Supplementary Information (SI) for Journal of Materials Chemistry C.

Broad-band Emissive Phenanthroimidazole-based Donor-Acceptor Luminogens for Hybrid White Light Emitting Diodes and Sensors for Picric Acid Detection

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Contents:

Experimental section

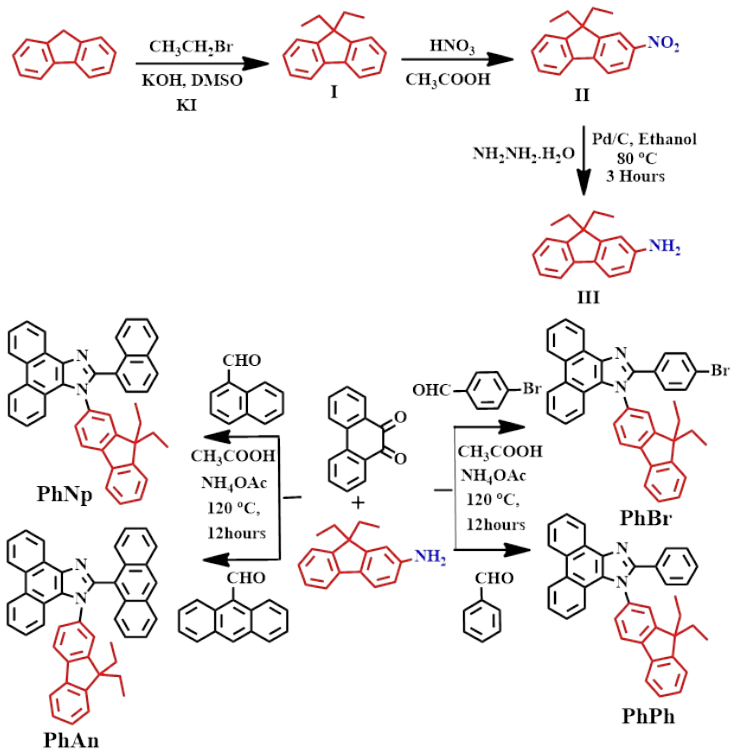
Materials:

All the reaction carried out under nitrogen atmosphere. Commercially available reagents (sigma aldrich) were used as purchased without any further purification. All the reaction were monitored by thin-layer chromatography (TLC) with silica gel 60 F_{254} Aluminium plates (Merck). Column chromatography was carried out using silica gel (Sigma-Aldrich).

General information for Measurements:

^{1}H NMR and ^{13}C NMR spectra were measured using an AV 400 Avance-III 400 MHz FT-NMR spectrometer (Bruker Biospin International, Switzerland) with tetramethylsilane (TMS) as the internal standard reference. The absorption and photoluminescence (PL) excitation and emission spectra of the synthesized luminophores were measured using a SHIMADZU UV-2450 spectrophotometer and a HORIBAFLUOROMAX – 4P spectrophotometer, respectively. The absolute fluorescence quantum yield was measured with Edinburgh Spectrofluorometer, FS5 with Integrating Sphere SC-30. The electrochemical properties of the fluorophores were measured by using Cyclic voltammetry (CV) experiments were performed in dimethyl formamide (DMF) solution containing 0.1 M tert-butyl ammonium perchlorate(Bu_4NClO_4) using as the supporting electrolyte, and the scan rate was continued at 100 mV s^{-1} using an AUTOLAB 302N Modular potentiostat at room temperature. The working (glass-carbon rod), auxiliary (counter, Pt wire) and reference (Ag/AgCl wire) electrode were used for CV analysis.

The CIE color chromaticity coordinates of the fluorophores were calculated from the emission spectral values by using MATLAB software.



Scheme 1. Synthetic Scheme of the synthesized fluorophores

Synthesis of 9,9-diethyl-9H-fluorene (Intermediate I):

To a mechanically stirred mixture of 9H-fluorene (2.5 g, 10.199 mmol) were dissolved in DMSO (20 mL) in 60 °C after that portion of powdered KOH (2.48 g, 44.36 mmol), KI (0.169 g, 1.019 mmol) were added then drop wise over 45 minutes Bromoethane (1.076 mL, 10 mmol) was added in room temperature, the reaction mixture was left over night with stirring. The reaction mass poured into water and the precipitate obtained was extracted from ethyl acetate. The organic extract was washed with brine solution and water and then concentrated

with rotavapour. The compound was purified on silica gel column chromatography using hexane/ethyl acetate mixture in 9/1 as eluent. Yield: 90% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.38 – 8.06 (m, 2H), 7.83 (dd, J = 8.0, 4.7 Hz,2H), 7.58 – 7.24 (m, 4H), 2.24 – 2.07 (m, 4H), 0.36 – 0.27 (m, 6H).**^{13}C NMR (101 MHz, $CDCl_3$)** δ 151.51 (s), 151.19 (s), 148.07 (s), 147.14 (s), 139.14 (s), 129.30 (s), 127.49 (s), 123.36 (s), 123.28 (s) 121.19 (s), 119.76 (s), 118.33 (s), 77.36 (s), 77.04 (s), 76.72 (s), 56.72 (s), 8.40 (s).

Synthesis of 9,9-diethyl-2-nitro-9H-fluorene (Intermediate II):

To a mechanically stirred mixture of Intermediate I (2.0 g, 8.99 mmol) were dissolved in glacial acetic acid (20 ml) after mixing, drop wise HNO_3 (2.26 ml, 53.95 mmol), was added in room temperature, the reaction mixture was left over 28 hours at 70 °C with stirring. After completion of reaction neutralise the reaction mixture with NaOH. The reaction mass poured into water and the precipitate obtained was extracted from ethyl acetate. The organic extract was washed with brine solution and water and then concentrated with rotavapour. The compound was purified on silica gel column chromatography using hexane/ethyl acetate mixture. Yield: 85 %. Yellow colour solid was obtained. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.04 – 7.75 (m, 2H), 7.67 – 7.38 (m, 5H), 2.21 (q, J = 7.3 Hz, 4H), 0.81 – 0.17 (m, 6H). **^{13}C NMR (101 MHz, CDCl3)** δ 150.01 (s), 141.71 (s), 127.29 (d, J = 17.6 Hz), 126.99 (s), 124.27 (s), 123.05 (s), 120.15 (s), 119.83 (s), 77.56 (s), 77.24 (s), 76.92 (s), 56.21 (s), 32.93 (s), 8.70 (s).

Synthesis of 9,9-diethyl-9H-fluoren-2-amine (Intermediate III):

To a mechanically stirred mixture of Intermediate II (200 mg, 0.749 mmol) were dissolved in ethanol (15 ml) and hydrazine (0.5 ml, 10 mmol) then by keeping reaction mixture in ice bath and add carefully portion wise 10 % palladium/carbon (50 mg, 0.469 mmol), the reaction mixture was left over for reflux for 8 hours with stirring. After completion of reaction neutralise the reaction mixture with NaOH. The reaction mass poured into water and the precipitate obtained was extracted from ethyl acetate. The organic extract was washed with brine solution

and water and then concentrated with rotavapour. The compound was purified on silica gel column chromatography using hexane/ethyl acetate mixture. Yield: 70 %. brown colour solid was obtained. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.22 – 8.08 (m, 2H), 7.79 – 7.66 (m, 2H), 7.45 – 7.28 (m, 3H), 2.11 – 1.92 (m, 4H), 0.27 – 0.15 (m, 6H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 151.52 (s), 151.21 (s), 148.06 (s), 147.16 (s), 139.14 (s), 129.30 (s), 127.49 (s), 123.32 (d, J = 7.2 Hz), 121.19 (s), 119.76 (s), 118.33 (s), 77.37 (s), 77.05 (s), 76.74 (s), 56.72 (s), 32.51 (s), 8.41 (s).

Synthesis of 2-(4-bromophenyl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro[9,10-d]imidazole (PhBr)

A mixture of 9,10-phenanthrenequinone (0.8 g, 3.84 mmol), 4-bromobenzaldehyde (1.38 g, 4.22 mmol), Intermediate III (0.687 g, 4.608 mmol) and ammonium acetate (1.183 g, 15.36 mmol) were added in acetic acid (30 mL), and the reaction mixture was heated to reflux for 12 hours under nitrogen atmosphere. After cooling to room temperature, the mixture was poured into ice water and extracted with CH_2Cl_2 three times the reaction mixture was added to the ice water and the product was extracted with CH_2Cl_2 three times. The extracted organic phase was dried over Na_2SO_4 and solvent was removed under reduced pressure. The raw product was purified by column chromatography using ethyl acetate/petroleum ether as eluent to yield a white powder (90%). **^{1}H NMR (400 MHz, $CDCl_3$) δ** 8.89 (d, *J* = 7.9 Hz, 1H), 8.80 (d, *J* = 8.3 Hz, 1H), 8.74 (d, *J* = 8.3 Hz, 1H), 7.92 (d, *J* = 7.9 Hz, 1H), 7.85 (dd, *J* = 5.8, 2.8 Hz, 1H), 7.78 (t, *J* = 7.5 Hz, 1H), 7.69 (t, *J* = 7.0 Hz, 1H), 7.53 (dd, *J* = 20.6, 8.0 Hz, 4H), 7.49 – 7.37 (m, 7H), 7.21 (t, *J* = 7.6 Hz, 1H), 2.17 – 1.95 (m, 4H), 0.47 (t, *J* = 7.3 Hz, 3H), 0.33 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (101 MHz, $CDCl_3$) δ** 152.19 (s), 143.40 (s), 140.08 (s), 131.38 (s), 130.82 (s), 128.32 (s), 127.61 (s), 127.36 (s), 126.19 (s), 125.72 (s), 123.64 (s), 123.08 (s), 122.73 (s), 121.07 (s), 56.71 (s), 32.99 (s), 8.31 (d, *J* = 17.9 Hz). **HRMS (m/z, ESI, $[M+H]^+$, (m/z, ESI, [M+3]+):** calcd. for $C_{38}H_{29}BrN_2$, 594.5622, 596.5781 found 594.1610, 596.1593.

Synthesis of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-phenyl-1H-phenanthro[9,10-d]imidazole (PhPh)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (d, *J* = 7.9 Hz, 1H), 8.80 (d, *J* = 8.4 Hz, 1H), 8.74 (d, *J* = 8.3 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.86 – 7.82 (m, 1H), 7.78 (t, *J* = 7.4 Hz, 1H), 7.68 (dd, *J* = 9.5, 3.6 Hz, 3H), 7.52 (dd, *J* = 11.3, 4.2 Hz, 2H), 7.48 – 7.38 (m, 5H), 7.29 – 7.17 (m, 4H), 2.16 – 1.95 (m, 4H), 0.47 (t, *J* = 7.3 Hz, 3H), 0.30 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (101 MHz, $CDCl_3$) δ** 128.82 (s), 128.23 (d, *J* = 10.1 Hz), 127.72 (s), 127.30 (s), 126.13 (s), 125.58 (s), 124.91 (s), 124.12 (s), 123.78 (s), 123.10 (d, *J* = 9.6 Hz), 122.81 (s), 121.07 (d, *J* = 5.0 Hz), 120.34 (s), 56.68 (s), 33.19 – 33.06 (m), 32.88 (d, *J* = 22.3 Hz), 8.42 (s), 8.22 (s). **HRMS (m/z, ESI, $[M+H]^+$):** calcd. for $C_{38}H_{30}N_2$, 515.2487, found 515.2486.

Synthesis of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-(naphthalen-1-yl)-1H-phenanthro[9,10-d]imidazole (PhNp)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 (d, *J* = 7.7 Hz, 1H), 8.85 (d, *J* = 8.3 Hz, 1H), 8.79 (d, *J* = 8.3 Hz, 1H), 7.97 (d, *J* = 7.1 Hz, 1H), 7.79 (dd, *J* = 14.5, 7.8 Hz, 3H), 7.67 (ddd, *J* = 18.8, 15.5, 7.5 Hz, 3H), 7.59 – 7.45 (m, 5H), 7.39 – 7.29 (m, 5H), 7.28 – 7.21 (m, 2H), 1.94 (dddd, *J* = 46.3, 28.2, 14.0, 6.8 Hz, 4H), 0.40 (t, *J* = 7.2 Hz, 3H), 0.22 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, $CDCl_3$) δ** 151.10 (s), 150.80 (s), 150.05 (s), 142.48 (s), 140.17 (s), 137.33 (s), 136.58 (s), 133.28 (d, *J* = 19.7 Hz), 129.77 (s), 129.51 (s), 129.27 (s), 128.23 (d, *J* = 18.9 Hz), 127.93 (s), 127.42 (d, *J* = 5.6 Hz), 127.07 (d, *J* = 7.8 Hz), 126.75 (s), 126.36 – 125.82 (m), 125.60 (s), 125.05 (s), 124.45 (s), 124.15 (s), 123.14 (d, *J* = 9.3 Hz), 122.89 (s), 121.23 (s), 120.36 (s), 120.10 (s), 56.38 (s), 32.61 (s), 7.87 (s). **HRMS (m/z, ESI, $[M+H]^+$):** calcd. for $C_{42}H_{32}N_2$, 565.2644, found 565.2640.

Synthesis of 2-(anthracen-9-yl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro[9,10-d]imidazole (PhAn)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (d, *J* = 7.7 Hz, 1H), 8.88 (d, *J* = 8.4 Hz, 1H), 8.83 (d, *J* = 8.2 Hz, 1H), 7.99 – 7.89 (m, 2H), 7.86 – 7.70 (m, 4H), 7.61 – 7.35 (m, 9H), 7.28 – 7.15 (m, 6H), 1.97 – 1.63 (m, 4H), 0.33 (t, *J* = 7.3 Hz, 3H), -0.68 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (101 MHz, $CDCl_3$) δ** 149.91 (s), 142.32 (s), 140.06 (s), 132.37 (d, *J* = 17.2 Hz), 130.85 (s), 129.14 (s), 128.43 (s), 127.74 (s), 126.92 (s), 126.60 – 125.88 (m), 125.24 (d, *J* = 10.8 Hz), 124.14 (s), 123.18 (s), 122.75 (s), 122.49 (s), 121.27 (s), 119.91 (s), 56.20 (s), 32.63 (s), 7.58 (s). **HRMS (m/z, ESI, $[M+H]^+$):** calcd. for $C_{46}H_{34}N_2$, 615.2800, found 615.2797.

SI1. NMR (^{1}H, ^{13}C) spectra of fluorophores.

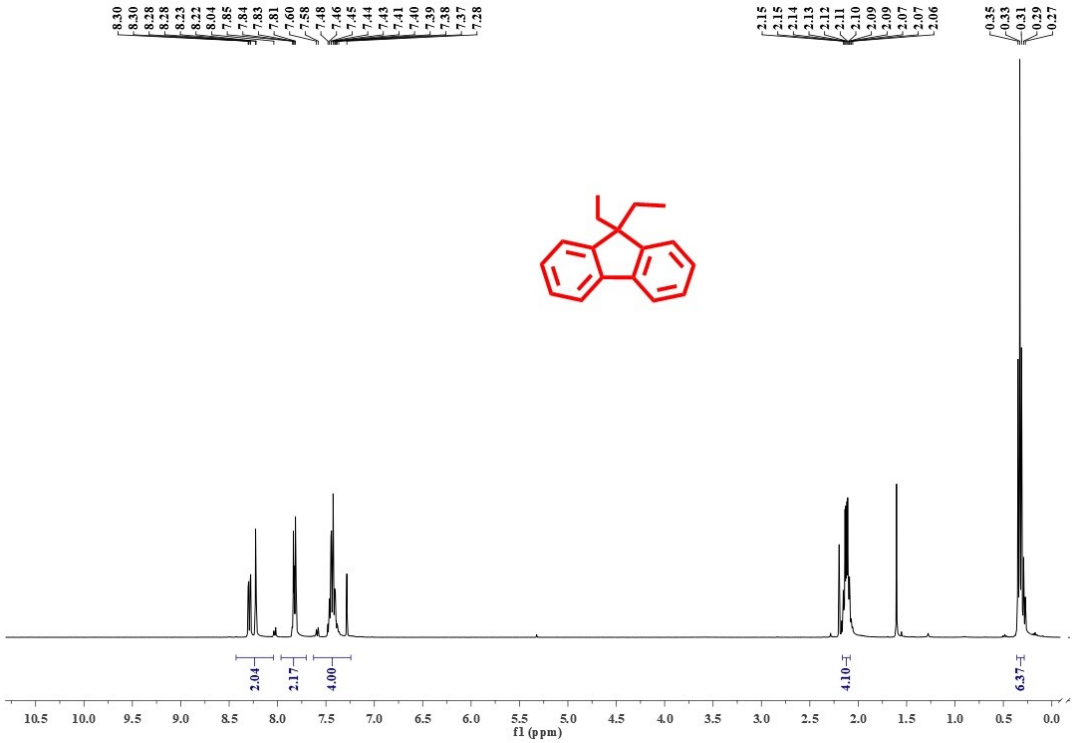


Fig. S1 ^{1}H NMR spectra of 9,9-diethyl-9H-fluorene (Intermediate I) in $CDCl_3$.

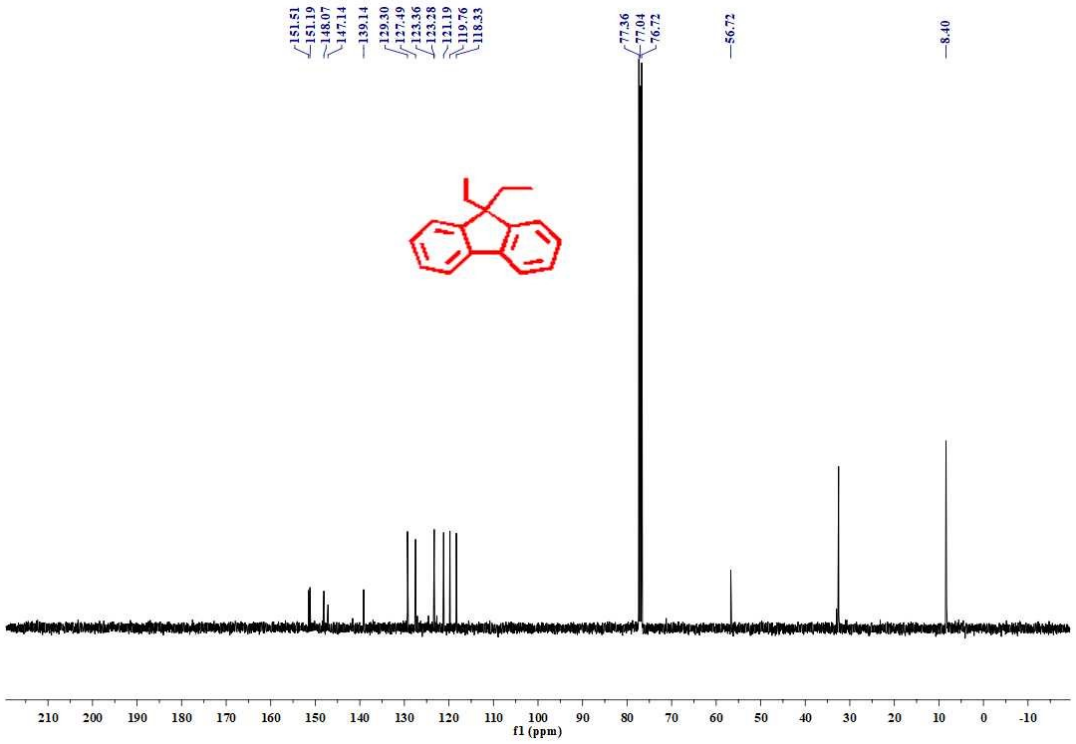


Fig. S2 ^{13}C NMR spectra of 9,9-diethyl-9H-fluorene (Intermediate I) in $CDCl_3$.

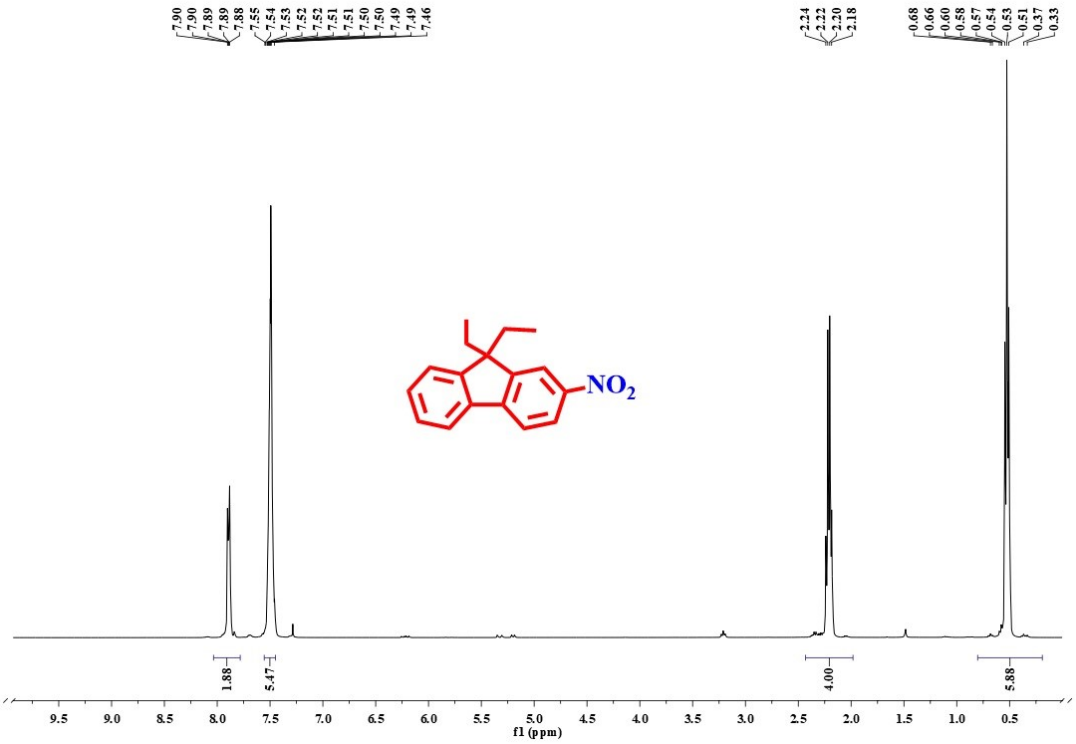


Fig. S3 ^{1}H NMR spectra of 9,9-diethyl-2-nitro-9H-fluorene (Intermediate II) in $CDCl_3$.

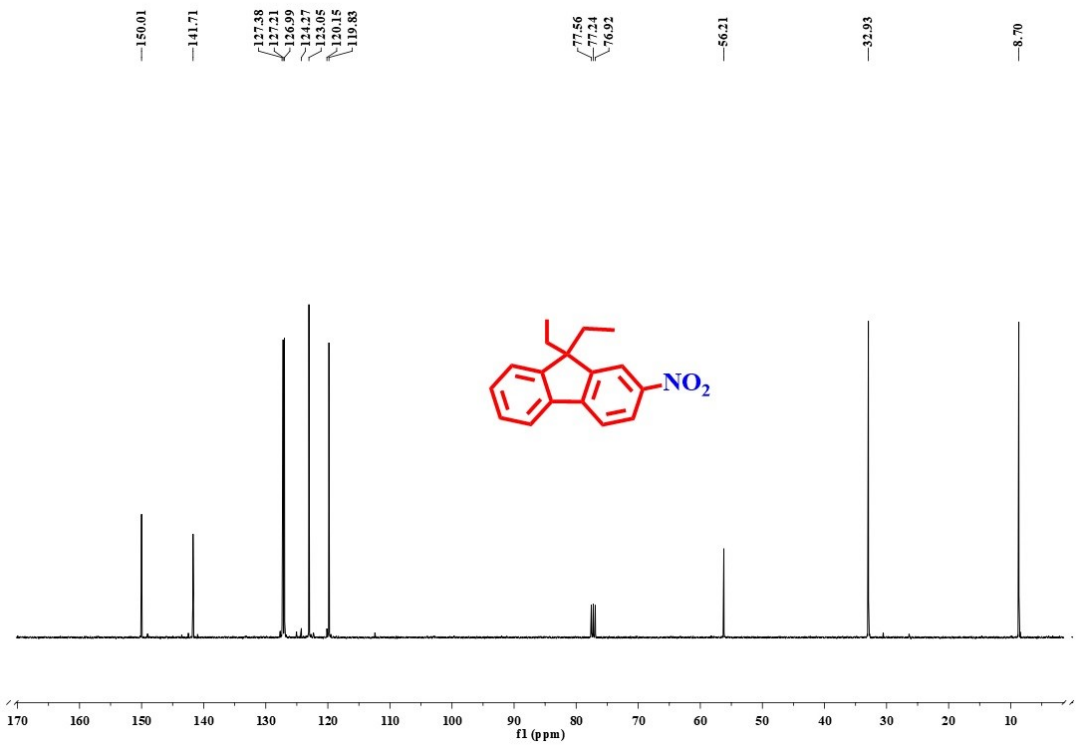


Fig. S4 ^{13}C NMR spectra of 9,9-diethyl-2-nitro-9H-fluorene (Intermediate II) in $CDCl_3$.

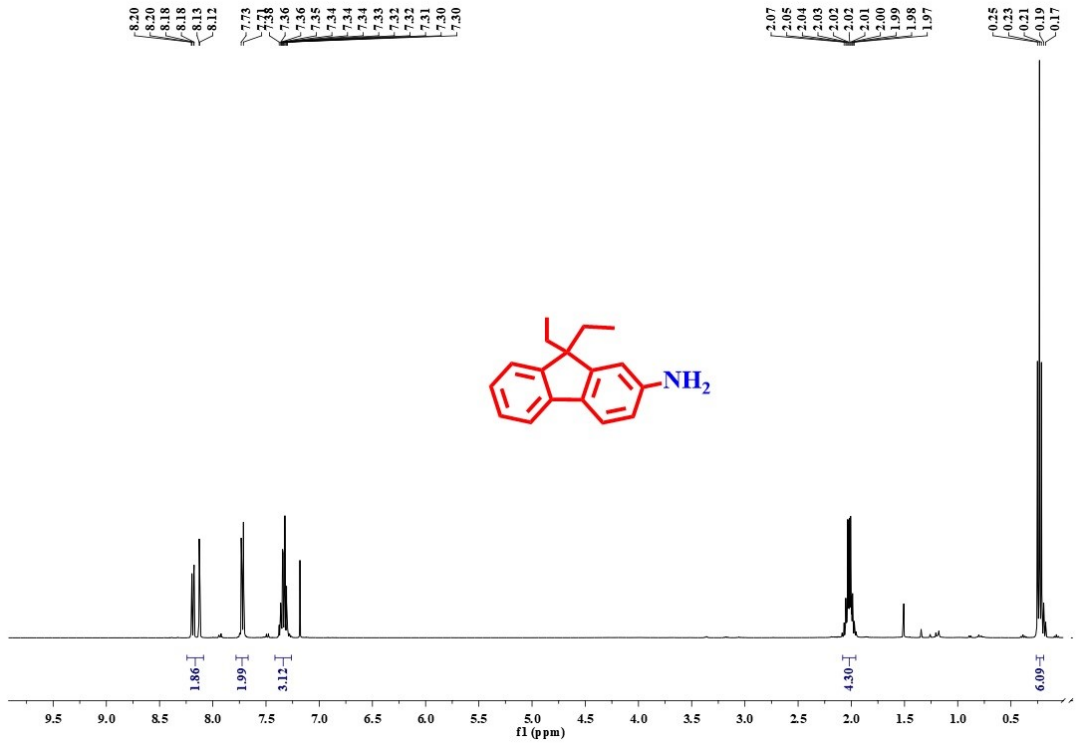


Fig. S5 ^{1}H NMR spectra of 9,9-diethyl-9H-fluoren-2-amine (Intermediate III) in $CDCl_3$.

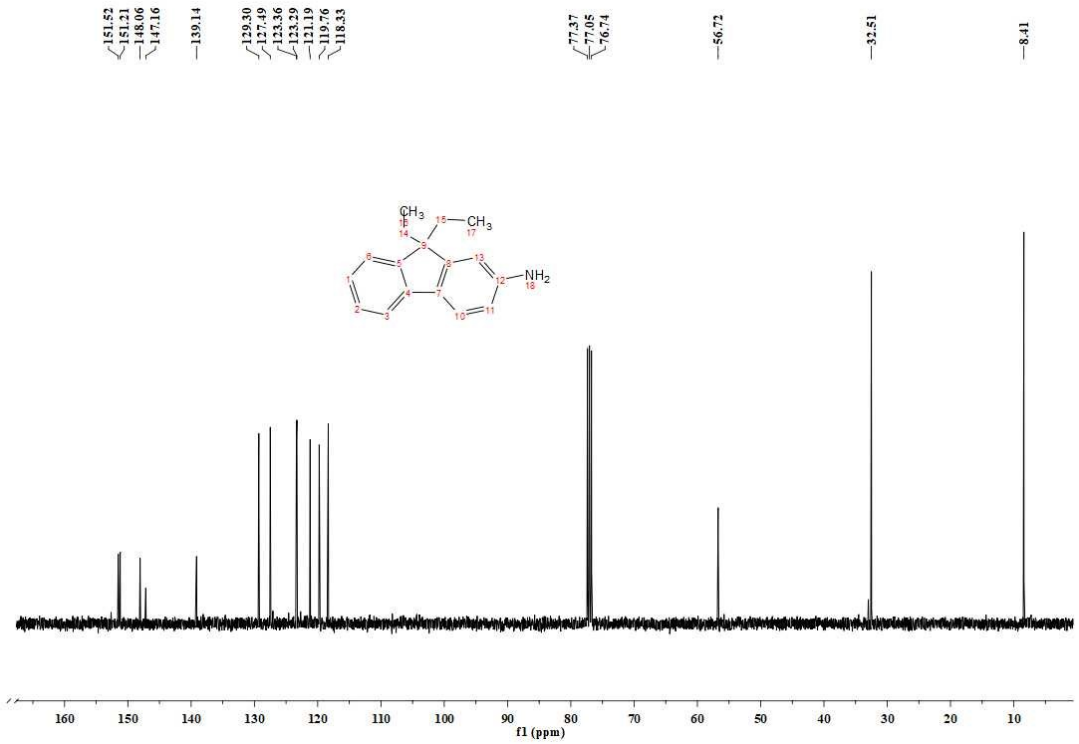


Fig. S6 ^{13}C NMR spectra of 9,9-diethyl-9H-fluoren-2-amine (Intermediate III) in $CDCl_3$.

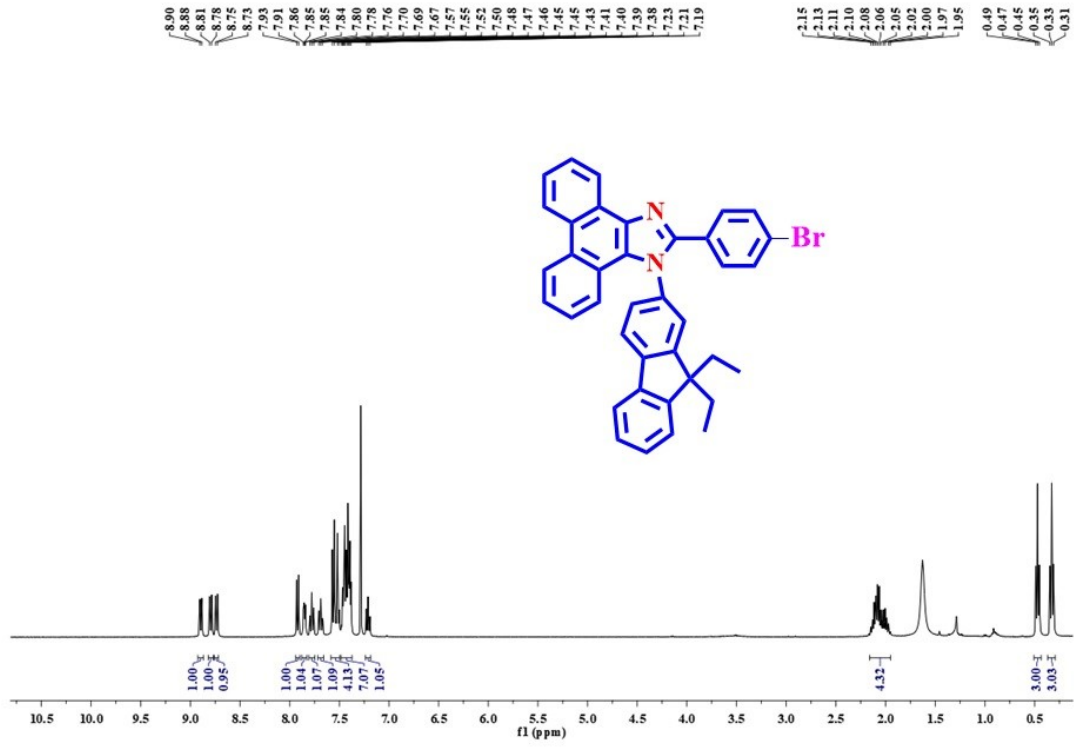


Fig. S7 ^{1}H NMR spectra of 2-(4-bromophenyl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro[9,10-d]imidazole (PhBr) in $CDCl_3$.

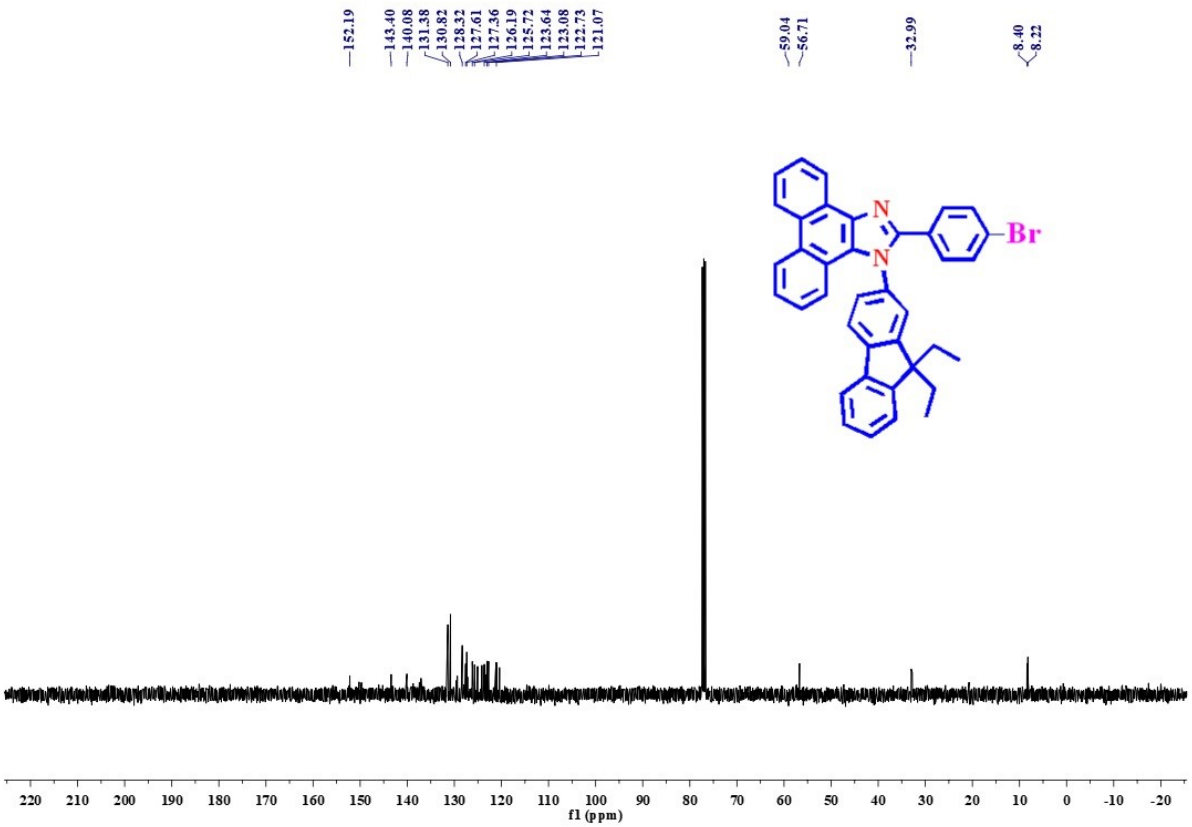


Fig. S8 ^{13}C NMR spectra of 2-(4-bromophenyl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro[9,10-d]imidazole (PhBr) in $CDCl_3$.

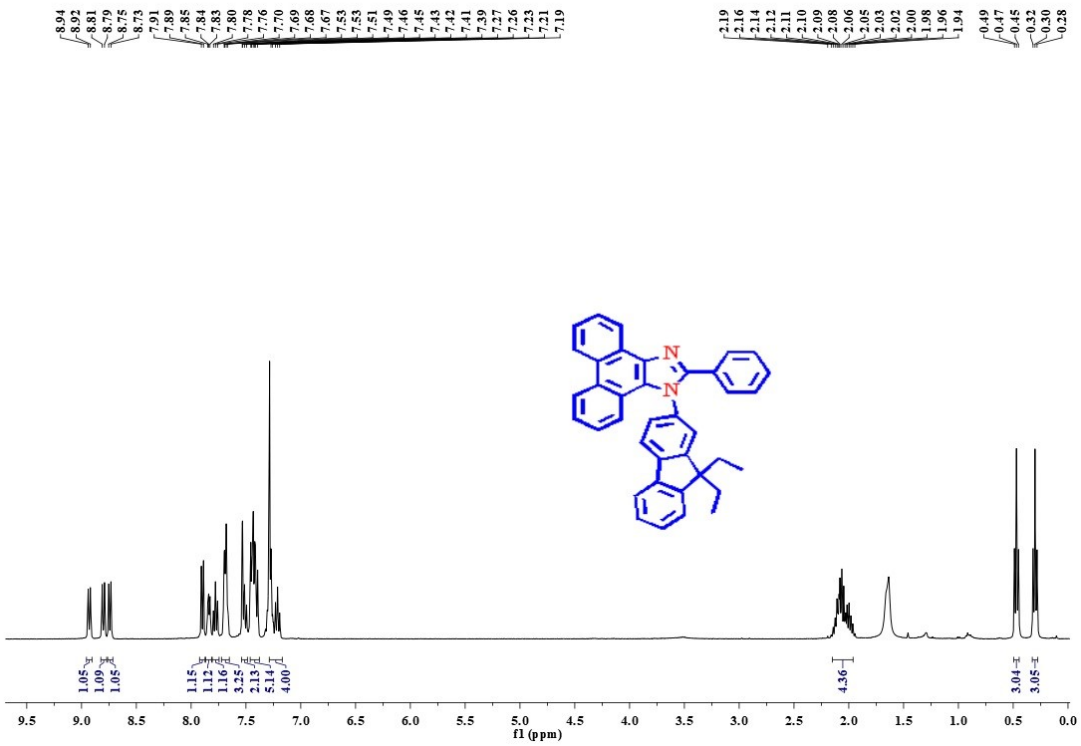


Fig. S9 ^{1}H NMR spectra of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-phenyl-1H-phenanthro[9,10-d]imidazole (PhPh) in $CDCl_3$.

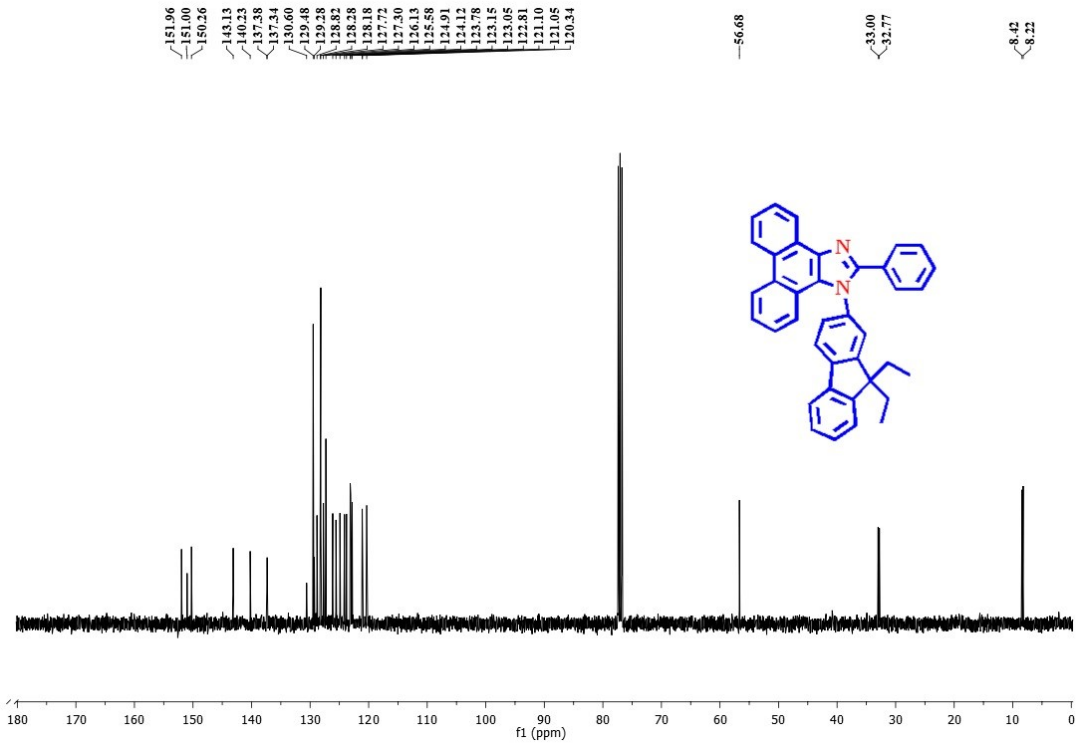


Fig. S10 ^{13}C NMR spectra of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-phenyl-1H-phenanthro[9,10-d]imidazole (PhPh) in $CDCl_3$.

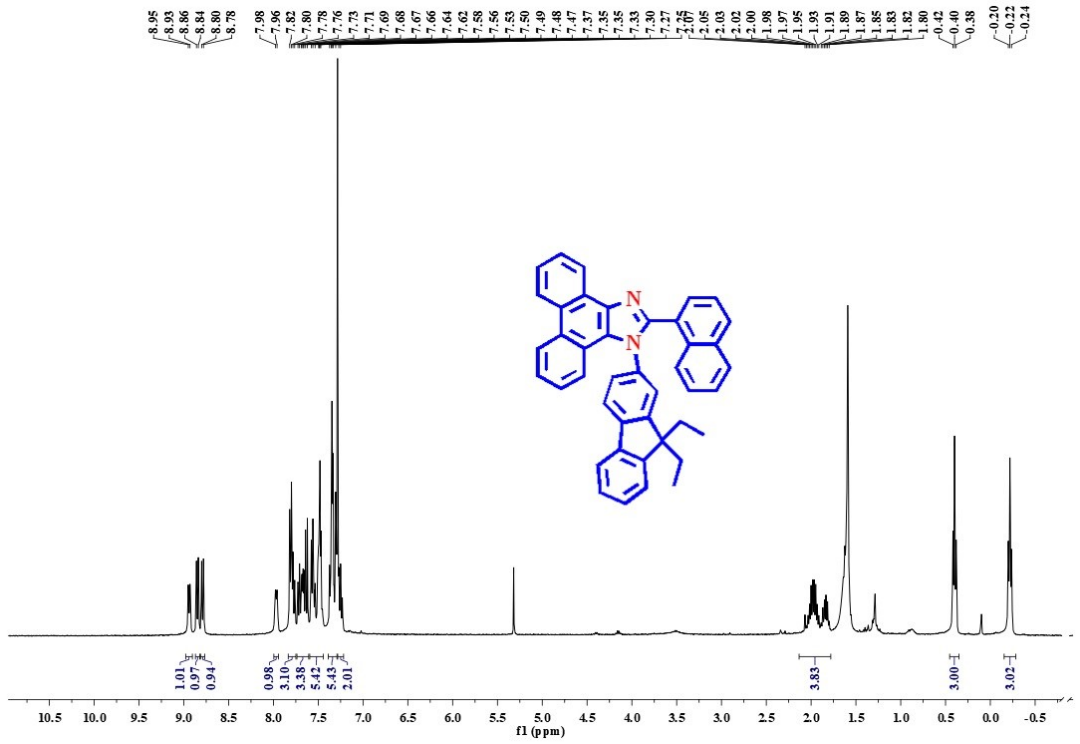


Fig. S11 ^{1}H NMR spectra of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-(naphthalen-1-yl)-1H-phenanthro[9,10-d]imidazole in (PhNp) $CDCl_3$.

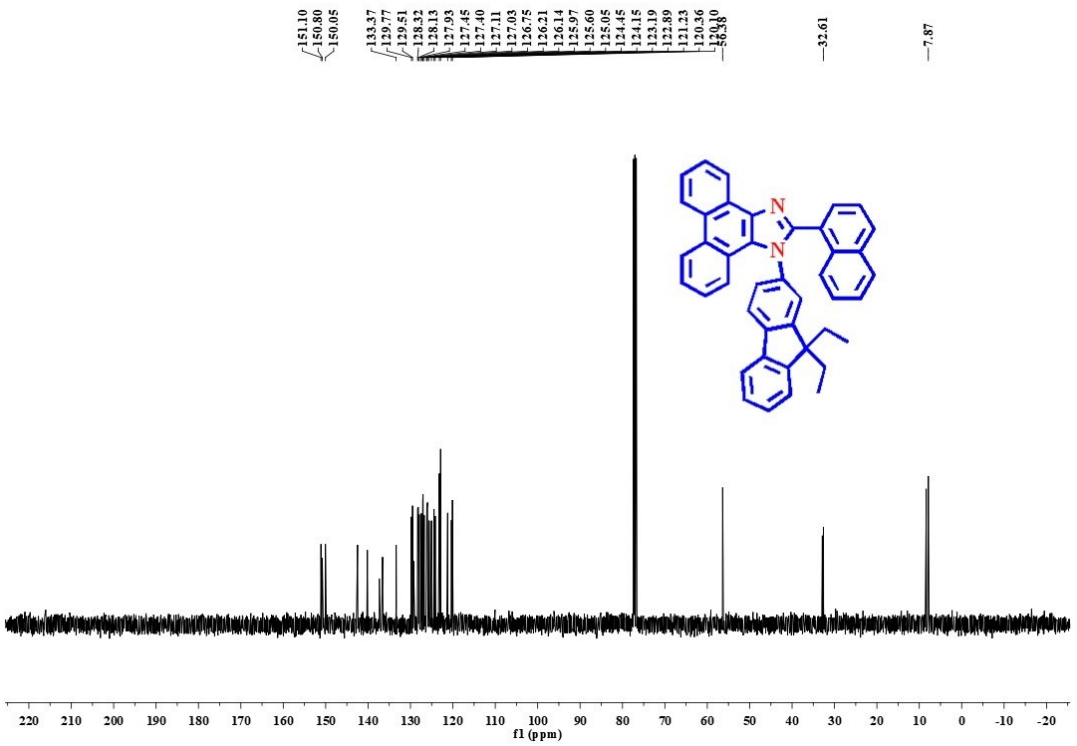


Fig. S12 ^{13}C NMR spectra of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-(naphthalen-1-yl)-1H-phenanthro[9,10-d]imidazole (PhNp) in $CDCl_3$.

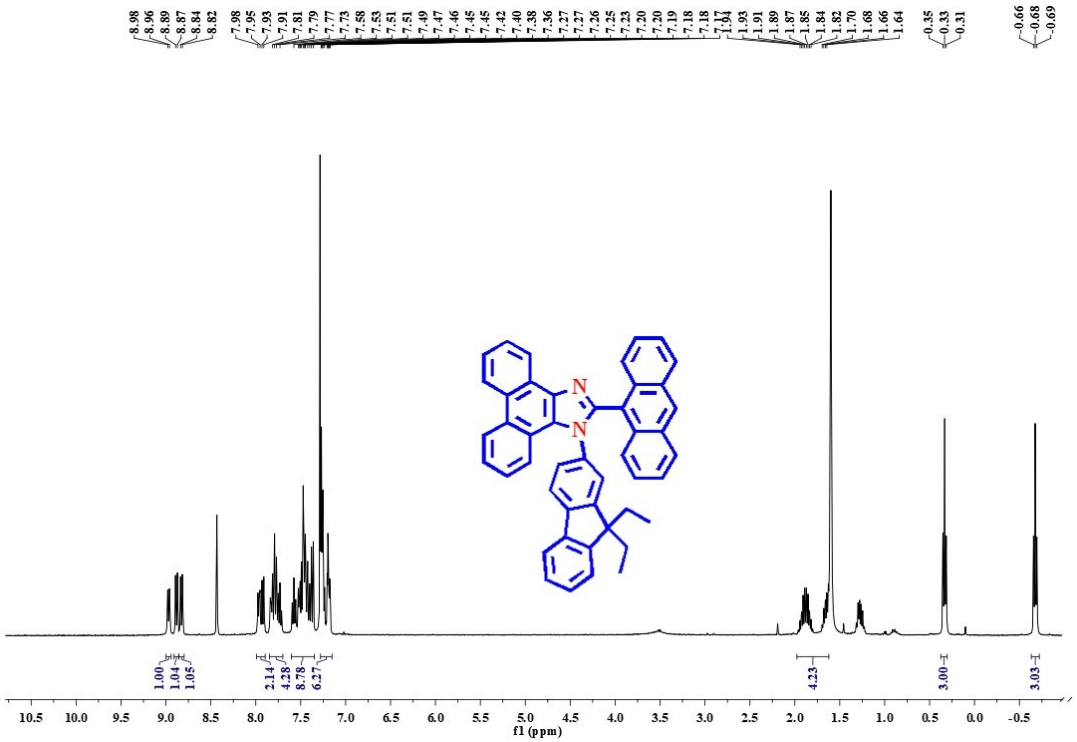


Fig. S13 ^{1}H NMR spectra of 2-(anthracen-9-yl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro[9,10-d]imidazole (PhAn) in $CDCl_3$.

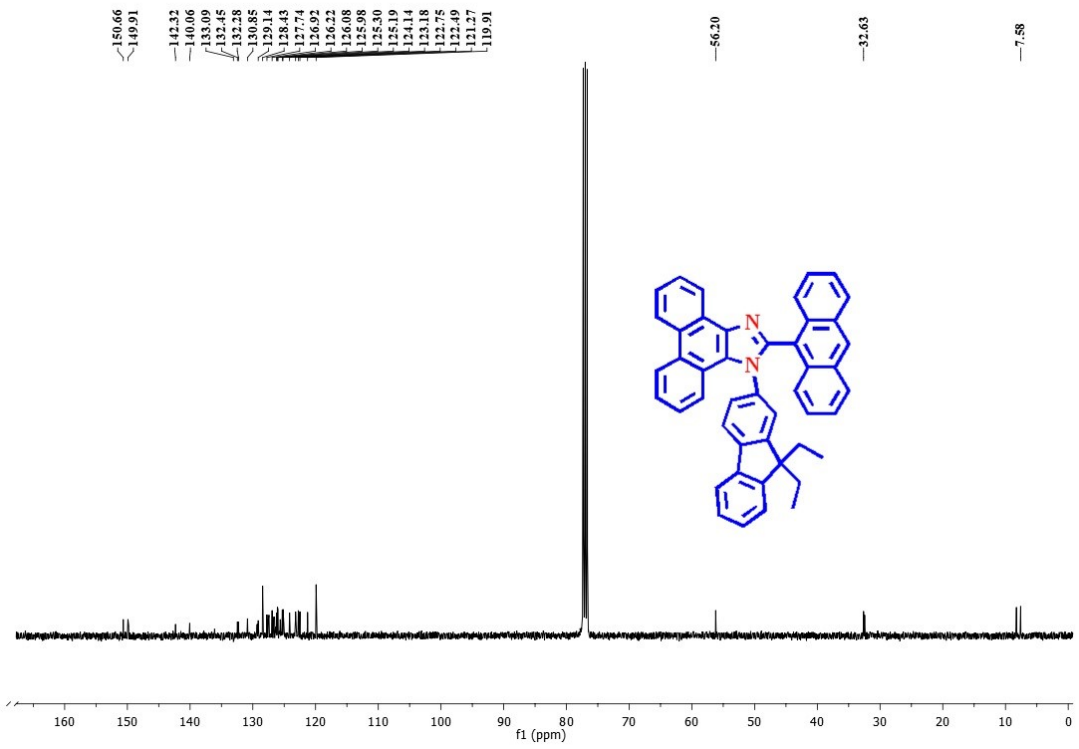


Fig. S14 ^{13}C NMR spectra of 2-(anthracen-9-yl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro[9,10-d]imidazole (PhAn) in $CDCl_3$.

SI2. Mass spectra of fluorophores.

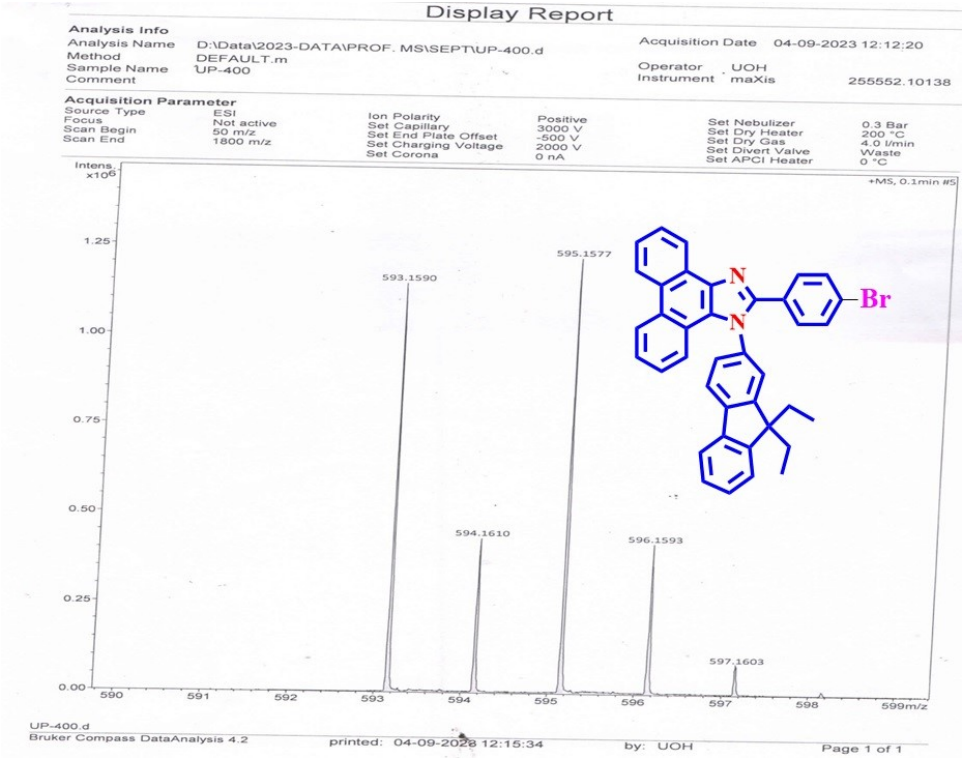


Fig. S15 Mass spectra of 2-(4-bromophenyl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro[9,10-d]imidazole (PhBr).

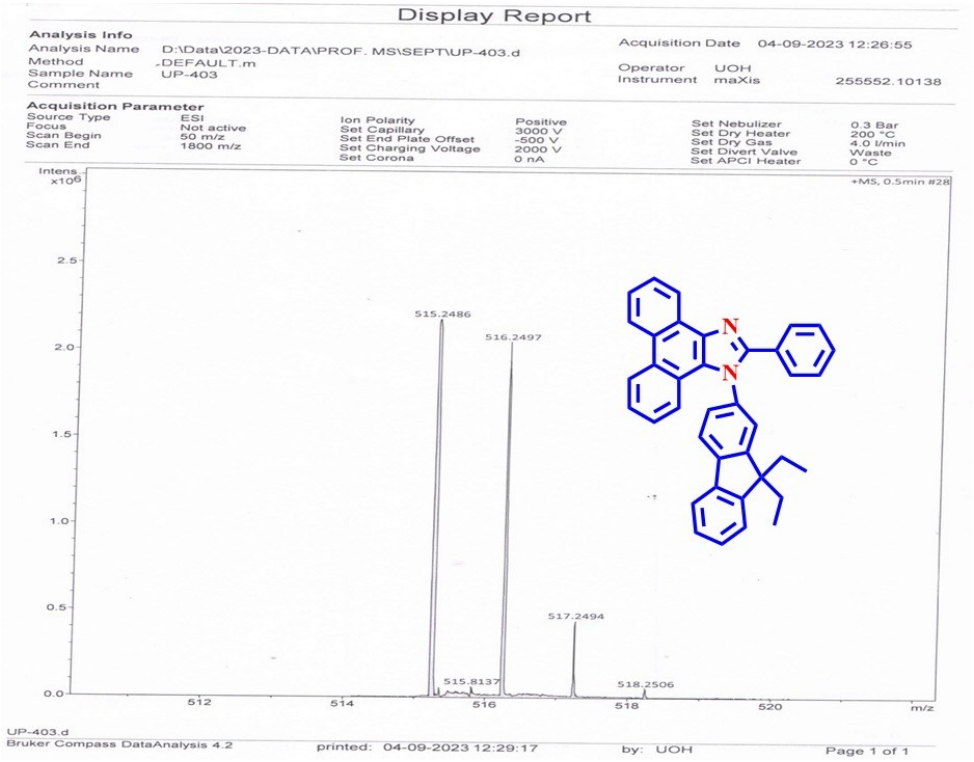


Fig. S16 Mass spectra of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-phenyl-1H-phenanthro[9,10-d]imidazole (PhPh).

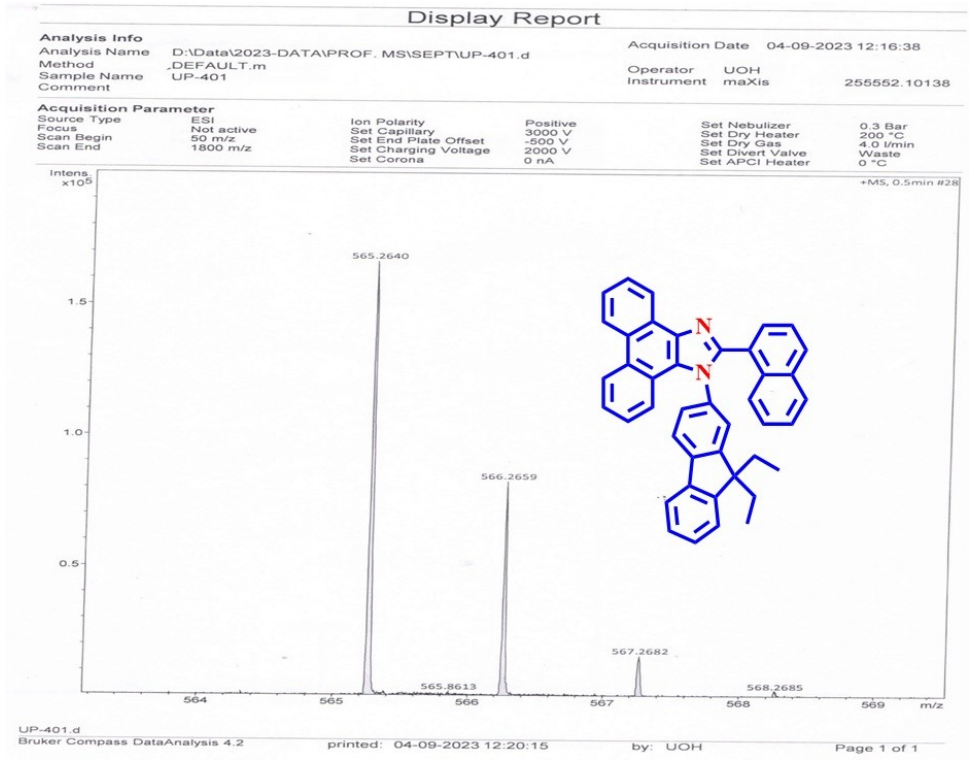


Fig. S17 Mass spectra of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-(naphthalen-1-yl)-1H-phenanthro[9,10-d]imidazole (PhNp).

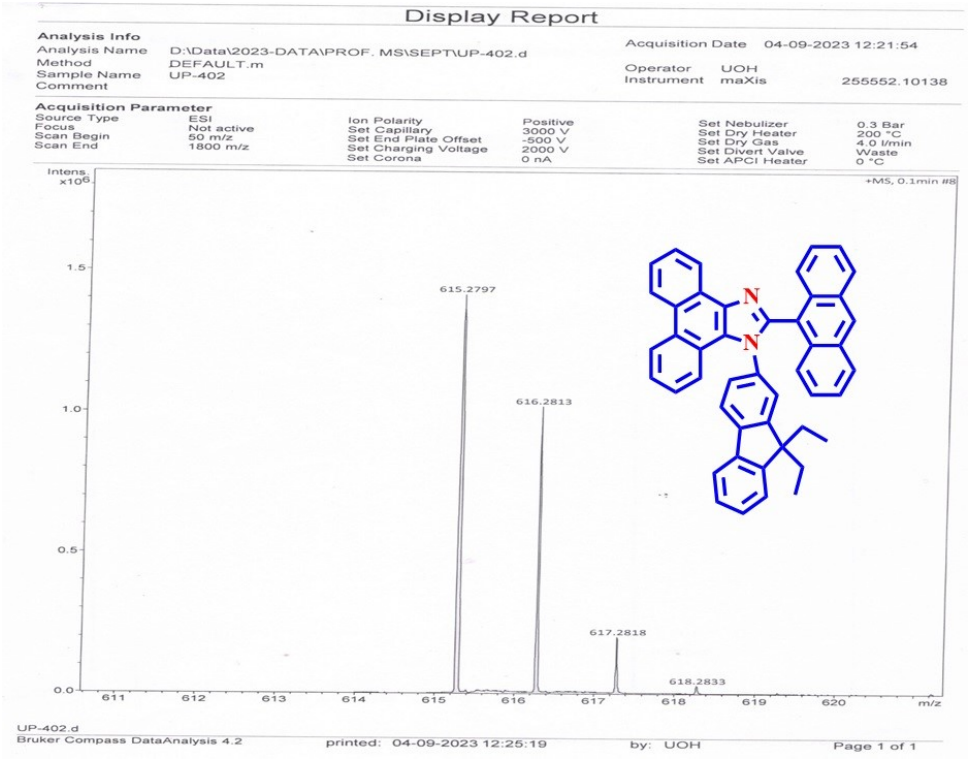


Fig. S18 Mass spectra of 2-(anthracen-9-yl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro[9,10-d]imidazole (PhAn).

SI3. NMR (^{1}H) spectra of fluorophores with PA in equivalent in $CDCl_3$.

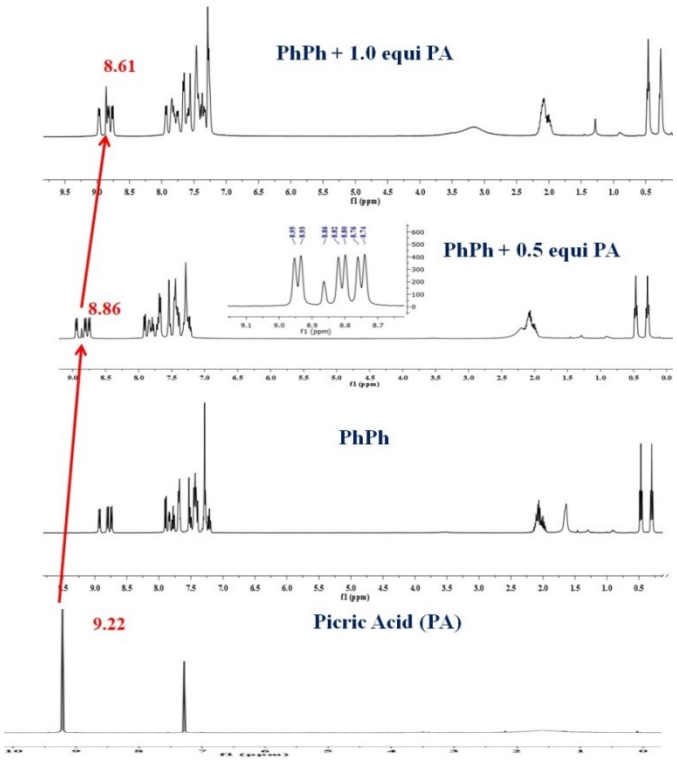


Fig. S19 ^{1}H NMR spectrum of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-phenyl-1H-phenanthro[9,10-d]imidazole (PhPh) with PA (0, 0.5, 1.0 equiv) in $CDCl_3$.

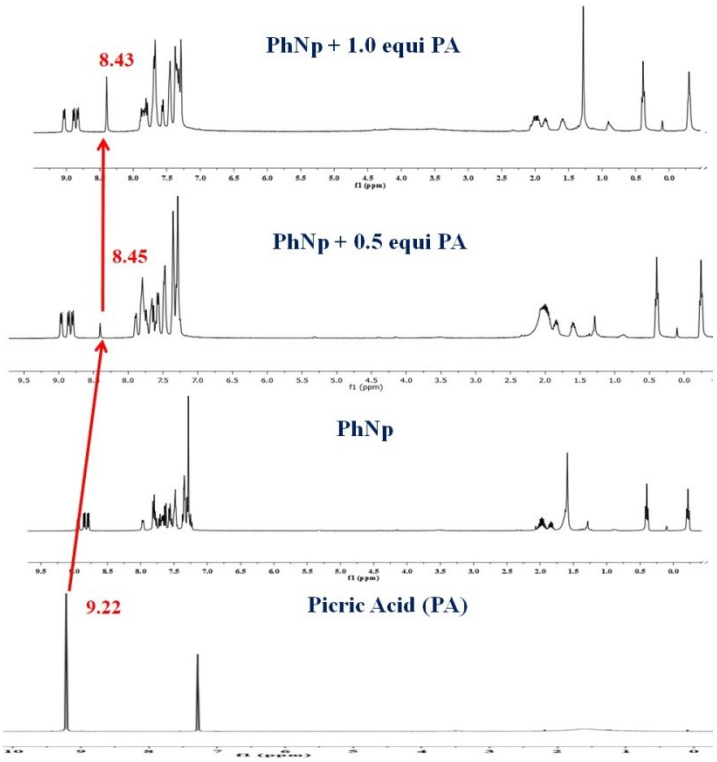


Fig. S20 ^{1}H NMR spectrum of 1-(9,9-diethyl-9H-fluoren-2-yl)-2-(naphthalen-1-yl)-1H-phenanthro[9,10-d]imidazole (PhNp) with PA (0, 0.5, 1.0 equiv) in $CDCl_3$.

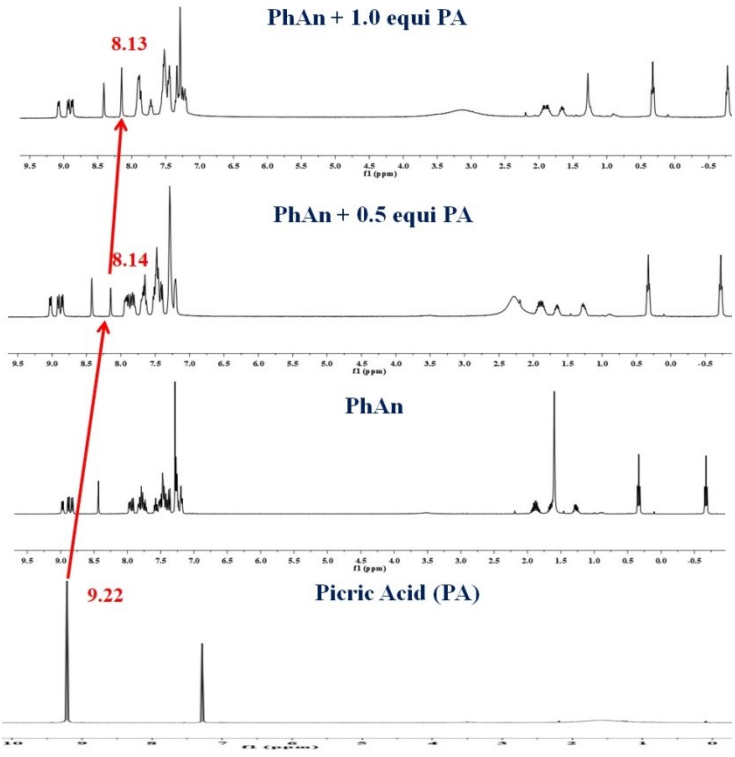


Fig. S21 ^{1}H NMR spectrum of 2-(anthracen-9-yl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro[9,10-d]imidazole (PhAn) with PA (0, 0.5, 1.0 equiv) in $CDCl_3$.

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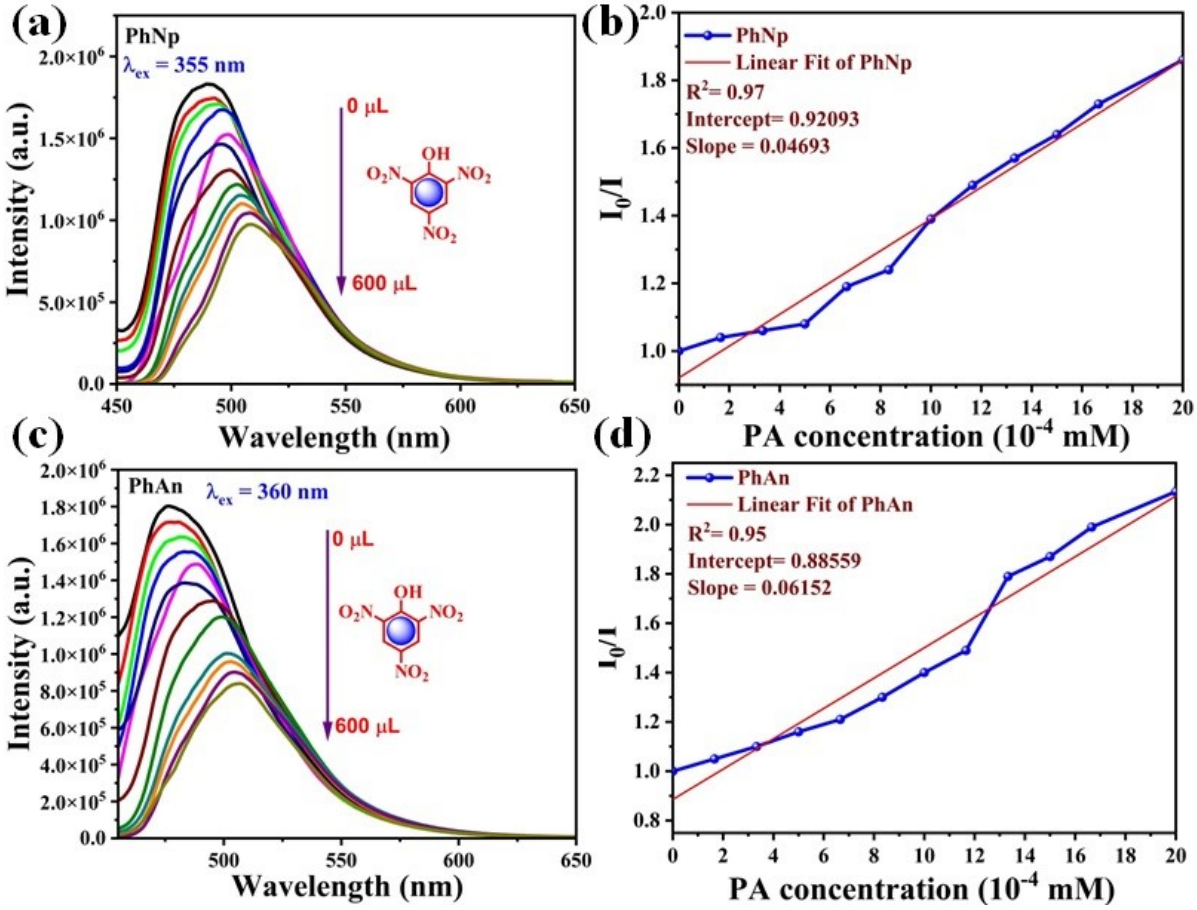


Fig. S22 (a) and (c) Change in the fluorescence of PhNp and PhAn upon the addition of PA excited at 355 nm and 360 nm in THF solvent (1x10^{-5} M). (b) and (d) Stern– Volmer plots of PhNp and PhAn using PA as a quencher.

Table ST1: Single crystal data of PhBr, PhPh, PhNp and PhAn.

Name	PhBr	PhPh	PhNp	PhAn
CCDC No.	2304012	2304798	2304013	2304812
Empirical Formula	C38 H29 Br N2	C42 H33 N2	C38 H30 N2	C46 H34 N2
Formula weight (g/mol)	593.54	565.7	514.64	614.75
Crystal System	monoclinic	orthorhombic	monoclinic	orthorhombic
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Space group	P 1 21/c 1 (14)	P 21 21 21 (19)	P 1 21/c 1 (14)	P b c a (61)
Cell Length (Å)	a=12.521(10) b=24.47(2) c=9.614(9)	a=12.798(3) b=13.832(3) c=17.083(3)	a=12.8246(6) b=11.3473(7) c=18.9588(10)	a=9.0799(6) b=19.2446(12) c=39.209(3)
Cell Angle (º)	β=94.93(3)	α= β = γ = 90	β=95.767(2)	α= β = γ = 90
Cell Volume (Å^3)	2934.73(400)	3024.07(100)	2745.01(30)	6851.34(80)

Z	4	4	4	8
Calculated Density (g/cm^3)	1.34328	1.24245	1.24521	1.19189
F(000)	1224.0	1192.0	1088.0	2592.0
h_{max} , k_{max} , l_{max}	16,31,12	16,17,21	16,14,24	10, 22, 46
Refinement method	SHELXL-2018/3	SHELXL-2018/3	SHELXL-2018/3	SHELXL-2018/3

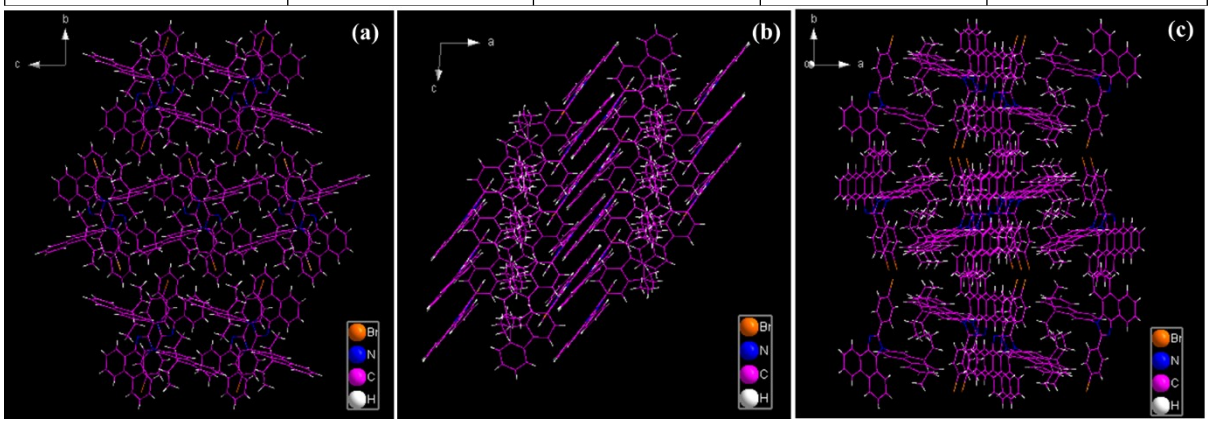


Fig. S23: (a) PhBr crystal packing view from (b) x-axis, (c) y-axis and z-axis respectively.

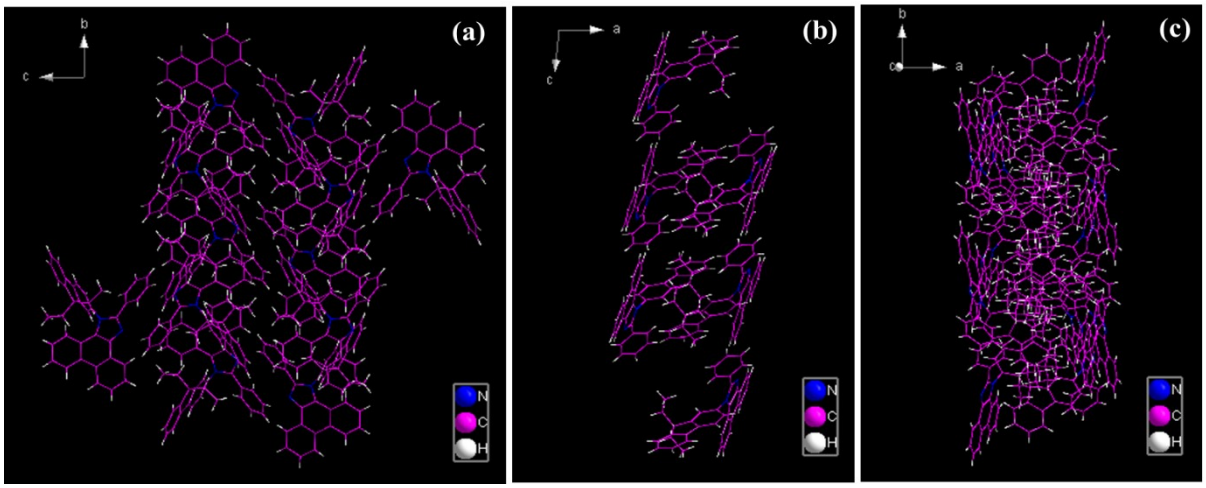


Fig. S24: (a) PhPh crystal packing view from (b) x-axis, (c) y-axis and z-axis respectively.

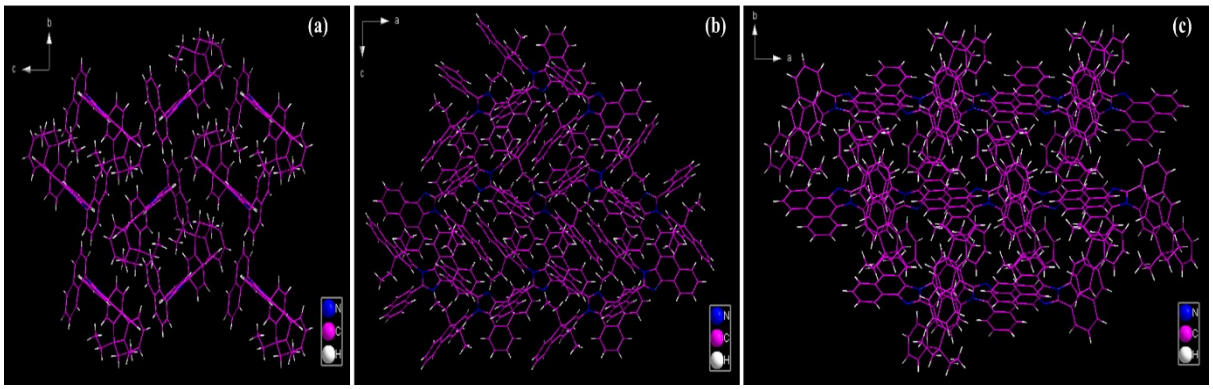


Fig. S25: (a) PhNp crystal packing view from (b) x-axis, (c) y-axis and z-axis respectively.

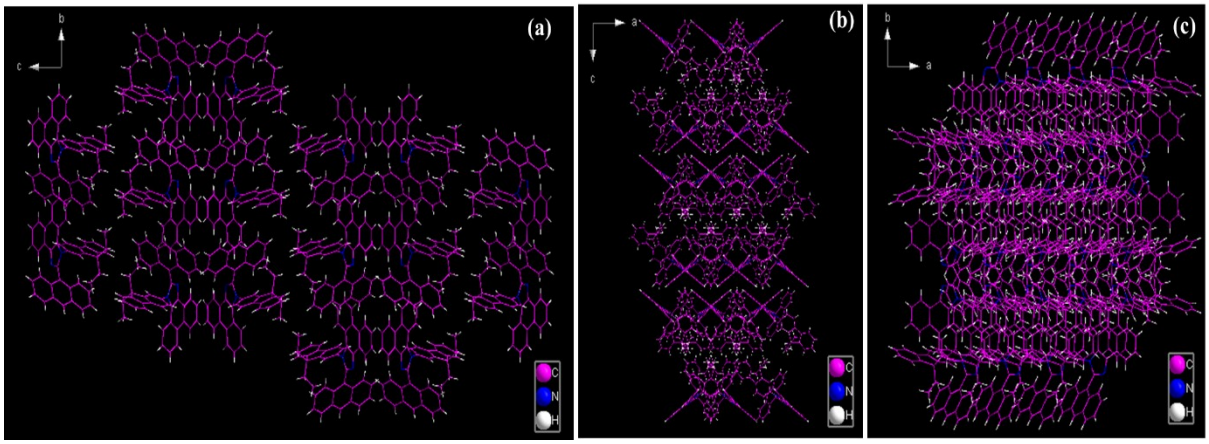


Fig. S26: (a) PhAn crystal packing view from (b) x-axis, (c) y-axis and z-axis respectively.

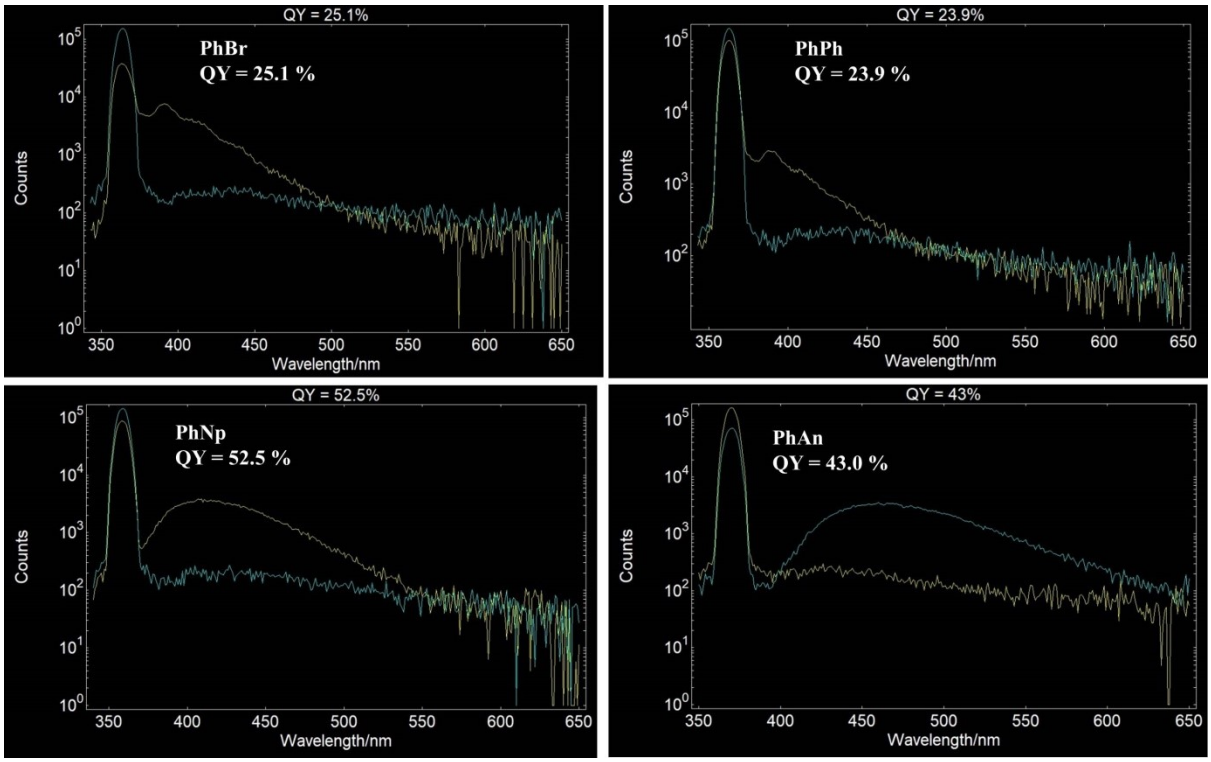


Fig. S27: Quantum Yield of respective fluorophores PhBr, PhPh, PhNp, and PhAn.

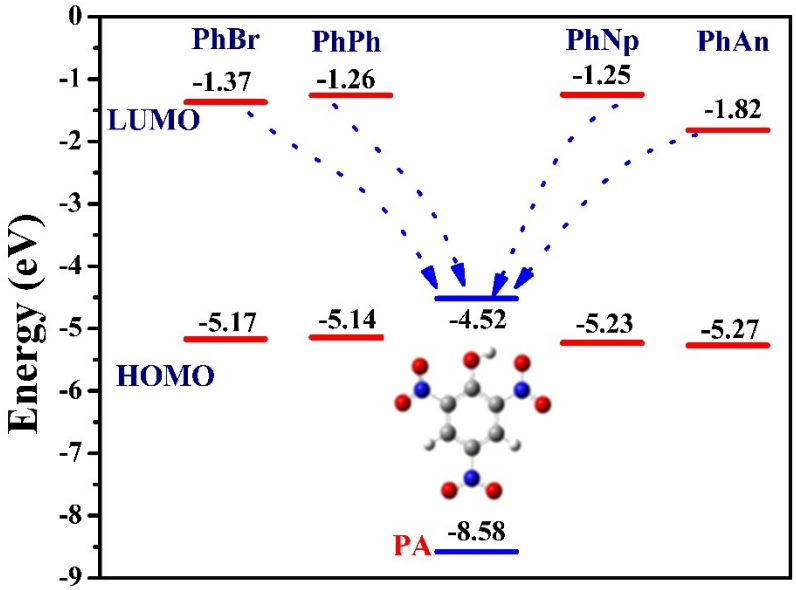
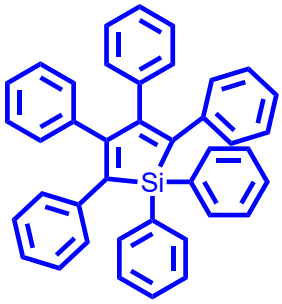
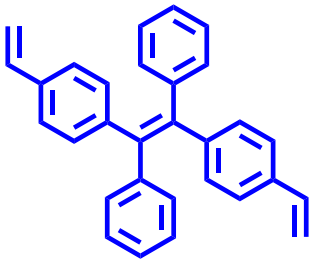
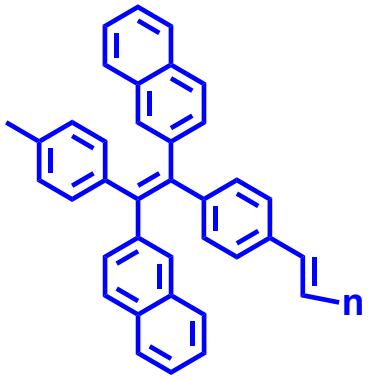
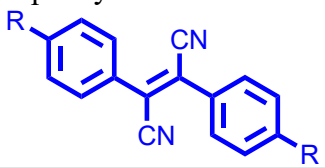
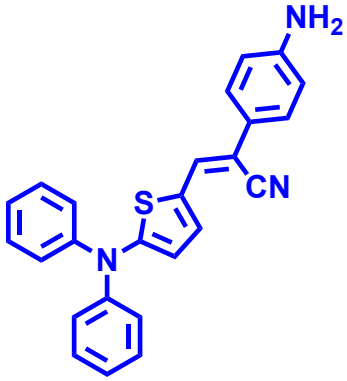
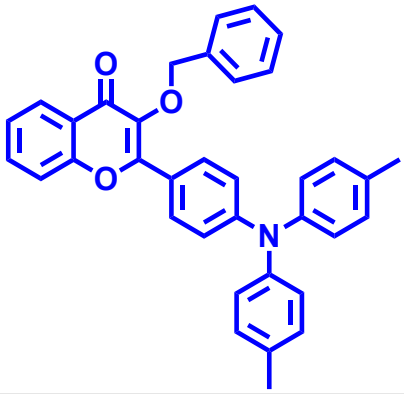
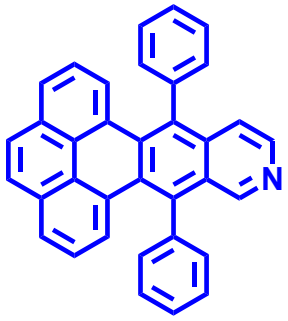
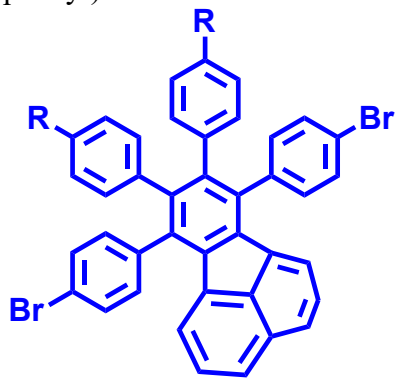
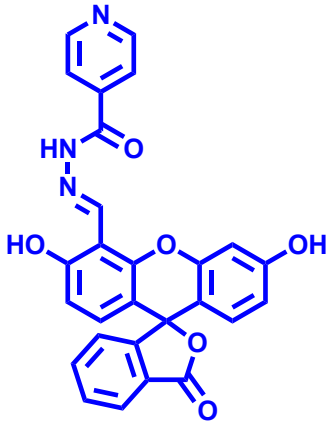
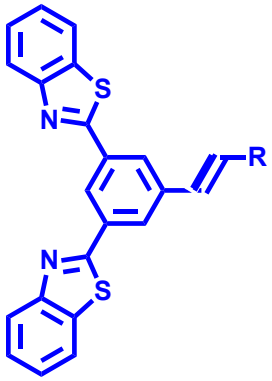


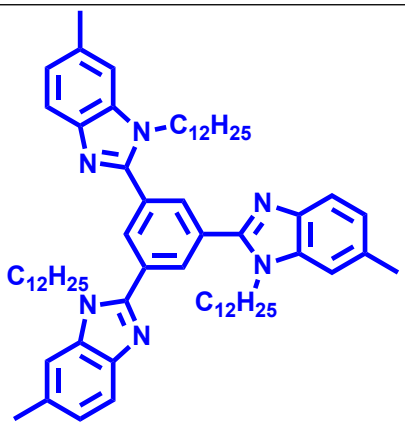
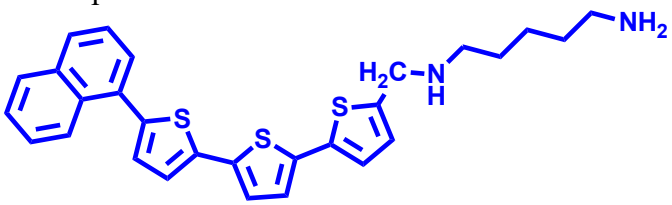
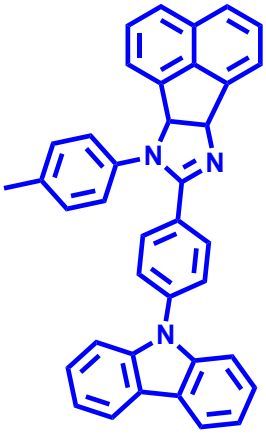
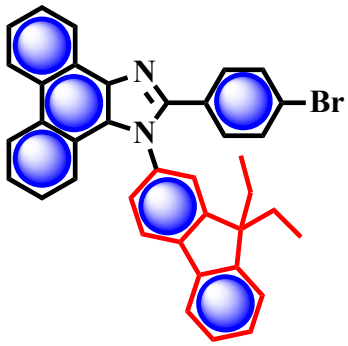
Fig. S28: Electron transfer process between fluorophores (PhBr, PhPh, PhNp, and PhAn) and PA.

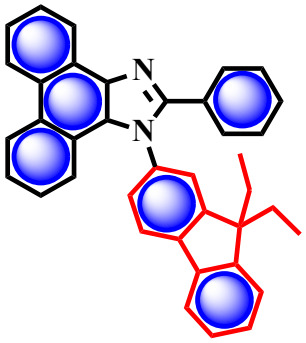
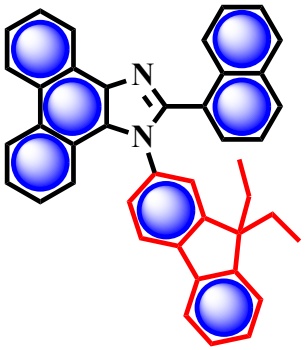
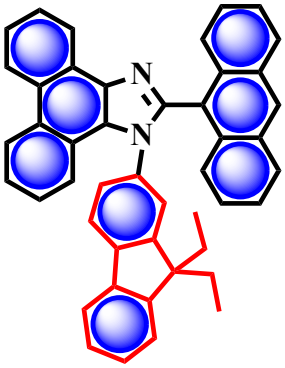
Table ST2: The Comparison of our luminophores with other reported PA sensors.

S. No	Fluorophores	Solvent	Quenching constant (M^{-1})	Detection limit (M)	Ref.
1	Hexaphenylsilole 	THF/Water	-	4.81 ppb	1
2	Tetraphenylethene 	Water	2.7×10^5	0.4 ppm	2
3	Polymers based on di (naphthalen-2-yl)-1,2-diphenylethene	H2O/THF (9/1)	4.70×10^4	1.81×10^{-6}	3

					
4	Triazine-COF	THF	8.71×10^4	10.7 ppm	4
5	poly(silylenevinylene)	THF	8.491×10^3	1.0 ppm	5
6	Diphenylfumaronitriles 	H2O/THF (8/2)	5.60×10^4	1.80×10^{-10}	6
7	Imidazole derivatives	H2O/DMF (9/1)	1.30×10^4	3.55×10^{-6}	7
8	Thiophene aromatic amine derivatives 	THF	-	5.70×10^{-6}	8
9	3-(Benzyloxy)-2-(4-(di-p-tolylamino)phenyl)-4H-chromen-4-one 	Water	1.93×10^4	3.70×10^{-9}	9
10	[P(dimethylacrylamide*co*-Benzophenone acrylamide-*co*-glycidyl methacrylate]	Water	7.75×10^4	5.60×10^{-7}	10

11	9,14-diphenylpyreno [4,5-g]isoquinoline 	MeCN	-	2.42 × 10^{-6}	11
12	7,10-bis(4-bromophenyl)-8,9-bis(4-(2-(2-(2-methoxyethoxy) ethoxy)ethoxy)-phenyl)-fluoranthene 	EtOH	5.60 × 10^5	2.6 ppb	12
13	Fluorescein derivatives 	EtOH	2.50 × 10^5	1.10 × 10^{-7}	13
14	1,3-Bis(benzo[d]thiazol-2-yl)benzene derivatives 	H2O/THF (9/1)	1.54 × 10^5	29.1 ppb	14
15	1,3,5-tri(1H- benzo[d]imidazol-2- yl)benzene derivative	THF	1.15x10^5	50 ppb	15

					
16	tetraphenylethylene	THF	$5.7x10^4$	1.45 ppb	16
17	Terthiophene 	THF/water	$5.7x10^3$	70 ppb	17
18	AC-2 	THF	2.5×10^3	450 ppb	18
19	**PhBr** 	THF	9.09×10^{-2}	3.72ppb	This work
20	**PhPh**	THF	2.49×10^{-2}	5.15ppb	This work

					
21	**PhNp** 	THF	4.69×10^{-2}	3.64ppb	This work
22	**PhAn** 	THF	6.15×10^{-2}	3.46ppb	This work

TGA and DSC:

The stability of compounds of all the fluorophores was evaluated by using Thermal Gravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC) and the temperature ranged from 25 °C to 800 °C and 25 °C to 500 °C respectively under a scanning rate of 10 °C/min in N_2 atmosphere. DSC thermograms have indicated endothermic peaks corresponding to melting points 270.36 °C, 237.09 °C, 243.49 °C, and 335.49 °C for PhBr, PhPh, PhNp, and PhAn respectively. The glass transition (Tg) temperatures were identified as 370.65 °C, 383.58 °C, 403.07 °C, and 404.10 °C for PhBr, PhPh, PhNp, and PhAn respectively.

Table ST3: Melting points of the fluorophores

Fluorophores	Melting Point (°C) by DSC	5 % wt loss by TGA (T_g (°C))
PhBr	270.36	216
PhPh	237.09	325
PhNp	243.49	211
PhAn	335.49	171

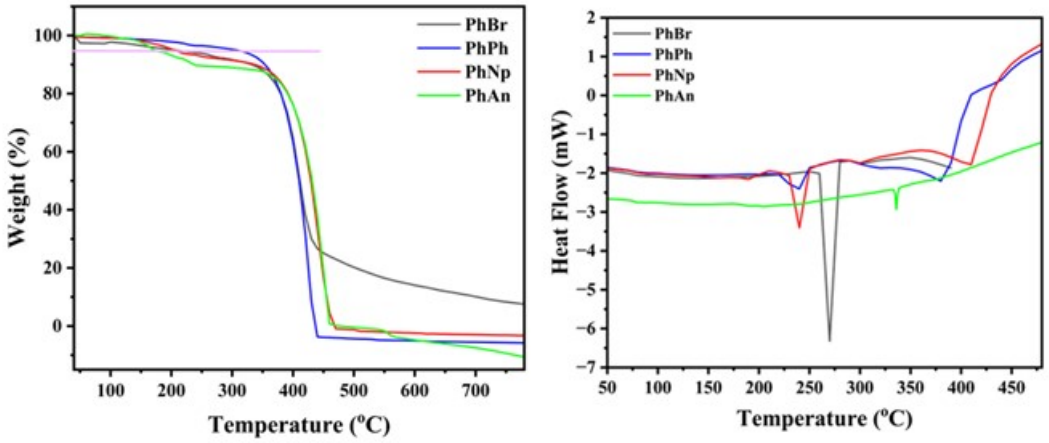


Fig. S29: TGA and DSC of PhBr, PhPh, PhNp, and PhAn

Table ST 4: CRI, LER, CCT, x, y coordinates and R9 values of fluorophores

Fluorophore	PhAn : Eu -1 : Eu -2	CRI	LER (lm W^{-1})	CCT (K)	(x, y)	R9
PhAn + Eu-1	1:1	90	236	8354	(0.29, 0.29)	57
PhAn + Eu-2	1:1	90	243	7613	(0.30, 0.30)	49
PhAn + Eu-1	1:2	84	233	7470	(0.30, 0.28)	64
PhAn + Eu-2	1:2	85	225	8628	(0.29, 0.27)	39

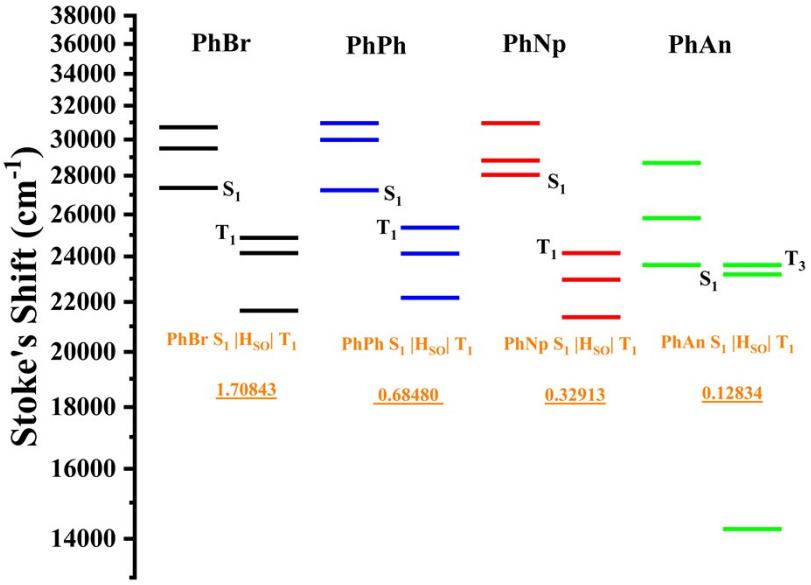


Fig SI30. Plot of singlet and triplet levels calculated by TD-DFT with SOC values of PhBr, PhPh, PhNp, PhAn

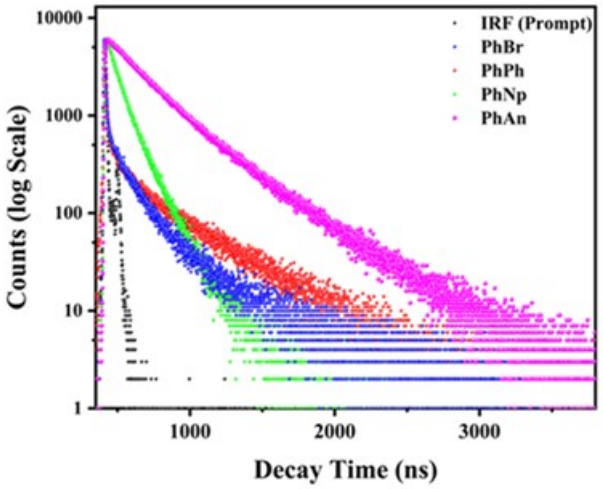


Fig SI31. Fluorescence lifetime of PhBr, PHPh, PhNp, PhAn at 77 K

Table ST5: Computed Vertical Transitions and Their Oscillator Strengths and Configurations

PhBr

Excited State 1: Triplet-A 2.6825 eV 462.20 nm f=0.0000 <S**2>=2.000

150 ->158	-0.10272
152 ->156	-0.13649
152 ->157	-0.12956
153 ->154	0.25779
153 ->155	0.53062
153 ->157	-0.13399
153 ->158	0.17293

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -4146.73944784
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.9945 eV 414.03 nm f=0.0000 <S**2>=2.000
146 ->156 0.10797
148 ->160 -0.13106
151 ->154 0.60602
151 ->155 -0.15539

Excited State 3: Triplet-A 3.0828 eV 402.18 nm f=0.0000 <S**2>=2.000
149 ->155 -0.12515
150 ->155 -0.14401
150 ->162 0.12429
152 ->155 -0.12315
152 ->156 -0.26236
152 ->157 -0.23236
153 ->155 -0.26960
153 ->157 -0.12453
153 ->158 0.38850

Excited State 4: Singlet-A 3.3914 eV 365.59 nm f=0.0189 <S**2>=0.000
153 ->154 0.69765

Excited State 5: Singlet-A 3.6568 eV 339.05 nm f=0.4806 <S**2>=0.000
152 ->158 0.10281
153 ->155 0.64320
153 ->156 0.16715
153 ->157 0.13846

Excited State 6: Singlet-A 3.8071 eV 325.66 nm f=0.0754 <S**2>=0.000
152 ->155 0.16688
152 ->158 0.11167
153 ->155 -0.23436
153 ->156 0.59863
153 ->157 0.16638

PhPh

Excited State 1: Triplet-A 2.7255 eV 454.90 nm f=0.0000 <S**2>=2.000
133 ->141 0.10330
135 ->138 -0.12131
135 ->139 -0.16445
135 ->140 -0.13586
136 ->137 0.21628
136 ->138 0.52087

136 ->140 -0.17619
136 ->141 0.17322
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1575.63415551
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.9916 eV 414.44 nm f=0.0000 <S**2>=2.000
129 ->139 0.11342
130 ->142 -0.14006
134 ->137 0.61332
135 ->137 -0.10659
136 ->137 -0.10485

Excited State 3: Triplet-A 3.1438 eV 394.38 nm f=0.0000 <S**2>=2.000
131 ->138 -0.14663
132 ->143 -0.12050
133 ->138 0.13064
133 ->144 -0.11940
135 ->138 -0.14433
135 ->139 -0.26260
135 ->140 -0.20379
136 ->138 -0.30680
136 ->140 -0.11463
136 ->141 0.37053

Excited State 4: Singlet-A 3.3761 eV 367.24 nm f=0.0129 <S**2>=0.000
136 ->137 0.70202

Excited State 5: Singlet-A 3.7166 eV 333.60 nm f=0.2178 <S**2>=0.000
135 ->138 0.12624
135 ->140 -0.10485
135 ->141 0.13310
136 ->138 0.51645
136 ->139 0.36612
136 ->140 0.19578

Excited State 6: Singlet-A 3.8368 eV 323.15 nm f=0.1732 <S**2>=0.000
135 ->138 0.11514
136 ->138 -0.42503
136 ->139 0.54027

PhNp

Excited State 1: Triplet-A 2.6487 eV 468.10 nm f=0.0000 <S**2>=2.000
144 ->155 0.15305
147 ->150 0.54250
147 ->151 0.24569
149 ->150 0.27048
This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -1729.27799684
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.8463 eV 435.60 nm f=0.0000 <S**2>=2.000
145 ->157 0.13079
147 ->150 -0.11414
148 ->152 -0.32061
149 ->150 0.18128
149 ->151 -0.14439
149 ->152 0.12010
149 ->153 0.47611
149 ->154 -0.11108

Excited State 3: Triplet-A 2.9942 eV 414.08 nm f=0.0000 <S**2>=2.000
142 ->154 0.13374
143 ->156 -0.14448
146 ->150 -0.27182
146 ->151 0.52736
148 ->151 -0.16120

Excited State 4: Singlet-A 3.4765 eV 356.63 nm f=0.0696 <S**2>=0.000
149 ->150 0.70201

Excited State 5: Singlet-A 3.5729 eV 347.01 nm f=0.0240 <S**2>=0.000
149 ->151 0.70073

Excited State 6: Singlet-A 3.8372 eV 323.11 nm f=0.0200 <S**2>=0.000
148 ->150 0.14649
148 ->153 0.23185
149 ->152 0.61950

PhAn

Excited State 1: Triplet-A 1.7684 eV 701.10 nm f=0.0000 <S**2>=2.000
161 ->163 0.68309
162 ->163 0.14134
161 <-163 0.13424
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1882.95055232
Copying the excited state density for this state as the 1-particle RhoCI density.
Excited State 2: Triplet-A 2.8752 eV 431.23 nm f=0.0000 <S**2>=2.000
158 ->171 0.12990
160 ->165 -0.34942

162 ->163 -0.12209
162 ->165 0.17679
162 ->166 0.47518
162 ->167 -0.15328

Excited State 3: Triplet-A 2.9267 eV 423.63 nm f=0.0000 <S**2>=2.000
161 ->163 -0.13930
162 ->163 0.67893

Excited State 4: Singlet-A 2.9310 eV 423.01 nm f=0.0016 <S**2>=0.000
162 ->163 0.69905

Excited State 5: Singlet-A 3.2009 eV 387.34 nm f=0.1150 <S**2>=0.000
161 ->163 0.69338

Excited State 6: Singlet-A 3.5568 eV 348.58 nm f=0.0002 <S**2>=0.000
160 ->163 0.70197

Optimized Cartesian coordinates and energies of luminophores:

Table ST6: Optimized Cartesian coordinates:

PhBr

70

symmetry c1

Atomic Type	**X**	**Coordinates (Angstroms) Y**	**Z**
C	3.193715000	-4.006837000	-0.561278000
C	2.553557000	-2.781437000	-0.532414000
C	3.273175000	-1.580861000	-0.328782000
C	4.695105000	-1.641076000	-0.132864000
C	5.306066000	-2.913702000	-0.173128000
C	4.582613000	-4.074077000	-0.384355000
C	2.678445000	-0.270593000	-0.283421000
C	5.482798000	-0.425477000	0.112553000
C	4.836817000	0.840349000	0.181689000

C	3.416073000	0.877368000	-0.016191000
C	5.575242000	2.014450000	0.430105000
H	5.039501000	2.956770000	0.472682000
C	6.944515000	1.955442000	0.608015000
C	7.600895000	0.714595000	0.538731000
C	6.884946000	-0.445401000	0.296789000
H	2.616329000	-4.913020000	-0.718814000
H	1.481106000	-2.746383000	-0.663134000
H	6.376613000	-2.996190000	-0.029229000
H	5.092546000	-5.032494000	-0.406711000
H	7.511222000	2.862254000	0.797812000
H	8.677105000	0.661347000	0.674785000
H	7.427636000	-1.382176000	0.248979000
C	0.199066000	-0.628275000	-0.669217000
C	-0.647825000	-0.939389000	0.402249000
C	-0.080529000	-1.078943000	-1.964902000
C	-1.777955000	-1.717185000	0.169357000
H	-0.406540000	-0.556331000	1.387263000
C	-1.221857000	-1.842772000	-2.205471000
H	0.597143000	-0.821392000	-2.772368000
C	-2.865100000	-2.165237000	1.153132000
C	-2.070677000	-2.153031000	-1.139827000
H	-1.445645000	-2.180473000	-3.212963000
C	-3.811788000	-2.920168000	0.211442000
C	-3.330118000	-2.900947000	-1.113301000
C	-4.981055000	-3.618294000	0.505936000
C	-4.022479000	-3.540787000	-2.143131000

C	-5.677786000	-4.257997000	-0.525634000
H	-5.354539000	-3.681857000	1.522696000
C	-5.205705000	-4.215509000	-1.840923000
H	-3.646601000	-3.521917000	-3.162282000
H	-6.593074000	-4.797092000	-0.299644000
H	-5.757846000	-4.718228000	-2.629353000
N	1.363038000	0.176862000	-0.435487000
C	-3.515917000	-0.891687000	1.778337000
H	-2.722765000	-0.319195000	2.272963000
H	-3.868366000	-0.260057000	0.954807000
C	-4.661610000	-1.106795000	2.772136000
H	-5.529215000	-1.574174000	2.299188000
H	-4.363010000	-1.726286000	3.623788000
H	-4.989757000	-0.141633000	3.171001000
C	-2.334127000	-3.164255000	2.228193000
H	-1.878961000	-4.009776000	1.699433000
H	-3.203387000	-3.576140000	2.753673000
C	-1.341595000	-2.624381000	3.262925000
H	-1.100050000	-3.408908000	3.987214000
H	-0.400514000	-2.310624000	2.803607000
H	-1.745528000	-1.776441000	3.824951000
C	0.236564000	2.472111000	-0.263588000
C	0.355406000	3.670962000	0.465233000
C	-0.943172000	2.253193000	-0.994604000
C	-0.668672000	4.610646000	0.480669000
H	1.271225000	3.852547000	1.015633000
C	-1.975791000	3.189890000	-0.984275000

H	-1.063682000	1.360867000	-1.594444000
C	-1.833745000	4.359096000	-0.242948000
H	-0.566478000	5.527297000	1.050188000
H	-2.879384000	3.013049000	-1.556300000
C	1.391075000	1.557624000	-0.235510000
N	2.614830000	1.986222000	0.016143000
Br	-3.252903000	5.640326000	-0.221439000

PhPh

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symmetry c1

Atomic Type	**Coordinates (Angstroms) X**	**Y**	**Z**
C	-5.158956880	0.336261200	0.015267290
C	-3.803038490	0.285808710	-0.028544030
C	-3.068420010	1.474597710	-0.040031560
C	-3.728335900	2.712157000	0.000066600
C	-5.126573190	2.739756080	0.041979940
C	-5.826814100	1.574888570	0.049240750
C	-1.676414320	1.481575030	-0.090961140
C	-2.977970090	3.914448890	0.000056960
C	-1.576317100	3.865355920	-0.040050740
C	-0.971008680	2.611828390	-0.090970200
C	-0.831162500	5.047569380	-0.028582230
H	0.237874610	5.010415510	-0.054644710
C	-1.472206180	6.243447260	0.015219910
C	-2.878307700	6.299204730	0.049202860

C	-3.617076980	5.158383150	0.041960540
H	-5.724174180	-0.572230110	0.023808510
H	-3.299982120	-0.658201580	-0.054599250
H	-5.643635090	3.676148220	0.068752510
H	-6.896046060	1.599621060	0.081354680
H	-0.904421320	7.150336260	0.023746570
H	-3.370291320	7.248847440	0.081309370
H	-4.685423890	5.211465440	0.068740190
C	-0.591967150	-0.715293280	-0.277266230
C	0.708075860	-1.231059250	-0.387624060
C	-1.702727980	-1.544081380	-0.404295150
C	0.867002780	-2.582759530	-0.626212100
H	1.577809870	-0.567283450	-0.285312700
C	-1.552676520	-2.916646310	-0.646499530
H	-2.714030770	-1.120695590	-0.314282420
C	2.130003420	-3.383672990	-0.785942040
C	-0.272996970	-3.434411920	-0.757123110
H	-2.434403690	-3.565114620	-0.745890780
C	1.625831490	-4.780860580	-1.022128840
C	0.197043520	-4.795968310	-1.002382300
C	2.335938540	-5.946586550	-1.236850980
C	-0.495374710	-5.979227140	-1.198128010
C	1.626122790	-7.140550150	-1.434172150
H	3.434673690	-5.946162410	-1.253932870
C	0.234646730	-7.156136580	-1.415030480
H	-1.594125440	-5.998951480	-1.184443230
H	2.181296020	-8.074536940	-1.606002840

H	-0.303789950	-8.102514530	-1.571711760
N	-0.730217790	0.359416710	-0.087620200
C	3.001025120	-3.311403850	0.482008430
H	3.397835520	-2.323189410	0.586285610
H	2.404819150	-3.548541600	1.338281820
C	4.159027020	-4.320123670	0.367483670
H	3.849084630	-5.265237490	0.761939730
H	4.431664020	-4.434909390	-0.660812640
H	5.000917840	-3.961087580	0.921751600
C	2.962404410	-2.881217080	-1.980197730
H	2.315320640	-2.689682710	-2.810557400
H	3.681115840	-3.625702490	-2.252402370
C	3.691714800	-1.582925390	-1.587584660
H	4.746433270	-1.715405160	-1.709724170
H	3.357795340	-0.782694020	-2.214503760
H	3.477644210	-1.348617540	-0.565736520
C	0.891559820	0.849823700	1.610276610
C	2.254931020	0.565327640	1.684456970
C	0.142645080	0.985670800	2.779844400
C	2.870279850	0.417723610	2.927851640
H	2.845440210	0.458580510	0.762965940
C	0.757816900	0.837619680	4.022897700
H	-0.932322040	1.209929000	2.721105330
C	2.121816230	0.554012630	4.096943440
H	3.945284110	0.193864490	2.986124880
H	0.167854960	0.944615760	4.944836410
H	2.606610640	0.437533310	5.077012800

C	0.406594350	0.966801390	0.630265780
N	0.452755220	2.254864020	-0.087635400

PhNp

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symmetry c1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.308689000	-4.055004000	-1.091459000
C	1.897557000	-2.766094000	-0.805123000
C	2.824997000	-1.764957000	-0.435050000
C	4.217780000	-2.100403000	-0.335655000
C	4.592130000	-3.427726000	-0.641484000
C	3.668448000	-4.387877000	-1.014682000
C	2.471070000	-0.405809000	-0.118879000
C	5.211956000	-1.104452000	0.085057000
C	4.798265000	0.212930000	0.430633000
C	3.402849000	0.525969000	0.322741000
C	5.736525000	1.174863000	0.856111000
H	5.373994000	2.165484000	1.109364000
C	7.078243000	0.854553000	0.939222000
C	7.506618000	-0.439334000	0.595197000
C	6.593475000	-1.392965000	0.178959000
H	1.575325000	-4.805308000	-1.371956000
H	0.845045000	-2.524133000	-0.859741000
H	5.634442000	-3.716284000	-0.577253000
H	3.999209000	-5.397422000	-1.239704000
H	7.798990000	1.598544000	1.265765000

H	8.560237000	-0.696283000	0.654770000
H	6.962745000	-2.378655000	-0.079174000
C	-0.056733000	-0.211618000	-0.433480000
C	-0.981319000	-0.426996000	0.596951000
C	-0.404234000	-0.442786000	-1.769550000
C	-2.255015000	-0.889369000	0.281780000
H	-0.684271000	-0.218036000	1.617823000
C	-1.682322000	-0.896114000	-2.090450000
H	0.331092000	-0.266427000	-2.547164000
C	-3.442247000	-1.166027000	1.211848000
C	-2.606626000	-1.109393000	-1.065551000
H	-1.952485000	-1.063551000	-3.128759000
C	-4.512688000	-1.583717000	0.195345000
C	-4.004934000	-1.543340000	-1.119286000
C	-5.818502000	-2.017554000	0.413593000
C	-4.799877000	-1.897954000	-2.210792000
C	-6.617555000	-2.371149000	-0.679906000
H	-6.222479000	-2.095270000	1.417748000
C	-6.114362000	-2.306825000	-1.982548000
H	-4.403548000	-1.863832000	-3.221771000
H	-7.637930000	-2.703465000	-0.512657000
H	-6.746844000	-2.585722000	-2.820155000
N	1.251964000	0.277833000	-0.109211000
C	-3.798159000	0.158828000	1.956607000
H	-2.906005000	0.487044000	2.502404000
H	-3.978786000	0.927631000	1.196730000
C	-4.984475000	0.120711000	2.925111000

H	-5.924704000	-0.092465000	2.409802000
H	-4.853456000	-0.625150000	3.715662000
H	-5.095080000	1.094902000	3.412402000
C	-3.189231000	-2.359481000	2.184303000
H	-2.929338000	-3.233697000	1.576147000
H	-4.144445000	-2.604353000	2.663076000
C	-2.126919000	-2.170056000	3.272092000
H	-2.097532000	-3.053473000	3.918099000
H	-1.125956000	-2.046848000	2.850282000
H	-2.335149000	-1.306441000	3.911676000
C	1.530968000	1.563786000	0.352624000
N	2.808296000	1.730949000	0.617075000
C	0.489618000	2.600181000	0.560701000
C	-0.153317000	3.255763000	-0.538583000
C	0.173241000	2.962769000	1.857208000
C	0.188444000	3.000645000	-1.894263000
C	-1.160904000	4.238351000	-0.261792000
C	-0.812059000	3.940021000	2.124087000
H	0.693449000	2.482262000	2.679832000
C	-0.448862000	3.658115000	-2.922125000
H	0.979515000	2.291048000	-2.111490000
C	-1.806923000	4.889630000	-1.347198000
C	-1.474689000	4.553383000	1.086811000
H	-1.043611000	4.198669000	3.152919000
C	-1.464088000	4.605416000	-2.648551000
H	-0.167258000	3.454781000	-3.951113000
H	-2.574303000	5.627423000	-1.127837000

H	-2.239421000	5.300029000	1.284308000
H	-1.962269000	5.114068000	-3.468535000

PhAn

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symmetry c1

C	-1.883826000	-4.342945000	1.196670000
C	-1.597849000	-3.012605000	0.949923000
C	-2.600355000	-2.118704000	0.508614000
C	-3.939790000	-2.598141000	0.318331000
C	-4.185033000	-3.964117000	0.581948000
C	-3.188035000	-4.823120000	1.009819000
C	-2.376064000	-0.725443000	0.231252000
C	-5.011625000	-1.698931000	-0.130379000
C	-4.732995000	-0.325352000	-0.382478000
C	-3.386838000	0.130690000	-0.188616000
C	-5.751480000	0.549818000	-0.810622000
H	-5.491550000	1.587680000	-0.990240000
C	-7.040754000	0.087042000	-0.993577000
C	-7.334790000	-1.265847000	-0.750507000
C	-6.342479000	-2.134543000	-0.329439000
H	-1.097184000	-5.010463000	1.535831000
H	-0.589598000	-2.650230000	1.100533000
H	-5.183744000	-4.362730000	0.449389000
H	-3.419894000	-5.866550000	1.201497000
H	-7.823197000	0.764181000	-1.323569000
H	-8.345995000	-1.635837000	-0.892821000
H	-6.608329000	-3.170238000	-0.152623000

C	0.103442000	-0.296453000	0.660676000
C	0.970814000	-0.788798000	-0.323737000
C	0.527563000	-0.146140000	1.984688000
C	2.265711000	-1.149515000	0.032486000
H	0.614794000	-0.864787000	-1.344333000
C	1.832256000	-0.485529000	2.341194000
H	-0.163982000	0.246923000	2.721901000
C	3.401833000	-1.674593000	-0.852471000
C	2.697663000	-0.982075000	1.364622000
H	2.165408000	-0.352508000	3.366104000
C	4.535130000	-1.793271000	0.174680000
C	4.103653000	-1.385401000	1.453502000
C	5.833047000	-2.271738000	0.008625000
C	4.965903000	-1.420507000	2.550922000
C	6.699257000	-2.305817000	1.107593000
H	6.179718000	-2.627408000	-0.956202000
C	6.271221000	-1.878546000	2.367954000
H	4.628177000	-1.103740000	3.533733000
H	7.713432000	-2.672656000	0.979222000
H	6.955374000	-1.912133000	3.210696000
N	-1.235087000	0.075122000	0.296320000
C	3.694246000	-0.609055000	-1.955656000
H	2.765788000	-0.434898000	-2.511320000
H	3.916115000	0.337773000	-1.450411000
C	4.815415000	-0.922560000	-2.951272000
H	5.789258000	-0.996134000	-2.459995000
H	4.638781000	-1.854800000	-3.497281000

H	4.885636000	-0.119804000	-3.692451000
C	3.110851000	-3.090609000	-1.438206000
H	2.903592000	-3.762045000	-0.596747000
H	4.039261000	-3.459013000	-1.889825000
C	1.980253000	-3.209313000	-2.465586000
H	1.932238000	-4.234871000	-2.845799000
H	1.004417000	-2.982858000	-2.027884000
H	2.128819000	-2.549860000	-3.326693000
C	-1.632023000	1.353079000	-0.087371000
N	-2.913442000	1.409261000	-0.380760000
C	-0.678970000	2.491875000	-0.146523000
C	-0.520166000	3.328014000	0.979953000
C	0.056500000	2.726202000	-1.328655000
C	-1.281868000	3.156484000	2.179767000
C	0.443381000	4.403042000	0.934162000
C	1.019212000	3.802198000	-1.363041000
C	-0.116241000	1.939372000	-2.511837000
C	-1.094058000	3.978160000	3.260031000
H	-2.036138000	2.377564000	2.211459000
C	0.609840000	5.233926000	2.086048000
C	1.190875000	4.604297000	-0.230435000
C	1.773622000	4.019367000	-2.558341000
H	-0.868914000	1.158127000	-2.513140000
C	0.623053000	2.184797000	-3.639542000
C	-0.132308000	5.028355000	3.217510000
H	-1.689335000	3.836016000	4.157207000
H	1.340151000	6.037496000	2.040577000

H	1.921424000	5.409578000	-0.258040000
C	1.586982000	3.233763000	-3.663595000
H	2.498176000	4.829329000	-2.570261000
H	0.466299000	1.583425000	-4.530283000
H	0.002068000	5.667964000	4.084701000
H	2.163589000	3.411973000	-4.566345000

Table ST7: Computed Vertical Transitions and Their Oscillator Strengths and Configurations

PICRIC ACID

PhBr + PA

Excited State 1: Triplet-A 2.5401 eV 488.11 nm f=0.0000 <S**2>=2.000
211 -> 212 0.68551
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -5067.72536279
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.8326 eV 437.70 nm f=0.0000 <S**2>=2.000
196 -> 212 -0.20715
196 -> 214 0.16363
196 -> 216 -0.35348
196 -> 226 -0.11001
197 -> 212 0.12234
197 -> 214 -0.12714
197 -> 216 0.26602
198 -> 216 0.12677
207 -> 212 0.19185
207 -> 216 0.18828
211 -> 216 0.14170

Excited State 3: Triplet-A 2.8878 eV 429.33 nm f=0.0000 <S**2>=2.000
191 -> 212 -0.16173
196 -> 216 0.16486
197 -> 212 -0.12217
201 -> 212 -0.10017
206 -> 212 0.20733
207 -> 212 0.13591
211 -> 214 0.28925
211 -> 216 0.42400

Excited State 4: Singlet-A 3.1808 eV 389.79 nm f=0.1020 <S**2>=0.000
211 -> 212 0.69499

Excited State 5: Singlet-A 3.5113 eV 353.10 nm f=0.0044 <S**2>=0.000

207 -> 212 0.19099
210 -> 212 0.67372

Excited State 6: Singlet-A 3.5555 eV 348.71 nm f=0.0066 <S**2>=0.000
201 -> 212 -0.14115
201 -> 216 0.12108
207 -> 212 0.60652
210 -> 212 -0.20476

PhPh+ PA

Excited State 1: Triplet-A 2.6659 eV 465.08 nm f=0.0000 <S**2>=2.000
193 -> 195 -0.13307
194 -> 195 0.64833
194 -> 196 -0.15877
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2496.61994852
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.8379 eV 436.88 nm f=0.0000 <S**2>=2.000
176 -> 199 0.10698
178 -> 199 -0.17528
179 -> 195 -0.28006
179 -> 196 0.11227
179 -> 198 0.11923
179 -> 199 0.36403
180 -> 195 0.12325
180 -> 199 -0.18012
190 -> 195 0.20396
190 -> 199 -0.16525

Excited State 3: Triplet-A 2.8454 eV 435.74 nm f=0.0000 <S**2>=2.000
192 -> 200 -0.20527
192 -> 201 -0.16321
192 -> 202 -0.11974
193 -> 195 0.18973
193 -> 196 0.40530
193 -> 197 -0.10101
193 -> 200 -0.25804
193 -> 201 0.18475
194 -> 196 0.13126

Excited State 4: Singlet-A 3.3003 eV 375.67 nm f=0.0993 <S**2>=0.000
193 -> 195 -0.11293
194 -> 195 0.67956

Excited State 5: Singlet-A 3.5331 eV 350.92 nm f=0.0269 <S**2>=0.000
190 -> 195 -0.15307
193 -> 195 0.65373

194 -> 195 0.12713
194 -> 196 0.10623

Excited State 6: Singlet-A 3.5558 eV 348.69 nm f=0.0047 <S**2>=0.000
193 -> 195 -0.13504
194 -> 196 0.66160
194 -> 197 -0.16841

PhNp+ PA

Excited State 1: Triplet-A 2.6037 eV 476.19 nm f=0.0000 <S**2>=2.000
207 -> 208 0.68571
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2650.26442603
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.6805 eV 462.54 nm f=0.0000 <S**2>=2.000
200 -> 217 0.14814
203 -> 209 0.14908
204 -> 209 -0.13794
205 -> 209 0.53790
205 -> 211 -0.31990

Excited State 3: Triplet-A 2.8244 eV 438.97 nm f=0.0000 <S**2>=2.000
190 -> 212 0.14603
192 -> 208 -0.18477
192 -> 210 -0.10113
192 -> 212 -0.30239
193 -> 208 -0.17683
193 -> 210 -0.10374
193 -> 212 -0.30918
194 -> 208 -0.11973
194 -> 212 -0.21065
202 -> 208 0.17445
202 -> 212 0.20546

Excited State 4: Singlet-A 3.2646 eV 379.78 nm f=0.1116 <S**2>=0.000
207 -> 208 0.69469

Excited State 5: Singlet-A 3.5685 eV 347.44 nm f=0.0060 <S**2>=0.000
193 -> 208 0.10498
196 -> 208 -0.17593
196 -> 212 0.14493
202 -> 208 0.61096
205 -> 208 0.14774

Excited State 6: Singlet-A 3.5868 eV 345.67 nm f=0.0011 <S**2>=0.000
206 -> 208 0.70300

PhAn+ PA

Excited State 1: Triplet-A 1.7725 eV 699.48 nm f=0.0000 <S**2>=2.000
220 -> 221 0.69535
220 <- 221 0.13299
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2803.93438907
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.6045 eV 476.05 nm f=0.0000 <S**2>=2.000
219 -> 222 0.68284

Excited State 3: Triplet-A 2.8239 eV 439.06 nm f=0.0000 <S**2>=2.000
202 -> 225 0.13440
204 -> 222 -0.17321
204 -> 225 -0.25144
204 -> 226 0.13878
205 -> 222 -0.15502
205 -> 225 -0.23880
205 -> 226 0.13178
206 -> 222 -0.15982
206 -> 225 -0.24889
206 -> 226 0.13739
215 -> 222 0.17420
215 -> 225 0.18204
215 -> 226 -0.10015

Excited State 4: Singlet-A 3.1595 eV 392.41 nm f=0.0861 <S**2>=0.000
219 -> 221 -0.23248
220 -> 221 0.65913

Excited State 5: Singlet-A 3.1897 eV 388.71 nm f=0.0167 <S**2>=0.000
219 -> 221 0.66720
220 -> 221 0.22878

Excited State 6: Singlet-A 3.2088 eV 386.39 nm f=0.0181 <S**2>=0.000
219 -> 222 -0.17544
220 -> 222 0.67977

Optimized Cartesian coordinates and energies of luminophores:

Table ST8: Optimized Cartesian coordinates:

PhBr + PA

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symmetry c1

C	0.377502000	5.049899000	0.023053000
C	1.230537000	3.912233000	-0.154825000
C	3.199308000	5.315339000	0.115630000
C	2.375984000	6.436691000	0.286819000
C	1.000367000	6.298659000	0.242630000
H	4.279356000	5.416234000	0.156480000
H	2.813823000	7.414908000	0.459834000
H	0.391165000	7.181465000	0.390139000
C	0.566032000	2.649673000	-0.352229000
C	-0.812395000	2.527088000	-0.317302000
C	-1.698959000	3.647054000	-0.189913000
C	-3.100474000	3.518452000	-0.266109000
C	-1.085274000	4.922894000	-0.021289000
C	-3.903515000	4.639108000	-0.163246000
H	-3.550729000	2.546855000	-0.436853000
C	-1.944584000	6.039156000	0.086742000
C	-3.320813000	5.902507000	0.020995000
H	-4.980365000	4.531889000	-0.240979000
H	-1.532607000	7.033000000	0.211423000
H	-3.949511000	6.784214000	0.101125000
C	0.012612000	0.490031000	-0.612940000
N	1.064274000	1.354179000	-0.557812000
N	-1.116532000	1.186718000	-0.464718000
C	-4.566839000	-0.211640000	-0.056060000
C	-5.931769000	-0.137574000	-0.557722000
C	-6.966607000	-0.910615000	-0.079167000
C	-6.741308000	-1.778453000	0.994323000

C	-5.486761000	-1.867444000	1.585750000
C	-4.449235000	-1.086170000	1.103445000
H	-7.949741000	-0.840737000	-0.526111000
H	-5.323909000	-2.531792000	2.424245000
O	-3.606980000	0.356869000	-0.633780000
H	-2.091086000	0.759844000	-0.431644000
N	-3.184214000	-1.188612000	1.793242000
N	-6.257855000	0.797416000	-1.634047000
N	-7.835998000	-2.580834000	1.511179000
O	-2.905141000	-2.245550000	2.371800000
O	-7.158703000	0.477541000	-2.413732000
O	-8.938027000	-2.467962000	0.967359000
O	-7.601189000	-3.330513000	2.463505000
O	-5.648363000	1.866735000	-1.682786000
O	-2.428287000	-0.205556000	1.781712000
C	2.442163000	0.938211000	-0.663136000
C	4.448393000	0.712174000	-1.982831000
C	4.386706000	-0.053068000	0.337772000
C	5.073543000	0.118704000	-0.883275000
H	4.977630000	0.844237000	-2.921385000
C	5.275312000	-0.747182000	1.375572000
C	6.425660000	-0.424677000	-0.738863000
C	6.565511000	-0.934268000	0.567836000
C	7.480693000	-0.472773000	-1.652250000
C	7.789635000	-1.466105000	0.968248000
C	8.693711000	-1.030034000	-1.248110000
H	7.365880000	-0.079013000	-2.658207000

C	8.847287000	-1.517542000	0.053579000
H	7.938486000	-1.832040000	1.978656000
H	9.525707000	-1.077379000	-1.944058000
H	9.800272000	-1.937677000	0.360989000
C	5.586613000	0.157273000	2.608880000
H	6.035916000	1.085216000	2.236265000
H	6.371827000	-0.339567000	3.189690000
C	4.602751000	-2.100333000	1.769527000
H	3.604566000	-1.876503000	2.163428000
H	4.438434000	-2.670598000	0.848041000
C	4.423027000	0.499982000	3.544814000
H	3.934076000	-0.392514000	3.947275000
H	4.793427000	1.078909000	4.396673000
H	3.662574000	1.110497000	3.050190000
C	5.344498000	-2.981101000	2.779536000
H	6.303830000	-3.330318000	2.389162000
H	5.528988000	-2.464289000	3.726538000
H	4.743772000	-3.867818000	3.004732000
C	3.122170000	1.126303000	-1.869239000
H	2.612889000	1.595559000	-2.704879000
C	2.633106000	4.072520000	-0.100083000
H	3.277920000	3.213355000	-0.219046000
C	3.058024000	0.344629000	0.444415000
H	2.486654000	0.200719000	1.354270000
C	0.114725000	-0.966572000	-0.821321000
C	0.642159000	-1.472588000	-2.019408000
C	-0.321249000	-1.853736000	0.173463000

C	0.729984000	-2.846184000	-2.224594000
C	-0.238514000	-3.229956000	-0.029118000
C	0.288178000	-3.713400000	-1.225093000
Br	0.408478000	-5.595261000	-1.505558000
H	1.129423000	-3.240089000	-3.151673000
H	-0.725763000	-1.472465000	1.104190000
H	0.973440000	-0.795315000	-2.799059000
H	-0.584654000	-3.912230000	0.738115000

PhPh+ PA

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symmetry c1

C	0.762380000	4.381939000	0.281321000
C	1.493174000	3.200580000	-0.076965000
C	3.595230000	4.406339000	0.158117000
C	2.893104000	5.559583000	0.533970000
C	1.511109000	5.540206000	0.586949000
H	4.679083000	4.418727000	0.098357000
H	3.429127000	6.472160000	0.775680000
H	0.996062000	6.450234000	0.867806000
C	0.702660000	2.030504000	-0.361724000
C	-0.680165000	2.058588000	-0.345183000
C	-1.446682000	3.227396000	-0.032901000
C	-2.856268000	3.239133000	-0.066019000
C	-0.706370000	4.396875000	0.305642000
C	-3.543118000	4.396172000	0.251066000
H	-3.405805000	2.348845000	-0.353929000
C	-1.449751000	5.553209000	0.633011000

C	-2.834187000	5.553839000	0.609545000
H	-4.627485000	4.399722000	0.213700000
H	-0.940592000	6.469772000	0.904655000
H	-3.371836000	6.462458000	0.863518000
C	-0.221765000	-1.402687000	-1.326973000
C	-1.293195000	-1.727755000	-2.179878000
C	0.644301000	-2.419823000	-0.892603000
C	-1.481649000	-3.042214000	-2.596405000
H	-1.978937000	-0.953996000	-2.506531000
C	0.446397000	-3.731370000	-1.315101000
H	1.452551000	-2.195397000	-0.208762000
C	-0.611335000	-4.046439000	-2.169311000
H	1.114066000	-4.511621000	-0.963800000
C	-0.085328000	-0.007091000	-0.897193000
N	1.059075000	0.714812000	-0.707802000
N	-1.128373000	0.799511000	-0.679808000
C	-4.547136000	-0.519243000	-0.161049000
C	-5.955700000	-0.284592000	-0.444275000
C	-6.978930000	-1.075510000	0.030912000
C	-6.681837000	-2.135884000	0.890718000
C	-5.370068000	-2.400159000	1.266672000
C	-4.339983000	-1.610684000	0.780569000
H	-8.003136000	-0.871827000	-0.252701000
H	-5.149884000	-3.216559000	1.941284000
O	-3.639964000	0.121704000	-0.754937000
H	-2.135000000	0.447359000	-0.613054000
N	-3.006936000	-1.931095000	1.266732000

N	-6.348059000	0.845753000	-1.286967000
N	-7.758067000	-2.961044000	1.411416000
O	-2.809853000	-3.057845000	1.730591000
O	-7.355959000	0.710341000	-1.985819000
O	-8.910506000	-2.689730000	1.062283000
O	-7.459478000	-3.887073000	2.170996000
O	-5.683356000	1.881063000	-1.229214000
O	-2.136641000	-1.053338000	1.223377000
H	-2.310746000	-3.280475000	-3.254978000
H	-0.762209000	-5.071578000	-2.493141000
C	2.393877000	0.192997000	-0.865377000
C	4.205705000	-0.488443000	-2.303358000
C	4.419448000	-0.635649000	0.127126000
C	4.947405000	-0.824858000	-1.169291000
H	4.613154000	-0.632102000	-3.299197000
C	5.415071000	-1.093050000	1.198664000
C	6.287599000	-1.402615000	-1.046778000
C	6.579863000	-1.569974000	0.321981000
C	7.211759000	-1.753443000	-2.032929000
C	7.826845000	-2.062986000	0.701005000
C	8.447332000	-2.269452000	-1.642391000
H	6.979615000	-1.622950000	-3.086103000
C	8.753259000	-2.417572000	-0.285925000
H	8.094253000	-2.167111000	1.747239000
H	9.178831000	-2.548840000	-2.394500000
H	9.723288000	-2.808301000	0.006631000
C	5.917840000	0.082226000	2.094795000

H	6.352409000	0.841552000	1.434168000
H	6.751083000	-0.298018000	2.696445000
C	4.758862000	-2.244953000	2.023149000
H	3.829768000	-1.858603000	2.458255000
H	4.457005000	-3.027804000	1.317379000
C	4.898030000	0.747062000	3.025184000
H	4.420337000	0.030997000	3.701144000
H	5.400026000	1.494578000	3.647576000
H	4.113434000	1.268756000	2.470355000
C	5.598565000	-2.874067000	3.139077000
H	6.486489000	-3.376916000	2.747515000
H	5.922318000	-2.137904000	3.881417000
H	5.004640000	-3.627290000	3.666147000
C	2.921099000	0.032890000	-2.147692000
H	2.324052000	0.306785000	-3.011018000
C	2.904298000	3.247017000	-0.143316000
H	3.457752000	2.368584000	-0.442232000
C	3.127799000	-0.144610000	0.280102000
H	2.671609000	-0.018361000	1.255833000

PhNp+ PA

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symmetry c1

C	-0.273853000	4.683838000	-0.632010000
C	-1.154828000	3.607249000	-0.287210000
C	-3.077857000	4.920651000	-0.987832000
C	-2.227680000	5.982503000	-1.326555000
C	-0.860969000	5.858920000	-1.151612000

H	-4.150522000	5.010599000	-1.128218000
H	-2.637628000	6.902936000	-1.730718000
H	-0.230479000	6.693633000	-1.431221000
C	-0.526834000	2.415530000	0.220770000
C	0.846996000	2.297338000	0.333946000
C	1.758109000	3.362693000	0.037491000
C	3.148656000	3.251673000	0.243960000
C	1.180183000	4.570331000	-0.451381000
C	3.975911000	4.321526000	-0.042760000
H	3.565058000	2.335214000	0.648380000
C	2.064103000	5.635327000	-0.736329000
C	3.429194000	5.514877000	-0.540697000
H	5.044321000	4.235248000	0.126643000
H	1.679701000	6.577254000	-1.107952000
H	4.077782000	6.355832000	-0.766816000
C	-0.019956000	0.369986000	0.988693000
N	-1.054938000	1.188773000	0.649603000
N	1.122510000	1.028114000	0.801297000
C	4.448359000	-0.488452000	0.387012000
C	5.787513000	-0.594844000	0.947753000
C	6.794166000	-1.354848000	0.398357000
C	6.568789000	-2.015250000	-0.814783000
C	5.348535000	-1.904622000	-1.468520000
C	4.331782000	-1.144694000	-0.908574000
H	7.753486000	-1.432036000	0.893279000
H	5.191022000	-2.400668000	-2.416826000
O	3.514969000	0.057658000	1.028983000

H	2.094165000	0.573156000	0.840006000
N	3.114077000	-1.030392000	-1.685224000
N	6.111049000	0.140333000	2.171532000
N	7.632025000	-2.805442000	-1.409954000
O	2.884450000	-1.877641000	-2.554809000
O	6.918792000	-0.375811000	2.948720000
O	8.706836000	-2.869610000	-0.806281000
O	7.400965000	-3.369343000	-2.483621000
O	5.596300000	1.245631000	2.337621000
O	2.362316000	-0.070892000	-1.461894000
C	-2.441090000	0.807553000	0.776910000
C	-4.491369000	0.829981000	2.046647000
C	-4.360392000	-0.341591000	-0.094021000
C	-5.085603000	0.050466000	1.051061000
H	-5.049416000	1.129290000	2.928403000
C	-5.217186000	-1.215020000	-1.016387000
C	-6.436739000	-0.507846000	0.961135000
C	-6.536157000	-1.248043000	-0.234413000
C	-7.522863000	-0.386556000	1.830110000
C	-7.750094000	-1.842183000	-0.573367000
C	-8.726006000	-1.006328000	1.492396000
H	-7.439258000	0.184648000	2.750407000
C	-8.839103000	-1.723594000	0.297347000
H	-7.866981000	-2.386329000	-1.504680000
H	-9.581721000	-0.923716000	2.155613000
H	-9.784527000	-2.190975000	0.038456000
C	-5.478532000	-0.557041000	-2.406978000

H	-5.936303000	0.423392000	-2.230683000
H	-6.244590000	-1.154558000	-2.914078000
C	-4.540670000	-2.618456000	-1.125620000
H	-3.524833000	-2.475055000	-1.511058000
H	-4.418738000	-3.007661000	-0.108296000
C	-4.279394000	-0.392462000	-3.346377000
H	-3.778753000	-1.343098000	-3.554264000
H	-4.615097000	0.014548000	-4.305437000
H	-3.535875000	0.302472000	-2.946689000
C	-5.250244000	-3.670375000	-1.983587000
H	-6.228581000	-3.938265000	-1.576105000
H	-5.390732000	-3.339371000	-3.017418000
H	-4.649633000	-4.584935000	-2.014105000
C	-3.158132000	1.211525000	1.905994000
H	-2.670337000	1.816504000	2.663228000
C	-2.547111000	3.750651000	-0.476721000
H	-3.209850000	2.933864000	-0.226377000
C	-3.025459000	0.026281000	-0.225894000
H	-2.424288000	-0.287234000	-1.071031000
C	-0.163887000	-0.992486000	1.549510000
C	-0.296508000	-1.119257000	2.920430000
C	-0.189604000	-2.147233000	0.703218000
C	-0.479180000	-2.386931000	3.514945000
C	-0.390426000	-3.428121000	1.316998000
C	-0.008729000	-2.084950000	-0.704902000
C	-0.534131000	-3.512574000	2.726930000
C	-0.428501000	-4.587038000	0.495980000

H	0.217668000	-1.136186000	-1.179735000
C	-0.034355000	-3.232138000	-1.467459000
H	-0.680631000	-4.490738000	3.176965000
C	-0.258093000	-4.493345000	-0.865765000
H	-0.583183000	-5.553245000	0.968419000
H	0.146725000	-3.165882000	-2.535014000
H	-0.275595000	-5.387701000	-1.480980000
H	-0.259886000	-0.233787000	3.547423000
H	-0.577124000	-2.462520000	4.592924000

PhAn+ PA

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symmetry c1

C	0.318287000	4.773876000	0.429000000
C	1.177631000	3.660282000	0.154196000
C	3.135590000	5.013463000	0.653612000
C	2.306255000	6.109211000	0.930307000
C	0.933037000	5.984653000	0.818436000
H	4.213764000	5.106105000	0.739505000
H	2.737781000	7.058073000	1.233735000
H	0.319773000	6.848527000	1.042206000
C	0.522538000	2.434340000	-0.220816000
C	-0.855040000	2.328145000	-0.297667000
C	-1.745724000	3.427278000	-0.070479000
C	-3.142558000	3.317842000	-0.230422000
C	-1.141727000	4.663056000	0.302872000
C	-3.950218000	4.417724000	-0.008967000

H	-3.579268000	2.376410000	-0.546451000
C	-2.006269000	5.758423000	0.525460000
C	-3.377433000	5.639985000	0.377013000
H	-5.023879000	4.331871000	-0.141405000
H	-1.602009000	6.721824000	0.810964000
H	-4.010730000	6.504275000	0.552934000
C	-0.027403000	0.336802000	-0.797232000
N	1.024561000	1.166143000	-0.546930000
N	-1.156936000	1.028190000	-0.650293000
C	-4.485983000	-0.414067000	-0.041660000
C	-5.833074000	-0.576492000	-0.569204000
C	-6.826521000	-1.288450000	0.062302000
C	-6.578591000	-1.835972000	1.326241000
C	-5.349098000	-1.661300000	1.947928000
C	-4.345515000	-0.950424000	1.305850000
H	-7.792847000	-1.414206000	-0.408422000
H	-5.174152000	-2.068914000	2.934525000
O	-3.566162000	0.076630000	-0.744856000
H	-2.135248000	0.586419000	-0.631989000
N	-3.117307000	-0.760039000	2.050683000
N	-6.179939000	0.044206000	-1.848847000
N	-7.627794000	-2.573965000	2.006909000
O	-2.870520000	-1.522862000	2.990850000
O	-6.997801000	-0.542768000	-2.562759000
O	-8.711578000	-2.696858000	1.428815000
O	-7.376944000	-3.038064000	3.123134000
O	-5.673384000	1.131653000	-2.122146000

O	-2.374651000	0.178601000	1.729702000
C	2.403433000	0.742641000	-0.618721000
C	4.436498000	0.486989000	-1.889272000
C	4.324359000	-0.228335000	0.444777000
C	5.037931000	-0.080861000	-0.763806000
H	4.984477000	0.595290000	-2.820080000
C	5.186845000	-0.906336000	1.514530000
C	6.386358000	-0.622013000	-0.577871000
C	6.495837000	-1.107572000	0.740978000
C	7.462415000	-0.687804000	-1.465121000
C	7.709867000	-1.632529000	1.179322000
C	8.665565000	-1.237803000	-1.022702000
H	7.370993000	-0.312784000	-2.480601000
C	8.788789000	-1.701226000	0.290845000
H	7.834590000	-1.979654000	2.199681000
H	9.513471000	-1.297987000	-1.698277000
H	9.734206000	-2.115622000	0.628169000
C	5.469311000	0.015677000	2.741217000
H	5.933360000	0.935538000	2.366472000
H	6.235807000	-0.475183000	3.351615000
C	4.503467000	-2.253525000	1.911043000
H	3.491541000	-2.027825000	2.266242000
H	4.370460000	-2.839850000	0.994648000
C	4.281735000	0.379162000	3.638452000
H	3.773731000	-0.504724000	4.036396000
H	4.631272000	0.965664000	4.494037000
H	3.541379000	0.988984000	3.113608000

C	5.214682000	-3.114763000	2.959185000
H	6.188564000	-3.465244000	2.607528000
H	5.364873000	-2.582501000	3.903774000
H	4.610456000	-4.000853000	3.178025000
C	3.108500000	0.904837000	-1.813309000
H	2.613927000	1.342064000	-2.673757000
C	2.577515000	3.807361000	0.271831000
H	3.224881000	2.966715000	0.064160000
C	2.994035000	0.170553000	0.513883000
H	2.400560000	0.038138000	1.410694000
C	0.093823000	-1.072701000	-1.231171000
C	0.174632000	-1.342746000	-2.617014000
C	0.161348000	-2.106388000	-0.270212000
C	0.067352000	-0.328365000	-3.620225000
C	0.373795000	-2.705226000	-3.050045000
C	0.365459000	-3.462721000	-0.723156000
C	0.016427000	-1.878074000	1.134186000
C	0.157270000	-0.639262000	-4.952109000
H	-0.113743000	0.699018000	-3.321575000
C	0.466233000	-2.983893000	-4.448929000
C	0.473604000	-3.720028000	-2.093055000
C	0.444880000	-4.512990000	0.243483000
H	-0.216710000	-0.882529000	1.495845000
C	0.077370000	-2.918538000	2.025450000
C	0.363410000	-1.982545000	-5.376122000
H	0.059933000	0.145828000	-5.695785000
H	0.615431000	-4.014255000	-4.759593000

H	0.630841000	-4.743339000	-2.425721000
C	0.308438000	-4.251115000	1.579861000
H	0.603404000	-5.527840000	-0.110716000
H	-0.082258000	-2.724737000	3.080907000
H	0.429770000	-2.206412000	-6.436128000
H	0.355642000	-5.058086000	2.304419000

Table ST9: Computed Vertical Transitions and Their Oscillator Strengths and Configurations of the crystals of the fluorophores.

PhBr

Excited State 1: Singlet-A 3.4418 eV 360.23 nm f=0.0029 <S**2>=0.000
153 ->154 0.69761
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -4146.14737638
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6607 eV 338.69 nm f=0.5872 <S**2>=0.000
153 ->155 0.65375
153 ->156 -0.15760
153 ->157 0.12951

Excited State 3: Singlet-A 3.8148 eV 325.01 nm f=0.0839 <S**2>=0.000
152 ->155 -0.18010
152 ->158 -0.11123
153 ->155 0.21677
153 ->156 0.58882
153 ->157 -0.23020

Excited State 4: Singlet-A 3.9342 eV 315.14 nm f=0.0051 <S**2>=0.000
152 ->155 0.18574
153 ->156 0.32341
153 ->157 0.58008

Excited State 5: Singlet-A 4.1267 eV 300.45 nm f=0.0042 <S**2>=0.000
152 ->154 -0.12848
152 ->155 -0.35516
152 ->157 -0.10367
153 ->157 0.16535
153 ->158 0.54140

Excited State 6: Singlet-A 4.1782 eV 296.74 nm f=0.0073 <S**2>=0.000
152 ->154 0.68750
153 ->158 0.10694

Excited State 7: Singlet-A 4.3231 eV 286.80 nm f=0.1488 <S**2>=0.000
152 ->155 0.50930
152 ->156 0.21165
152 ->157 -0.16500
153 ->157 -0.16172
153 ->158 0.31858

Excited State 8: Singlet-A 4.4704 eV 277.35 nm f=0.0173 <S**2>=0.000
147 ->155 -0.14144
153 ->159 0.56519
153 ->160 -0.34338

Excited State 9: Singlet-A 4.5573 eV 272.06 nm f=0.1177 <S**2>=0.000
151 ->154 0.44411
151 ->155 0.49854
151 ->156 0.12113

Excited State 10: Singlet-A 4.5938 eV 269.90 nm f=0.2699 <S**2>=0.000
146 ->154 0.11121
147 ->154 -0.10901
151 ->154 -0.41179
151 ->155 0.47100
151 ->156 -0.15941
151 ->157 -0.12908

Triplet State

Excited State 1: Triplet-A 2.6625 eV 465.67 nm f=0.0000 <S**2>=2.000
150 ->155 0.10914
152 ->156 0.10039
152 ->157 -0.12770
153 ->154 0.14133
153 ->155 0.60561
153 ->158 0.13705
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -4146.17601486
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 3.0838 eV 402.05 nm f=0.0000 <S**2>=2.000
149 ->155 -0.12068
150 ->155 -0.11994
150 ->158 -0.11422
150 ->161 0.12294
152 ->155 -0.11106
152 ->156 0.24432
152 ->157 -0.28577
153 ->155 -0.20361
153 ->158 0.42741

Excited State 3: Triplet-A 3.2057 eV 386.76 nm f=0.0000 <S**2>=2.000
140 ->163 0.12304
146 ->156 0.10237
148 ->159 0.13266
148 ->160 0.11107
151 ->154 0.59906
151 ->155 -0.10981
151 ->156 -0.14288

Excited State 4: Triplet-A 3.3396 eV 371.26 nm f=0.0000 <S**2>=2.000
150 ->158 -0.13381
153 ->154 -0.25025
153 ->155 0.14046
153 ->156 -0.40583
153 ->157 0.40799

Excited State 5: Triplet-A 3.4477 eV 359.62 nm f=0.0000 <S**2>=2.000
153 ->154 0.63232
153 ->155 -0.11681
153 ->156 -0.18178
153 ->157 0.17869

Excited State 6: Triplet-A 3.5906 eV 345.30 nm f=0.0000 <S**2>=2.000
150 ->155 -0.13539
152 ->155 0.29819
152 ->156 -0.26940
152 ->157 0.30450
153 ->157 -0.11182
153 ->158 0.40366

Excited State 7: Triplet-A 3.7779 eV 328.18 nm f=0.0000 <S**2>=2.000
144 ->157 -0.10251
149 ->155 -0.19800
150 ->155 -0.19164
150 ->158 0.26261
152 ->154 0.11141
152 ->155 0.24315
152 ->156 0.14275
152 ->157 -0.13724
153 ->155 0.11448
153 ->157 0.20802
153 ->161 0.27381

Excited State 8: Triplet-A 3.8606 eV 321.15 nm f=0.0000 <S**2>=2.000
153 ->156 0.48090
153 ->157 0.39812
153 ->159 0.21072

Excited State 9: Triplet-A 3.8790 eV 319.63 nm f=0.0000 <S**2>=2.000
149 ->155 0.24684

150 ->158 -0.17230
152 ->154 0.15007
152 ->155 0.44563
152 ->156 0.11882
152 ->157 -0.16584
152 ->158 0.17873
153 ->161 -0.18776

Excited State 10: Triplet-A 3.9721 eV 312.14 nm f=0.0000 <S**2>=2.000
140 ->154 0.19683
146 ->156 0.17051
146 ->157 0.11039
146 ->160 0.14100
147 ->156 -0.11523
147 ->159 -0.11124
147 ->160 -0.13210
148 ->154 0.27881
148 ->156 0.21638
148 ->157 0.19352
148 ->159 -0.21164
148 ->160 -0.10038
151 ->156 -0.14250
151 ->157 -0.10035
151 ->163 0.17936

PhPh

Excited State 1: Singlet-A 3.4805 eV 356.23 nm f=0.0421 <S**2>=0.000
136 ->137 0.70019
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1575.19614361
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.7993 eV 326.34 nm f=0.1006 <S**2>=0.000
135 ->137 0.15432
135 ->138 0.10684
135 ->140 -0.10502
135 ->141 -0.12775
136 ->138 0.53747
136 ->139 -0.31338
136 ->140 0.18556

Excited State 3: Singlet-A 4.0119 eV 309.04 nm f=0.1833 <S**2>=0.000
135 ->138 -0.11137
136 ->138 0.32771
136 ->139 0.60062

Excited State 4: Singlet-A 4.0670 eV 304.85 nm f=0.0377 <S**2>=0.000
135 ->137 0.17405
135 ->138 0.19234
136 ->138 -0.22664

136 ->139 0.10872
136 ->140 0.59282

Excited State 5: Singlet-A 4.1415 eV 299.37 nm f=0.1356 <S**2>=0.000
135 ->137 0.65625
136 ->140 -0.21372

Excited State 6: Singlet-A 4.2914 eV 288.91 nm f=0.0782 <S**2>=0.000
135 ->138 0.26578
136 ->141 0.60929

Excited State 7: Singlet-A 4.4238 eV 280.27 nm f=0.3908 <S**2>=0.000
134 ->137 0.64985
134 ->139 0.10976
135 ->139 0.11296

Excited State 8: Singlet-A 4.5877 eV 270.25 nm f=0.0490 <S**2>=0.000
134 ->137 -0.12927
134 ->138 -0.12362
135 ->138 0.35682
135 ->139 0.50098
136 ->140 -0.12051

Excited State 9: Singlet-A 4.6281 eV 267.90 nm f=0.1355 <S**2>=0.000
129 ->137 -0.19880
133 ->137 -0.14303
134 ->138 -0.20764
134 ->139 0.25134
134 ->140 0.27096
135 ->138 -0.24787
135 ->139 0.16049
135 ->140 0.33363
136 ->141 0.13423

Excited State 10: Singlet-A 4.6804 eV 264.90 nm f=0.0015 <S**2>=0.000
132 ->137 -0.11492
132 ->138 -0.13088
136 ->142 0.51220
136 ->143 -0.40955

Triplet State

Excited State 1: Triplet-A 2.8410 eV 436.42 nm f=0.0000 <S**2>=2.000
133 ->141 -0.10280
135 ->138 -0.18984
135 ->139 0.12264
135 ->140 -0.13168
136 ->137 0.33420
136 ->138 0.38789

136 ->139 0.20023
136 ->140 -0.18442
136 ->141 -0.18243
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1575.21964531
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 3.0759 eV 403.09 nm f=0.0000 <S**2>=2.000
129 ->140 0.10859
134 ->137 0.56129
134 ->139 -0.15204
135 ->137 0.17264
136 ->137 0.13358

Excited State 3: Triplet-A 3.2763 eV 378.42 nm f=0.0000 <S**2>=2.000
132 ->143 -0.11291
133 ->138 -0.13776
133 ->144 -0.11249
135 ->138 0.22979
135 ->139 -0.19704
135 ->140 0.18165
136 ->137 0.18911
136 ->138 0.29248
136 ->140 0.10942
136 ->141 0.32969

Excited State 4: Triplet-A 3.3773 eV 367.11 nm f=0.0000 <S**2>=2.000
133 ->141 -0.10358
136 ->137 -0.27492
136 ->138 0.41722
136 ->139 -0.33833
136 ->140 0.26060

Excited State 5: Triplet-A 3.5579 eV 348.48 nm f=0.0000 <S**2>=2.000
133 ->138 0.11052
135 ->138 0.12427
136 ->137 0.44887
136 ->139 -0.31284
136 ->140 0.10297
136 ->141 -0.23877

Excited State 6: Triplet-A 3.6688 eV 337.95 nm f=0.0000 <S**2>=2.000
135 ->138 0.32850
135 ->139 -0.19269
135 ->140 0.16808
136 ->137 -0.21810
136 ->138 0.16652
136 ->139 0.13241
136 ->140 -0.27280
136 ->141 -0.32631

Excited State 7: Triplet-A 3.8433 eV 322.59 nm f=0.0000 <S**2>=2.000

127 ->138	0.11497
130 ->138	0.11462
131 ->138	0.16614
131 ->139	0.10896
132 ->142	0.10052
132 ->143	-0.20221
133 ->141	-0.28810
135 ->146	-0.11207
136 ->138	-0.12473
136 ->140	-0.13803
136 ->144	0.35092

Excited State 8: Triplet-A 3.8960 eV 318.24 nm f=0.0000 <S**2>=2.000

135 ->137	0.44858
135 ->138	0.29903
135 ->139	0.22949
135 ->140	-0.19552
135 ->141	-0.18962

Excited State 9: Triplet-A 3.9464 eV 314.17 nm f=0.0000 <S**2>=2.000

129 ->139	-0.13565
129 ->140	-0.13590
129 ->142	0.11247
130 ->140	-0.10348
134 ->139	0.19411
134 ->140	0.21789
134 ->145	0.11241
136 ->139	0.25798
136 ->140	0.30846
136 ->141	-0.13079

Excited State 10: Triplet-A 3.9934 eV 310.47 nm f=0.0000 <S**2>=2.000

124 ->137	0.14542
126 ->137	-0.11883
129 ->137	0.12758
129 ->142	-0.13323
130 ->137	0.13782
130 ->140	0.13869
130 ->142	0.17269
131 ->140	-0.13591
131 ->142	-0.18118
134 ->137	0.14658
134 ->139	0.19031
134 ->140	0.14905
134 ->145	-0.16947
135 ->140	0.12731
136 ->139	0.18733
136 ->140	0.15312

PhNp

Excited State 1: Singlet-A 3.5207 eV 352.15 nm f=0.0476 <S**2>=0.000
149 ->150 0.70355
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1728.62517954
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.7086 eV 334.32 nm f=0.0356 <S**2>=0.000
149 ->151 0.69725

Excited State 3: Singlet-A 3.9163 eV 316.58 nm f=0.0144 <S**2>=0.000
148 ->150 -0.15610
148 ->153 0.23621
149 ->152 0.61416
149 ->153 -0.11263

Excited State 4: Singlet-A 4.1039 eV 302.11 nm f=0.0542 <S**2>=0.000
148 ->150 0.66806
149 ->152 0.16321

Excited State 5: Singlet-A 4.2065 eV 294.74 nm f=0.0664 <S**2>=0.000
148 ->151 0.23487
148 ->152 -0.29605
149 ->153 0.56984

Excited State 6: Singlet-A 4.2701 eV 290.36 nm f=0.0409 <S**2>=0.000
146 ->150 0.29905
146 ->151 0.13287
147 ->150 0.51966
148 ->151 0.30042

Excited State 7: Singlet-A 4.2927 eV 288.83 nm f=0.0128 <S**2>=0.000
146 ->150 0.18324
147 ->150 -0.27388
148 ->151 0.24572
149 ->152 -0.11753
149 ->153 -0.10106
149 ->154 0.52152

Excited State 8: Singlet-A 4.3084 eV 287.77 nm f=0.0246 <S**2>=0.000
147 ->150 -0.24388
147 ->151 0.12037
148 ->151 0.45746
148 ->152 0.10330
149 ->153 -0.11965
149 ->154 -0.40861

Excited State 9: Singlet-A 4.3395 eV 285.71 nm f=0.0621 <S**2>=0.000
146 ->150 0.56273
147 ->150 -0.15679
147 ->151 0.17970
148 ->151 -0.26142
149 ->154 -0.13881

Excited State 10: Singlet-A 4.4693 eV 277.41 nm f=0.0583 <S**2>=0.000
144 ->150 -0.19305
146 ->151 -0.30046
147 ->150 0.19511
147 ->151 0.45522
147 ->155 -0.13021
149 ->155 -0.25407

Triplet State

Excited State 1: Triplet-A 2.7952 eV 443.56 nm f=0.0000 <S**2>=2.000
144 ->155 -0.13498
146 ->150 -0.24397
146 ->151 -0.13991
147 ->150 0.45842
147 ->151 0.28184
149 ->150 0.25440
149 ->151 0.10951
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1728.65184333
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.9677 eV 417.78 nm f=0.0000 <S**2>=2.000
145 ->157 0.12531
148 ->152 -0.32142
149 ->150 -0.16749
149 ->151 0.12418
149 ->152 0.13044
149 ->153 0.48919

Excited State 3: Triplet-A 3.1056 eV 399.23 nm f=0.0000 <S**2>=2.000
142 ->154 0.12339
143 ->156 -0.12912
146 ->150 -0.30803
146 ->151 0.43477
147 ->150 -0.15653
147 ->151 0.22576
148 ->150 -0.10837
148 ->151 0.14030

Excited State 4: Triplet-A 3.4588 eV 358.46 nm f=0.0000 <S**2>=2.000
149 ->150 0.11242

149 ->151 -0.18006
149 ->152 0.61299
149 ->153 -0.11793
149 ->154 0.10761

Excited State 5: Triplet-A 3.4637 eV 357.95 nm f=0.0000 <S**2>=2.000
147 ->150 -0.15845
148 ->152 -0.29574
149 ->150 0.52759
149 ->152 -0.13656
149 ->157 0.14304

Excited State 6: Triplet-A 3.6449 eV 340.16 nm f=0.0000 <S**2>=2.000
148 ->152 0.37699
149 ->150 0.21975
149 ->151 0.37789
149 ->152 0.12181
149 ->153 0.28637

Excited State 7: Triplet-A 3.7438 eV 331.17 nm f=0.0000 <S**2>=2.000
148 ->152 -0.18800
149 ->150 -0.18542
149 ->151 0.51789
149 ->153 -0.33667

Excited State 8: Triplet-A 3.8754 eV 319.92 nm f=0.0000 <S**2>=2.000
140 ->152 -0.13692
145 ->153 0.27167
148 ->152 0.10281
148 ->160 -0.11839
149 ->150 -0.13554
149 ->151 -0.12188
149 ->152 -0.11824
149 ->154 -0.10245
149 ->156 0.14942
149 ->157 0.43824
149 ->158 -0.11088

Excited State 9: Triplet-A 3.9558 eV 313.42 nm f=0.0000 <S**2>=2.000
148 ->150 0.49750
148 ->153 -0.40424

Excited State 10: Triplet-A 4.0234 eV 308.16 nm f=0.0000 <S**2>=2.000
136 ->151 0.14529
142 ->150 -0.15991
142 ->154 0.14247
142 ->156 -0.19808
143 ->150 -0.17615
143 ->151 0.14470
143 ->154 0.27901

143 ->155 -0.10100
143 ->156 0.20156
146 ->159 -0.17739
147 ->151 -0.11572

PhAn

Excited State 1: Singlet-A 3.0966 eV 400.39 nm f=0.0008 <S**2>=0.000
162 ->163 0.70213
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1882.23589179
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.3547 eV 369.58 nm f=0.1060 <S**2>=0.000
161 ->163 0.69539

Excited State 3: Singlet-A 3.6002 eV 344.38 nm f=0.0007 <S**2>=0.000
159 ->163 0.11945
160 ->163 0.69314

Excited State 4: Singlet-A 3.7756 eV 328.38 nm f=0.0182 <S**2>=0.000
162 ->164 0.69926

Excited State 5: Singlet-A 3.8040 eV 325.93 nm f=0.0019 <S**2>=0.000
159 ->163 0.69344
160 ->163 -0.11878

Excited State 6: Singlet-A 3.8518 eV 321.89 nm f=0.0040 <S**2>=0.000
157 ->163 0.13276
161 ->164 0.67685

Excited State 7: Singlet-A 3.9222 eV 316.11 nm f=0.0199 <S**2>=0.000
160 ->164 0.11900
160 ->166 -0.19681
160 ->167 0.14289
162 ->165 0.63436

Excited State 8: Singlet-A 3.9896 eV 310.77 nm f=0.0063 <S**2>=0.000
157 ->163 0.41142
158 ->163 0.28373
161 ->164 -0.19119
161 ->166 0.10905
161 ->167 0.33563
161 ->168 -0.27681

Excited State 9: Singlet-A 4.2321 eV 292.96 nm f=0.0929 <S**2>=0.000
160 ->164 0.65761
160 ->165 -0.10115
162 ->165 -0.11980

162 ->166 -0.18245

Excited State 10: Singlet-A 4.2562 eV 291.30 nm f=0.0366 <S**2>=0.000
160 ->164 0.20325
160 ->165 0.34869
162 ->166 0.52462
162 ->167 -0.20220

Triplet States

Excited State 1: Triplet-A 1.9720 eV 628.73 nm f=0.0000 <S**2>=2.000
161 ->163 0.68715
161 <-163 0.11882
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1882.27722094
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.9897 eV 414.71 nm f=0.0000 <S**2>=2.000
152 ->174 0.10372
158 ->171 -0.10634
159 ->165 -0.11556
160 ->165 0.42513
162 ->164 -0.15394
162 ->166 0.36268
162 ->167 -0.24777
162 ->168 -0.12742

Excited State 3: Triplet-A 3.0902 eV 401.22 nm f=0.0000 <S**2>=2.000
159 ->164 -0.15170
162 ->163 0.67218

Excited State 4: Triplet-A 3.1100 eV 398.66 nm f=0.0000 <S**2>=2.000
156 ->169 -0.11997
159 ->164 0.56708
159 ->167 -0.11066
160 ->164 0.17439
162 ->163 0.18329

Excited State 5: Triplet-A 3.4051 eV 364.11 nm f=0.0000 <S**2>=2.000
154 ->163 -0.32617
155 ->163 0.36144
156 ->163 0.10184
157 ->163 -0.20893
161 ->167 0.11720
161 ->169 -0.14912
161 ->170 0.34334

Excited State 6: Triplet-A 3.4657 eV 357.74 nm f=0.0000 <S**2>=2.000
162 ->165 0.65635

Excited State 7: Triplet-A 3.5433 eV 349.91 nm f=0.0000 <S**2>=2.000
157 ->163 0.43634
158 ->163 0.32209
160 ->163 0.33226
160 ->165 0.11115
161 ->167 -0.11208
161 ->168 0.13250

Excited State 8: Triplet-A 3.5577 eV 348.49 nm f=0.0000 <S**2>=2.000
157 ->163 -0.14414
158 ->163 -0.10299
160 ->165 0.43064
162 ->164 0.30401
162 ->166 -0.30349
162 ->167 0.17510

Excited State 9: Triplet-A 3.6160 eV 342.87 nm f=0.0000 <S**2>=2.000
154 ->163 0.11073
157 ->163 -0.23459
158 ->163 -0.11834
159 ->163 0.14785
160 ->163 0.59317

Excited State 10: Triplet-A 3.7883 eV 327.28 nm f=0.0000 <S**2>=2.000
157 ->163 0.12246
159 ->163 -0.34278
161 ->164 0.36760
161 ->167 0.23122
161 ->168 -0.20820
162 ->164 -0.28299
162 ->166 -0.12627

Optimized Cartesian coordinates and energies of Crystals:

Table ST10: Optimized Cartesian coordinates:

PhBr

70

symmetry c1

Br 3.370270000 5.626642000 0.123198000

C 1.931851000 4.367882000 0.163329000

C 2.058903000 3.204058000 0.916229000

C 0.767480000 4.630461000 -0.557313000

C	1.011238000	2.284068000	0.940570000
H	2.961412000	3.019609000	1.487546000
H	0.677085000	5.542973000	-1.135406000
C	-0.271529000	3.707378000	-0.527809000
C	-0.168106000	2.514349000	0.212293000
H	1.118885000	1.396560000	1.550110000
H	-1.187081000	3.898301000	-1.075533000
C	-1.336807000	1.618114000	0.202130000
N	-1.326074000	0.238141000	0.407977000
N	-2.557197000	2.064154000	-0.034409000
C	-0.167790000	-0.586941000	0.597244000
C	-2.650076000	-0.190540000	0.275222000
C	-3.374049000	0.967103000	0.012286000
C	0.623135000	-0.926579000	-0.507817000
C	0.157354000	-1.039484000	1.882294000
C	-3.263929000	-1.491292000	0.337112000
C	-4.797025000	0.949829000	-0.171582000
C	1.744220000	-1.723385000	-0.311897000
H	0.344453000	-0.563175000	-1.492271000
H	-0.478802000	-0.760850000	2.716196000
C	1.280945000	-1.842667000	2.079016000
C	-4.687751000	-1.532258000	0.150277000
C	-2.561676000	-2.700285000	0.551913000
C	-5.520909000	2.133651000	-0.416660000
C	-5.459963000	-0.306725000	-0.094822000
C	2.073933000	-2.182735000	0.979960000
C	2.750347000	-2.226037000	-1.345451000

H	1.528164000	-2.193323000	3.076597000
C	-5.316739000	-2.795701000	0.202327000
C	-3.219395000	-3.916029000	0.593912000
H	-1.489323000	-2.679006000	0.686193000
H	-4.972443000	3.068318000	-0.465399000
C	-6.892139000	2.093318000	-0.584343000
C	-6.863548000	-0.307578000	-0.269064000
C	3.291226000	-2.997937000	0.887048000
C	3.698940000	-3.034520000	-0.461411000
C	2.071848000	-3.111443000	-2.432548000
C	3.481702000	-1.053271000	-2.063527000
H	-6.389060000	-2.863676000	0.064211000
C	-4.609412000	-3.964803000	0.419721000
H	-2.655027000	-4.828733000	0.760613000
H	-7.447621000	3.007555000	-0.771650000
C	-7.565076000	0.861774000	-0.508123000
H	-7.418838000	-1.236615000	-0.215493000
C	4.016171000	-3.671109000	1.872424000
C	4.836220000	-3.747571000	-0.826090000
H	1.406951000	-2.468877000	-3.023877000
H	2.856026000	-3.448945000	-3.122167000
C	1.287499000	-4.323161000	-1.922235000
H	4.197192000	-1.492518000	-2.770385000
H	2.743090000	-0.519388000	-2.675152000
C	4.207905000	-0.055922000	-1.157138000
H	-5.133056000	-4.915524000	0.451263000
H	-8.642866000	0.823187000	-0.636362000

C	5.156608000	-4.384193000	1.498675000
H	3.703148000	-3.643838000	2.912433000
C	5.563763000	-4.422618000	0.160916000
H	5.162667000	-3.784673000	-1.862039000
H	1.926016000	-5.003174000	-1.350686000
H	0.869881000	-4.884874000	-2.763648000
H	0.454173000	-4.022524000	-1.280098000
H	3.513642000	0.456754000	-0.484938000
H	4.706818000	0.708819000	-1.760451000
H	4.969970000	-0.549192000	-0.546534000
H	5.732522000	-4.913324000	2.252048000
H	6.453241000	-4.981588000	-0.114415000

PhPh

70

symmetry c1

N	-1.166133000	0.704277000	-0.270635000
C	0.223067000	0.434126000	-0.503943000
C	-2.200984000	-0.233378000	-0.205519000
C	-1.755186000	1.955563000	-0.077696000
C	1.017522000	-0.049408000	0.547204000
C	0.767673000	0.654644000	-1.772943000
C	-3.345179000	0.516111000	0.041172000
C	-2.233956000	-1.661220000	-0.382475000
N	-3.058691000	1.852940000	0.108091000
C	-1.068904000	3.260226000	-0.099378000
H	0.565884000	-0.210877000	1.521628000
C	2.360319000	-0.312284000	0.309683000

H	0.126849000	1.028644000	-2.564281000
C	2.117496000	0.392335000	-2.011911000
C	-4.631871000	-0.095079000	0.212829000
C	-3.511074000	-2.295417000	-0.208043000
C	-1.115261000	-2.450646000	-0.737828000
C	-1.834431000	4.377755000	-0.483124000
C	0.269198000	3.462593000	0.277556000
C	2.911100000	-0.093361000	-0.971063000
C	3.421185000	-0.831344000	1.280332000
H	2.535325000	0.564678000	-2.999282000
C	-4.713145000	-1.511806000	0.105978000
C	-5.779575000	0.673970000	0.490754000
C	-3.571344000	-3.697174000	-0.370364000
H	-0.159311000	-1.975026000	-0.907041000
C	-1.222116000	-3.820620000	-0.893450000
H	-2.871731000	4.222434000	-0.756625000
C	-1.274569000	5.650827000	-0.504059000
H	0.876140000	2.630191000	0.608896000
C	0.825348000	4.741382000	0.253638000
C	4.333243000	-0.456314000	-0.933329000
C	4.646912000	-0.892074000	0.369602000
C	3.636046000	0.144664000	2.475772000
C	3.053922000	-2.228757000	1.860071000
C	-5.983720000	-2.102121000	0.299969000
H	-5.668359000	1.750621000	0.563501000
C	-7.005633000	0.061939000	0.670005000
H	-4.518306000	-4.208239000	-0.244578000

C	-2.459045000	-4.451394000	-0.699674000
H	-0.347547000	-4.401536000	-1.171126000
H	-1.881694000	6.498717000	-0.807758000
C	0.061093000	5.839227000	-0.140330000
H	1.860481000	4.877382000	0.553320000
C	5.309477000	-0.425459000	-1.931177000
C	5.941389000	-1.298826000	0.675854000
H	2.707684000	0.169335000	3.060694000
H	4.395329000	-0.296649000	3.133950000
C	4.051103000	1.573049000	2.113746000
H	3.867236000	-2.533279000	2.531098000
H	2.167574000	-2.109044000	2.496238000
C	2.799553000	-3.337701000	0.836042000
H	-6.100101000	-3.177741000	0.236705000
C	-7.104158000	-1.337004000	0.575398000
H	-7.888016000	0.657250000	0.885866000
H	-2.550672000	-5.526930000	-0.817813000
H	0.499392000	6.832736000	-0.158984000
H	5.069434000	-0.089777000	-2.936153000
C	6.606326000	-0.835401000	-1.616371000
H	6.197297000	-1.637268000	1.676480000
C	6.920543000	-1.268799000	-0.324016000
H	5.006922000	1.590324000	1.582322000
H	4.160464000	2.176985000	3.019939000
H	3.306543000	2.061125000	1.477414000
H	2.579819000	-4.280466000	1.346764000
H	3.670646000	-3.499547000	0.194385000

H	1.944895000	-3.103634000	0.194849000
H	-8.063953000	-1.824686000	0.718988000
H	7.377575000	-0.818057000	-2.380682000
H	7.933800000	-1.585114000	-0.094375000

PhNp

76

symmetry c1

N	1.106716000	-0.034713000	-0.591800000
C	-0.260065000	-0.456526000	-0.695845000
C	1.557614000	1.286179000	-0.644945000
C	2.232600000	-0.825866000	-0.347777000
C	-1.141304000	-0.204150000	0.363077000
C	-0.699628000	-1.104148000	-1.857415000
N	2.861260000	1.364296000	-0.464022000
C	0.674683000	2.442782000	-0.906486000
C	3.291038000	0.072933000	-0.288022000
C	2.405156000	-2.239169000	-0.132436000
H	-0.774251000	0.301152000	1.251161000
C	-2.465773000	-0.606471000	0.245549000
H	0.008327000	-1.286834000	-2.659526000
C	-2.026723000	-1.517180000	-1.971899000
C	0.717327000	3.606495000	-0.061332000
C	-0.185904000	2.420413000	-1.992136000
C	4.643041000	-0.355443000	-0.073035000
C	3.751268000	-2.690836000	0.084929000
C	1.348904000	-3.179163000	-0.101992000
C	-2.909569000	-1.265619000	-0.918935000

C	-3.604556000	-0.442946000	1.250361000
H	-2.360778000	-2.022565000	-2.873213000
C	-0.150830000	4.708460000	-0.367616000
C	1.561754000	3.713977000	1.078316000
H	-0.202487000	1.552726000	-2.641552000
C	-1.032233000	3.511037000	-2.286799000
C	4.877662000	-1.748186000	0.100715000
C	5.709739000	0.565143000	-0.041860000
C	3.949450000	-4.072917000	0.298532000
H	0.331409000	-2.843564000	-0.246251000
C	1.589225000	-4.523662000	0.114671000
C	-4.335995000	-1.575729000	-0.762845000
C	-4.757769000	-1.103753000	0.496357000
C	-3.894484000	1.055996000	1.558698000
C	-3.299644000	-1.164973000	2.596141000
C	-1.016063000	4.631354000	-1.490399000
C	-0.132176000	5.860491000	0.464422000
H	2.236656000	2.899001000	1.306537000
C	1.550416000	4.844319000	1.864831000
H	-1.687218000	3.459179000	-3.151175000
C	6.217435000	-2.157843000	0.294931000
H	5.482362000	1.616799000	-0.180588000
C	7.005891000	0.127549000	0.154117000
H	4.951815000	-4.448311000	0.466010000
C	2.901346000	-4.976024000	0.311759000
H	0.758980000	-5.223462000	0.133961000
C	-5.230773000	-2.215885000	-1.622629000

C	-6.079009000	-1.272397000	0.897016000
H	-4.729653000	1.092683000	2.270000000
H	-3.026171000	1.464612000	2.091217000
C	-4.213517000	1.942073000	0.351577000
H	-2.461421000	-0.643431000	3.075800000
H	-4.163787000	-1.017130000	3.256412000
C	-2.982320000	-2.659647000	2.500825000
H	-1.663244000	5.476267000	-1.710523000
H	-0.792380000	6.688004000	0.217861000
C	0.698327000	5.930803000	1.557846000
H	2.205961000	4.903690000	2.728774000
H	6.452665000	-3.207631000	0.425647000
C	7.258003000	-1.245091000	0.321515000
H	7.826100000	0.839141000	0.175637000
H	3.098296000	-6.030349000	0.481367000
C	-6.555283000	-2.381468000	-1.213451000
H	-4.907460000	-2.580715000	-2.593597000
H	-6.417849000	-0.912952000	1.865142000
C	-6.976803000	-1.913943000	0.035699000
H	-4.420275000	2.965561000	0.679834000
H	-5.093075000	1.580781000	-0.189668000
H	-3.376165000	1.984545000	-0.350832000
H	-2.090975000	-2.843694000	1.893600000
H	-3.812379000	-3.218680000	2.058950000
H	-2.794745000	-3.071467000	3.497438000
H	0.703086000	6.816927000	2.185801000
H	8.274769000	-1.595969000	0.472232000

H -7.264269000 -2.877205000 -1.869925000

H -8.010434000 -2.049995000 0.340029000

PhAn

82

symmetry c1

C -0.090560000 -0.411945000 0.547574000

N 1.240062000 0.050271000 0.268468000

C -0.955790000 -0.699760000 -0.516187000

C -0.509530000 -0.558047000 1.874882000

C 1.585337000 1.372433000 0.001122000

C 2.420712000 -0.688426000 0.180256000

H -0.607937000 -0.568244000 -1.535787000

C -2.241979000 -1.141313000 -0.235047000

H 0.180283000 -0.317293000 2.676412000

C -1.798909000 -1.009248000 2.157684000

N 2.871075000 1.512167000 -0.239496000

C 0.579229000 2.466247000 0.001111000

C 3.401061000 0.245909000 -0.131482000

C 2.702648000 -2.090410000 0.335749000

C -2.663223000 -1.302342000 1.100648000

C -3.359255000 -1.504679000 -1.210963000

H -2.118306000 -1.122922000 3.189321000

C -0.054783000 2.831109000 -1.206600000

C 0.268282000 3.128855000 1.208395000

C 4.774584000 -0.127952000 -0.307897000

C 1.728063000 -3.068591000 0.639474000

C 4.070606000 -2.488009000 0.160548000

C	-4.050153000	-1.784640000	1.094582000
C	-4.470912000	-1.911521000	-0.244638000
C	-2.952018000	-2.671346000	-2.157737000
C	-3.770359000	-0.286199000	-2.090901000
C	-1.069664000	3.858866000	-1.191638000
C	0.265733000	2.219380000	-2.460725000
C	-0.746325000	4.156707000	1.211971000
C	0.926913000	2.828227000	2.443104000
C	5.112835000	-1.503139000	-0.158936000
C	5.762929000	0.827771000	-0.618214000
H	0.697307000	-2.769282000	0.775014000
C	2.069200000	-4.402228000	0.771379000
C	4.372515000	-3.860522000	0.304672000
C	-4.911334000	-2.100772000	2.147156000
C	-5.757147000	-2.356311000	-0.531796000
H	-3.808791000	-2.886231000	-2.809195000
H	-2.155293000	-2.306631000	-2.818804000
C	-2.495808000	-3.963625000	-1.475217000
H	-2.916728000	-0.030300000	-2.731223000
H	-4.569210000	-0.617882000	-2.766861000
C	-4.227904000	0.964381000	-1.335592000
C	-1.722197000	4.206690000	-2.415884000
C	-1.391953000	4.486287000	0.016070000
C	-0.382028000	2.584213000	-3.612080000
H	1.056078000	1.477018000	-2.491327000
C	-1.064979000	4.811817000	2.442449000
H	1.718015000	2.086018000	2.444980000

C	0.595600000	3.484270000	3.599405000
C	6.471367000	-1.856099000	-0.333120000
H	5.457631000	1.863596000	-0.722325000
C	7.080500000	0.444253000	-0.781861000
H	1.302821000	-5.135100000	1.005780000
C	3.402780000	-4.801626000	0.602467000
H	5.394107000	-4.198807000	0.178856000
H	-4.588713000	-2.003484000	3.180027000
C	-6.200770000	-2.546755000	1.850954000
C	-6.621030000	-2.673922000	0.522882000
H	-6.094795000	-2.458236000	-1.559874000
H	-1.601148000	-3.802406000	-0.866413000
H	-2.253134000	-4.723255000	-2.225010000
H	-3.276443000	-4.371633000	-0.826361000
H	-5.112908000	0.763458000	-0.724630000
H	-4.480575000	1.760045000	-2.043227000
H	-3.442027000	1.347325000	-0.678463000
C	-1.394020000	3.587130000	-3.591565000
H	-2.485216000	4.980208000	-2.391320000
H	-2.161274000	5.255027000	0.024298000
H	-0.115477000	2.114491000	-4.554345000
C	-0.417824000	4.485525000	3.603467000
H	-1.833167000	5.580521000	2.433275000
H	1.114929000	3.247308000	4.523324000
C	7.433838000	-0.908532000	-0.637004000
H	6.783052000	-2.888877000	-0.228964000
H	7.839641000	1.183436000	-1.020462000

H	3.678214000	-5.847086000	0.704370000
H	-6.883170000	-2.797148000	2.657841000
H	-7.627068000	-3.022290000	0.308125000
H	-1.895010000	3.862653000	-4.514744000
H	-0.667082000	4.992541000	4.530805000
H	8.467759000	-1.216270000	-0.763403000

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