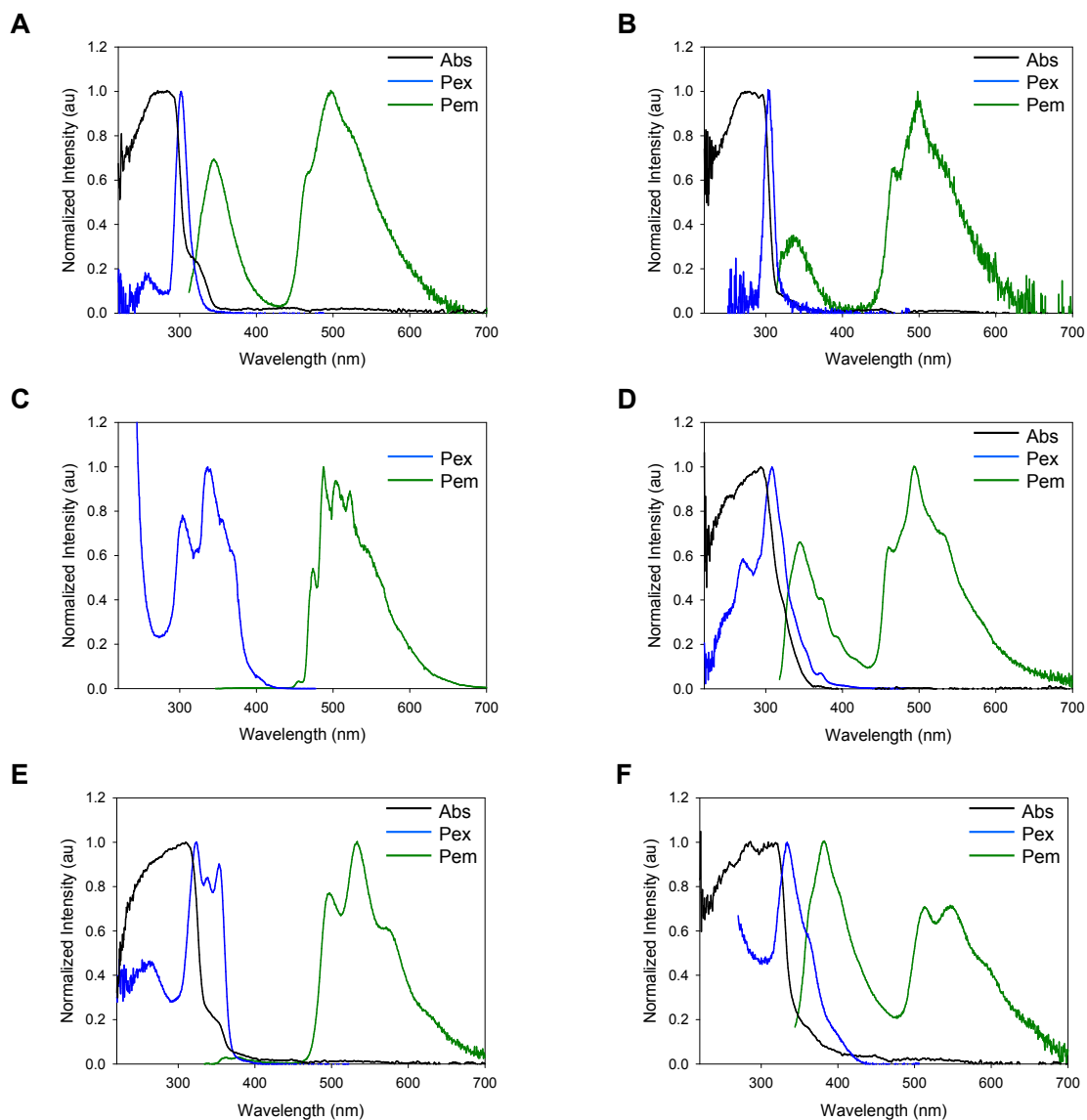


Fig. S12 Absorption spectra (Abs) and phosphorescence excitation (P_{ex}) and emission (P_{em}) spectra at 296 K of the compounds stated in the main text. For the time-resolved spectra, afterglows of 50–75 ms were measured. (A) Bz: excitation at 302 nm for P_{em} and emission at 498 nm for P_{ex} . (B) Bzd_5 : excitation at 301 nm for P_{em} and emission at 495 nm for P_{ex} . (C) IPA77K: excitation at 305 nm for P_{em} and emission at 456 nm for P_{ex} . (D) $IPAd_4$: excitation at 308 nm for P_{em} and emission at 495 nm for P_{ex} . (E) PMA: excitation at 324 nm for P_{em} and emission at 533 nm for P_{ex} . (F) TPA: excitation at 334 nm for P_{em} and emission at 516 nm for P_{ex} .

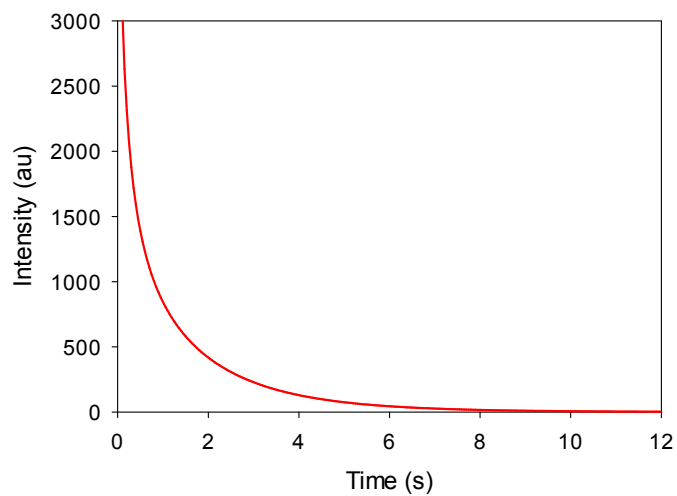


Fig. S13 Decay curve of the phosphorescence of IPA.

Table S1 Inductively coupled plasma atomic emission spectrometry (ICP-AES) analysis of IPA in comparison with the blank analysis in ppm.^a

	S	K	I	Na	P	U	Mg	Ca	Si	Fe	Cu
Blank	3.1	1.7	3.3	0.47	0.62	0.45	0.0022	0.0055	0.017	0.0083	0.011
IPA	3.3	1.4	3.0	0.58	0.67	0.47	0.0023	0.0062	0.029	0.011	0.0073

^aICP-AES was performed on Shimadzu ICPS-8100.

Table S2 Spectroscopic properties of the phosphorescent aromatic compounds.^a

Compound ^b	F _{ex} (nm)	F (nm)	P _{ex} (nm)	P (nm)	DF (nm)	Φ (%)
IPA	313	363	309	501	382	28
IPA at 77K ^c	302	355	305	456	-	ND ^d
IPAd ₂	315	366	308	500	382	32
IPAd ₄	310	346	308	495	345	20
TPA	319	341	334	516	383	18
PMA	338	379	324	533	-	9.2
Bz	260	308	301	495	344	13
Bzd ₁	260	308	301	499	344	13
Bzd ₅	260	308	301	495	335	13
2FBz	303	357	310	490	-	3.1
2ClBz	327	511	326	511	-	12
2BrBz	329	511	348	557	-	6.7
2IBz	398	501	395	566	-	14
3FBz	320	362	318	539	361	19
3ClBz	314	339	324	525	-	0.42
3BrBz	389	495	329	500	-	2
3IBz	400	506	388	553	-	1.3
4FBz	263	316	294	498	-	5.8
4ClBz	295	313	305	517	-	1.6
4BrBz	310	516	310	516	-	9.0
4IBz	400	505	338	554	-	0.038

^aPeak wavelengths of fluorescence excitation (F_{ex}), fluorescence (F), phosphorescence excitation (P_{ex}), phosphorescence (P), and delayed fluorescence (DF) and fluorescence quantum yield (Φ). ^bAbbreviation of compounds: IPA, isophthalic acid; IPAd₂, isophthalic acid-*d*₂ (*O*-deuterated); IPAd₄, isophthalic acid-*d*₄ (*C*-deuterated); TPA, terephthalic acid; PMA, pyromellitic acid; Bz, benzoic acid; Bzd₁, benzoic acid-*d*₁ (*O*-deuterated); Bzd₅, benzoic acid-*d*₅ (*C*-deuterated); general abbreviation for #XBz such as 2FBz, #-halogenated benzoic acid such as 2-fluorobenzoic acid. ^cAll the other entries employ room temperature. ^dNot determined.

Table S3 Lifetime parameters of phosphorescence.^a

Compound ^b	$\tau_1 / \text{s}^{-1} (A_1)$	$\tau_2 / \text{s}^{-1} (A_2)$	$\tau_3 / \text{s}^{-1} (A_3)$	$\tau_4 / \text{s}^{-1} (A_4)$	$\tau_5 / \text{s}^{-1} (A_5)$	$\tau_{\text{Ave}} / \text{s}^{-1}$
IPA	2.9 (4.7%)	1.6 (41%)	0.44 (30%)	0.14 (24%)	-	0.97
IPA at 77K ^c	7.2 (9.4%)	4.3 (91%)	-	-	-	4.4
IPAd ₂	2.8 (9.4%)	1.6 (43%)	0.22 (40%)	0.047 (7.2%)	-	1.1
IPAd ₄	4.3 (3.6%)	2.3 (2.1%)	0.69 (10%)	0.19 (27%)	0.081 (57%)	0.37
TPA	0.80 (24%)	0.46 (36%)	0.13 (40%)	-	-	0.41
PMA	1.2 (79%)	0.84 (16%)	0.35 (5.3%)	-	-	1.1
Bz	0.74 (5.6%)	0.41 (26%)	0.16 (69%)	-	-	0.26
Bzd ₁	0.94 (18%)	0.45 (41%)	0.16 (41%)	-	-	0.42
Bzd ₅	1.1 (3.9%)	0.36 (22%)	0.18 (74%)	-	-	0.26
2FBz	1.3 (3.2%)	0.61 (23%)	0.27 (41%)	0.089 (33%)	-	0.32
2ClBz	0.93 (0.090%)	0.19 (56%)	0.12 (43%)	-	-	0.16
2BrBz	0.31 (3.0%)	0.11 (64%)	0.042 (33%)	-	-	0.093
2IBz	0.016 (100%)	-	-	-	-	0.016
3FBz	1.1 (58%)	0.89 (32%)	0.091 (10%)	-	-	0.94
3ClBz	3.1 (0.35%)	0.52 (9.8%)	0.14 (31%)	0.038 (58%)	-	0.13
3BrBz	0.29 (3.4%)	0.098 (19%)	0.033 (46%)	0.012 (31%)	-	0.048
3IBz	0.96 (0.016%)	0.15 (1.1%)	0.095 (6.0%)	0.033 (83%)	0.012 (9.5%)	0.036
4FBz	1.1 (7.0%)	0.47 (34%)	0.21 (48%)	0.033 (11%)	-	0.34
4ClBz	0.69 (8.7%)	0.31 (46%)	0.092 (23%)	0.021 (22%)	-	0.23
4BrBz	0.41 (6.6%)	0.23 (9.7%)	0.098 (84%)	-	-	0.13
4IBz	0.020 (100%)	-	-	-	-	0.020

^aPhosphorescence decay curves were obtained at the peak wavelengths of phosphorescence (P) indicated in Table S2. Fractional lifetimes τ_n / s^{-1} , contribution coefficients A_n in parentheses and average lifetimes $\tau_{\text{ave}} / \text{s}$. ^bAbbreviation of compounds: IPA, isophthalic acid; IPAd₂, isophthalic acid-*d*₂ (*O*-deuterated); IPAd₄, isophthalic acid-*d*₄ (*C*-deuterated); TPA, terephthalic acid; PMA, pyromellitic acid; Bz, benzoic acid; Bzd₁, benzoic acid-*d*₁ (*O*-deuterated); Bzd₅, benzoic acid-*d*₅ (*C*-deuterated); general abbreviation for #XBz such as 2FBz, #-halogenated benzoic acid such as 2-fluorobenzoic acid. ^cAll the other entries employ room temperature.

Table S4 Lifetime parameters of delayed fluorescence.^a

Compound ^b	$\tau_1 / \text{s}^{-1} (A_1)$	$\tau_2 / \text{s}^{-1} (A_2)$	$\tau_3 / \text{s}^{-1} (A_3)$	$\tau_4 / \text{s}^{-1} (A_4)$	$\tau_{\text{Ave}} / \text{s}^{-1}$
IPA	0.66 (2.1%)	0.23 (32%)	0.097 (66%)	-	0.15
IPAd ₂	1.7 (0.21%)	0.43 (5.8%)	0.16 (46%)	0.061 (48%)	0.13
IPAd ₄	0.10 (11%)	0.045 (89%)	-	-	0.051
TPA	0.29 (12%)	0.11 (51%)	0.044 (37%)	-	0.11
Bz	0.17 (27%)	0.084 (73%)	-	-	0.11
Bzd ₁	0.32 (14%)	0.15 (63%)	0.061 (23%)	-	0.15
Bzd ₅	0.14 (58%)	0.10 (20%)	0.053 (22%)	-	0.10
3FBz	0.36 (28%)	0.19 (35%)	0.052 (36%)	-	0.19

^aDelayed fluorescence decay curves were obtained at the peak wavelengths of delayed fluorescence (DF) indicated in Table S2. Fractional lifetimes τ_n / s^{-1} , contribution coefficients A_n in parentheses and average lifetimes $\tau_{\text{Ave}} / \text{s}$. ^bAbbreviation of compounds: IPA, isophthalic acid; IPAd₂, isophthalic acid-*d*₂ (*O*-deuterated); IPAd₄, isophthalic acid-*d*₄ (*C*-deuterated); TPA, terephthalic acid; Bz, benzoic acid; Bzd₁, benzoic acid-*d*₁ (*O*-deuterated); Bzd₅, benzoic acid-*d*₅ (*C*-deuterated); 3FBz, 3-fluorobenzoic acid.

Notes and references for supplementary information

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