Supporting Information

Barbier single-atom polymerization induced emission as a one-pot approach for stimuli-responsive luminescent polymer

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Experimental details

Materials

THF was dried with sodium metal before use, and re-evaporated and purified with benzophenone as an indicator. Chemicals and other common reagents were obtained from commercial suppliers and used without further purification.

Characterization methods

Nuclear magnetic resonance (NMR) spectroscopy. The ^{1}H and ^{13}C NMR measurements were performed on Bruker-BioSpin AVANCE III HD 400 spectrometer in $CDCl_3$ using tetramethylsilane as an internal standard.

Gel permeation chromatography (GPC). Weight-average molecular weight (M_w) and polydispersity indices (PDI) of the polymers were estimated on an Agilent 1260 Infinity II equipped with a G7110B isocratic pump and G7162A refractive index detector. Polystyrene standards were utilized, and DMF was used as the eluent at a flow rate of 1.0 mL/min at 50 ^{o}C.

Fourier transform infrared (FT-IR) spectroscopy. FT-IR Spectra using KBr pellets were recorded on a TENSOR II FTIR Spectrometer (Bruker, Germany). The spectra were recorded from an accumulation of 16 scans in the range of 4000-400 cm^{-1} and were collected at room temperature. The OPUS v7.5 software auto-corrected the spectral base line and calculated the second derivative spectra.

UV-vis absorption. The spectra were recorded in THF with sample concentration of 0.1 mg/mL and sample transmittance at 500 nm were acquired in THF/water mixtures with different water fractions (f_w, vol%) on a Shimadzu UV-2450 UV-vis spectrophotometer at room temperature.

Luminescence spectroscopy. The spectrum was performed on a Shimadzu RF 5301pc fluorescence spectrophotometer in a quartz cuvette with a path length of 1 cm.

Aggregation-induced emission (AIE) property. The measurements of the polymer in solvent/nonsolvent mixtures were tested. In this study, THF was selected as good solvent for polymers and water as aggregation-inducing nonsolvent. The luminescence spectra of polymers in THF/water mixtures with different water content were recorded respectively on a Shimadzu RF-5301pc fluorescence spectrophotometer.

The detection of 2,4,6-trinitrotoluene (TNT). The detection was performed by luminescence quenching of aggregated polymer in the THF/water mixtures. The luminescence spectra (excitation @470 nm) of polymer solution (0.1 mg/mL in THF/water mixtures with 90% water fractions (vol%)) upon addition of different amounts of TNT were tested. Thus, the intensities and quenching ratio (the luminescence quenching efficiency = $(1- I/I_0) \times 100\%$, I and I_0 denote the luminescence intensity of polymer with and without TNT, respectively) of polymer solution upon addition of different amounts of TNT were acquired. Further, Corresponding Stern–Volmer plots of TNT was acquired, which can be used to detect the content of TNT. Meanwhile, test strips for the detection of TNT were made by dripping *p*-P(*p*-DMAPTPM) solution onto the filter papers and then dried it in air which showed yellow luminescence under irradiation with UV lamp @365 nm. Take the TNT solution and add it dropwise to the prepared test paper. After the solvent evaporates, there is no

emission under UV lamp @365nm, and the minimum detection limit visible to the human eye is 1 ng.

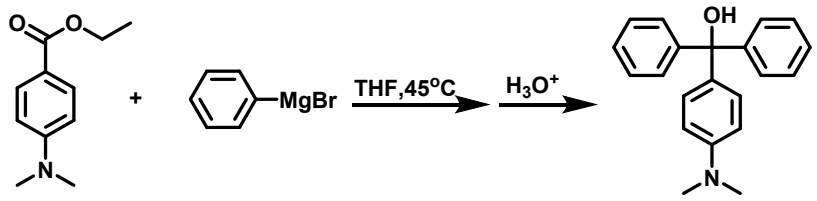
Theoretical calculation. All the molecules were fully optimized by density functional theory (DFT) methods with the B3LYP hybrid functional and the 6-311G* basis set implemented in the Gaussian 09 package. The vertical excitations and the excited state structure optimizations were performed using the time-dependent extension of DFT (TD-DFT) with the same functional and basis set. The environment layer is treated with the universal force field (UFF). All the atoms are allowed to relax both in the ground and excited state calculations.

Safety precautions.

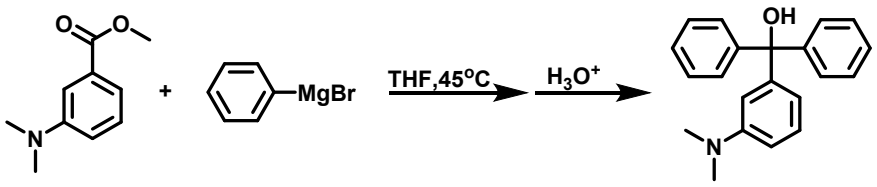
Note: Explosive TNT should be used with extreme caution. It only should be used in highly diluted solution. At the same time, it should be far away from the fire source and impact shall be avoided. After use, it should be post-treatment with a large amount of water.

Synthetic procedures

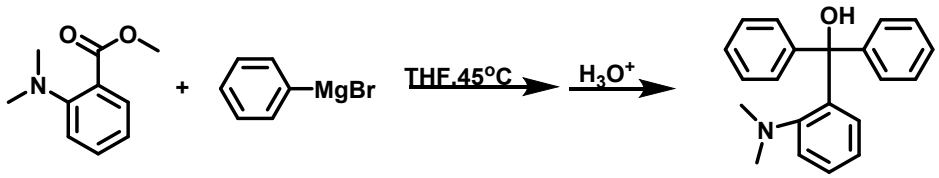
Synthesis of (4-dimethylamino)-triphenylmethanol (*p*-DMATPM). 0.1 g ethyl 4-dimethylaminobenzoate (1.0 equivalent) was dissolved in THF (1mL) and added to one flame-dried Schlenk tube, then 1.34 mL phenylmagnesium bromide (2.4 equivalent, 1 mol/L in THF) was added at 45°C through a syringe. After reaction for 12 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$. Then the solvent was removed by rotary evaporation under vacuum and the residue was chromatographed on silica gel (petroleum ether/ethyl acetate = 10:1) to yield *p*-DMATPM (0.128 g, 85.9%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.32-7.22 (broad, -C_6H_5-, 10H), 7.08 (d, Ar-H, 2H), 6.65 (d, Ar-H, 2H), 2.94 (s, -CH_3, 6H), 2.74 (s, -OH, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.57, 147.33, 134.75, 128.92, 127.79, 126.88, 111.85, 81.85, 40.40 ppm.



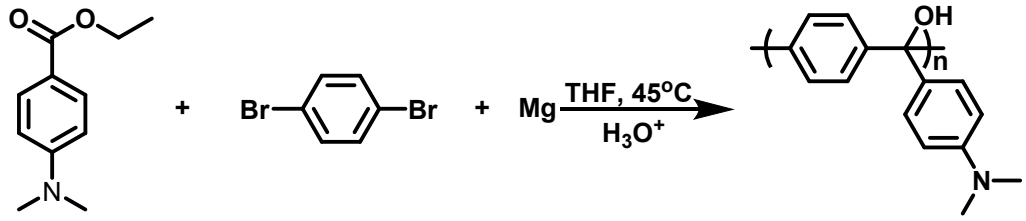
Synthesis of (3-dimethylamino)-triphenylmethanol (*m*-DMATPM). 0.2 g methyl 3-(dimethylamino)benzoate (1.0 equivalent) was dissolved in THF (2mL) and added to one flame-dried Schlenk tube, then 2.70 mL phenylmagnesium bromide (2.4 equivalent, 1 mol/L in THF) was added at 45°C through a syringe. After reaction for 12 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$. Then the solvent was removed by rotary evaporation under vacuum and the residue was chromatographed on silica gel (petroleum ether/ethyl acetate = 10:1) to yield *m*-DMATPM (0.304 g, 91.2%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.34-7.23 (broad, -C_6H_5-, 10H), 7.15 (t, Ar-H, 1H), 6.71 (t, Ar-H, 1H), 6.65 (dd, Ar-H, 1H), 6.52 (d, Ar-H, 1H), 2.87 (s, -CH_3, 6H), 2.83 (s, -OH, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 150.31, 147.77, 147.10, 128.55, 128.01, 127.82, 127.13, 116.78, 112.40, 111.48, 82.31, 40.61 ppm.



Synthesis of (2-dimethylamino)-triphenylmethanol (*o*-DMATPM) 0.1 g methyl 2-(dimethylamino)benzoate (1.0 equivalent) was dissolved in THF (1mL) and added to one flame-dried Schlenk tube, then 1.34 mL phenylmagnesium bromide (2.4 equivalent, 1 mol/L in THF) was added at 45°C through a syringe. After reaction for 12 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$. Then the solvent was removed by rotary evaporation under vacuum and the residue was chromatographed on silica gel (petroleum ether/ethyl acetate = 10:1) to yield *o*-DMATPM (0.142 g, 85.3%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.85 (s, -OH, 1H), 7.39-7.20 (broad, -C_6H_5-, Ar-H, 12H), 7.05 (t, Ar-H, 1H), 6.70 (dd, Ar-H, 1H), 2.38 (s, -CH_3, 6H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 152.10, 147.63, 143.01, 130.48, 128.29, 127.69, 126.90, 125.17, 123.55, 82.98, 45.62 ppm.

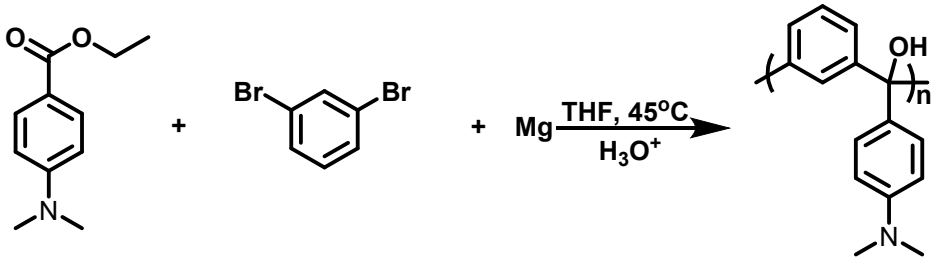


Synthesis of para-poly(*p*-dimethylaminotriphenylmethanol) (*p*-P(*p*-DMATPM)). To one flame-dried Schlenk tube containing freshly peeled Mg scraps (0.3 g, 2.4 equivalent), was added 1,4-dibromobenzene (1.22 g, 1.0 equivalent), ethyl 4-dimethylaminobenzoate (1 g ,1.0 equivalent) dissolved in THF (5 mL) at 45°C through a syringe. After 10 minutes, 50 μL of 1,2-dibromoethane was added to initiate the reaction. After the reaction was refluxed for 24 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with 10 mL saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$ and concentrated under reduced pressure. After the product was purified by precipitation into excessive petroleum ether, filtered and dried under vacuum, 0.803 g *p*-P(*p*-DMATPM) was obtained as a light-yellow powder with a yield of 69.2 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.01-6.74 (broad, Ar-H, 6H), 6.73-6.35 (broad, Ar-H, 2H), 3.10-2.97 (broad, -OH, 1H), 2.97-2.79 (-CH_3, 6H) ppm.

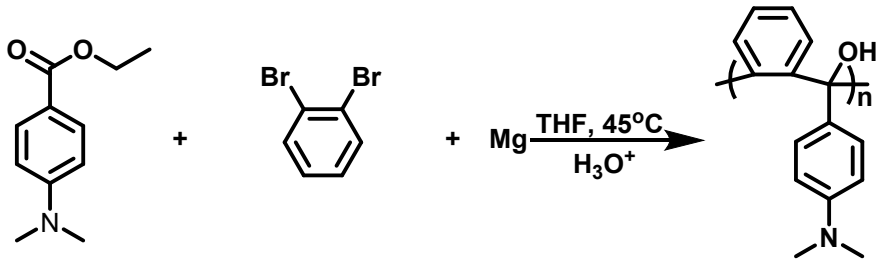


Synthesis of meta-poly(*p*-dimethylaminotriphenylmethanol) (*m*-P(*p*-DMATPM)). To one flame-dried Schlenk tube containing freshly peeled Mg scraps (0.3 g, 2.4 equivalent), was added

1,3-dibromobenzene (1.22 g, 1.0 equivalent), ethyl 4-dimethylaminobenzoate (1 g ,1.0 equivalent) dissolved in THF (5 mL) at 45°C through a syringe. After 10 minutes, 50 μL of 1,2-dibromoethane was added to initiate the reaction. After the reaction was refluxed for 24 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with 10 mL saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$ and concentrated under reduced pressure. After the product was purified by precipitation into excessive petroleum ether, filtered and dried under vacuum, 0.875 g *m*-P(*p*-DMATPM) was obtained as a light-yellow powder with a yield of 75.4 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.99-6.76 (broad, Ar-H, 6H), 6.74-6.34 (broad, Ar-H, 2H), 3.12-2.98 (broad, -OH, 1H), 2.98-2.66 (-CH_3, 6H) ppm.

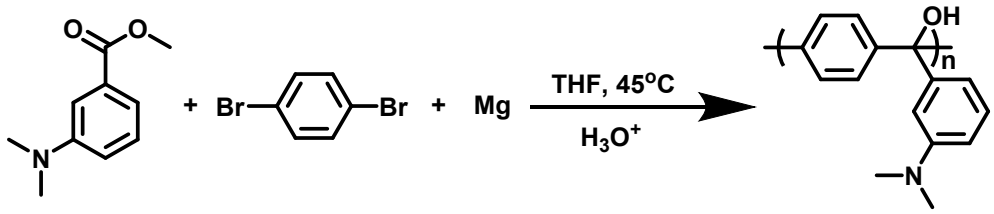


Synthesis of ortho-poly(*p*-dimethylaminotriphenylmethanol) (*o*-P(*p*-DMATPM)). To one flame-dried Schlenk tube containing freshly peeled Mg scraps (0.3 g, 2.4 equivalent), was added 1,2-dibromobenzene (1.22 g, 1.0 equivalent), ethyl 4-dimethylaminobenzoate (1 g ,1.0 equivalent) dissolved in THF (5 mL) at 45°C through a syringe. After 10 minutes, 50 μL of 1,2-dibromoethane was added to initiate the reaction. After the reaction was refluxed for 24 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with 10 mL saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$ and concentrated under reduced pressure. After the product was purified by precipitation into excessive petroleum ether, filtered and dried under vacuum, 0.664 g *o*-P(*p*-DMATPM) was obtained as a light-yellow powder with a yield of 57.3 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.10-6.80 (broad, Ar-H, 6H), 6.80-6.24 (broad, Ar-H, 2H), 3.13-2.97 (broad, -OH, 1H), 2.97-2.74 (-CH_3, 6H) ppm.

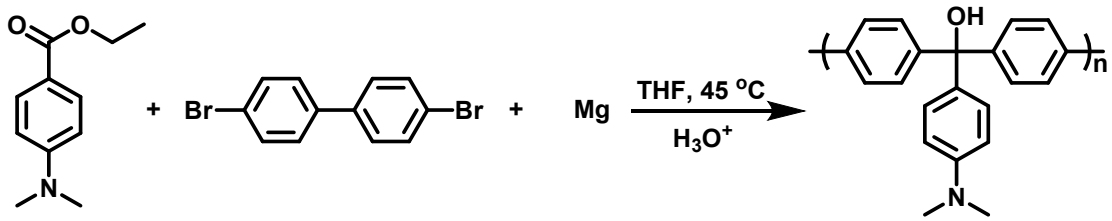


Synthesis of para-poly(*p*-dimethylaminotriphenylmethanol) (*p*-P(*m*-DMATPM)). To one flame-dried Schlenk tube containing freshly peeled Mg scraps (96 mg, 2.4 equivalent), was added 1,4-dibromobenzene (0.4 g, 1.0 equivalent), methyl 3-dimethylaminobenzoate (0.3 g ,1.0 equivalent) dissolved in THF (3 mL) at 45°C through a syringe. After 10 minutes, 10 μL of 1,2-dibromoethane was added to initiate the reaction. After the reaction was refluxed for 24 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with 10 mL saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$ and concentrated under reduced pressure. After

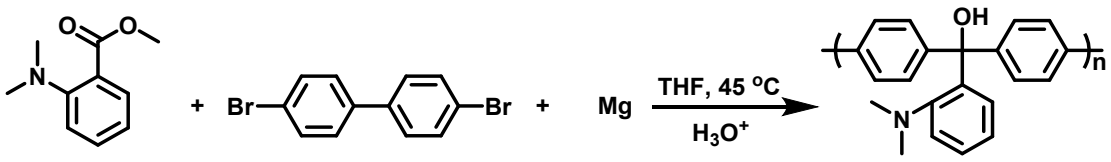
the product was purified by precipitation into excessive petroleum ether, filtered and dried under vacuum, 0.198 g *p*-P(*m*-DMATPM) was obtained as a light-yellow powder with a yield of 56.9 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.01-6.83 (broad, Ar-H, 6H), 6.83-6.22 (broad, Ar-H, 2H), 3.83-3.34 (broad, -OH, 1H), 3.24-2.27 (-CH_3, 6H) ppm.



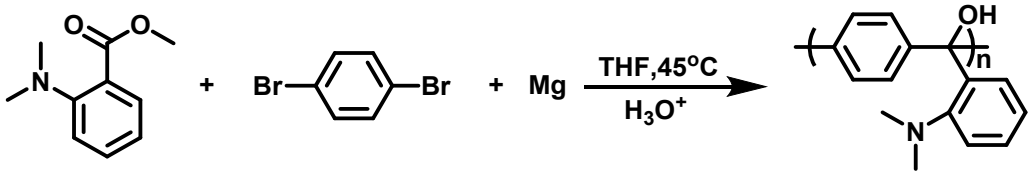
Synthesis of para-poly(*p*-dimethylaminophenyltriphenylmethanol) (*p*-P(*p*-DMAPTPM)). To one flame-dried Schlenk tube containing freshly peeled Mg scraps (0.3 g, 2.4 equivalent), was added 4,4'-dibromobiphenyl (1.61 g, 1.0 equivalent), ethyl 4-dimethylaminobenzoate (1 g ,1.0 equivalent) dissolved in THF (6 mL) at 45°C through a syringe. After 10 minutes, 50 μL of 1,2-dibromoethane was added to initiate the reaction. After the reaction was refluxed for 24 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with 10 mL saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$ and concentrated under reduced pressure. After the product was purified by precipitation into excessive petroleum ether, filtered and dried under vacuum, 1.228 g *p*-P(*p*-DMAPTPM) was obtained as a light-yellow powder with a yield of 78.4 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.11-6.81 (broad, Ar-H,10H), 6.77-6.29 (broad, Ar-H, 2H),3.14-3.05 (broad, -OH, 1H), 3.05-2.39 (-CH_3, 6H) ppm. ^{13}C NMR (100 MHz) δ = 133.65, 132.54, 131.64, 130.02, 129.28, 128.69, 128.45, 128.20, 128.07, 126.87, 126.35, 126.12, 112.27, 111.79, 111.54, 110.98, 110.36, 109.94, 81.31, 40.27 ppm.



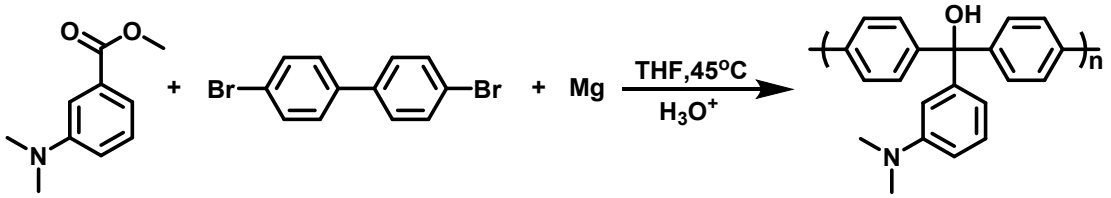
Synthesis of para-poly(*o*-dimethylaminophenyl Triphenylmethanol) (*p*-P(*o*-DMAPTPM)). To one flame-dried Schlenk tube containing freshly peeled Mg scraps (0.16 g, 2.4 equivalent), was added 4,4'-dibromobiphenyl (0.87 g, 1.0 equivalent), methyl 2-dimethylaminobenzoate (0.5 g ,1.0 equivalent) dissolved in THF (4 mL) at 45°C through a syringe. After 10 minutes, 20 μL of 1,2-dibromoethane was added to initiate the reaction. After the reaction was refluxed for 24 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with 10 mL saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$ and concentrated under reduced pressure. After the product was purified by precipitation into excessive petroleum ether, filtered and dried under vacuum, 0.616 g *p*-P(*p*-DMAPTPM) was obtained as a light-yellow powder with a yield of 71.3 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.01-9.90 (broad, -OH, 1H), 8.04-6.96 (broad, Ar-H, 11H), 6.92-6.76 (broad, Ar-H, 1H), 3.03-2.01 (-CH_3, 6H) ppm.



Synthesis of para-poly(*o*-dimethylaminotriphenylmethanol) (*p*-P(*o*-DMATPM)). To one flame-dried Schlenk tube containing freshly peeled Mg scraps (96mg, 2.4 equivalent), was added 1,4-dibromobenzene (0.40 g, 1.0 equivalent), methyl 2-dimethylaminobenzoate (0.3 g ,1.0 equivalent) dissolved in THF (3 mL) at 45°C through a syringe. After 10 minutes, 50 μL of 1,2-dibromoethane was added to initiate the reaction. After the reaction was refluxed for 24 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with 10 mL saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/ water, the organic solution was dried with anhydrous $MgSO_4$ and concentrated under reduced pressure. After the product was purified by precipitation into excessive petroleum ether, filtered and dried under vacuum, 0.218 g *p*-P(*o*-DMAPTPM) was obtained as a light-yellow powder with a yield of 57.6%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.01-9.90 (broad, -OH, 1H), 8.04-6.96 (broad, Ar-H, 11H), 6.92-6.76 (broad, Ar-H, 1H), 3.03-2.01 (-CH_3, 6H) ppm.



Synthesis of para-poly(*m*-dimethylaminophenyl Triphenylmethanol) (*p*-P(*m*-DMAPTPM)). To one flame-dried Schlenk tube containing freshly peeled Mg scraps (96mg, 2.4 equivalent), was added 4,4'-dibromobiphenyl (0.52 g, 1.0 equivalent), methyl 3-dimethylaminobenzoate (0.3 g ,1.0 equivalent) dissolved in THF (3 mL) at 45°C through a syringe. After 10 minutes, 10 μL of 1,2-dibromoethane was added to initiate the reaction. After the reaction was refluxed for 24 h, the solution was cooled to room temperature, followed by quenching and hydrolysis with 10 mL saturated aqueous ammonium chloride. After filtration and workup with dichloromethane/water, the organic solution was dried with anhydrous $MgSO_4$ and concentrated under reduced pressure. After the product was purified by precipitation into excessive petroleum ether, filtered and dried under vacuum, 0.314 g *p*-P(*m*-DMAPTPM) was obtained as a light-yellow powder with a yield of 62.1%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.01-6.95 (broad, Ar-H, 11H), 6.95-6.33 (broad, Ar-H, 1H), 3.01-2.97 (broad, -OH, 1H), 2.97-2.25 (-CH_3, 6H) ppm.



Result characterization data

Synthetic characterization

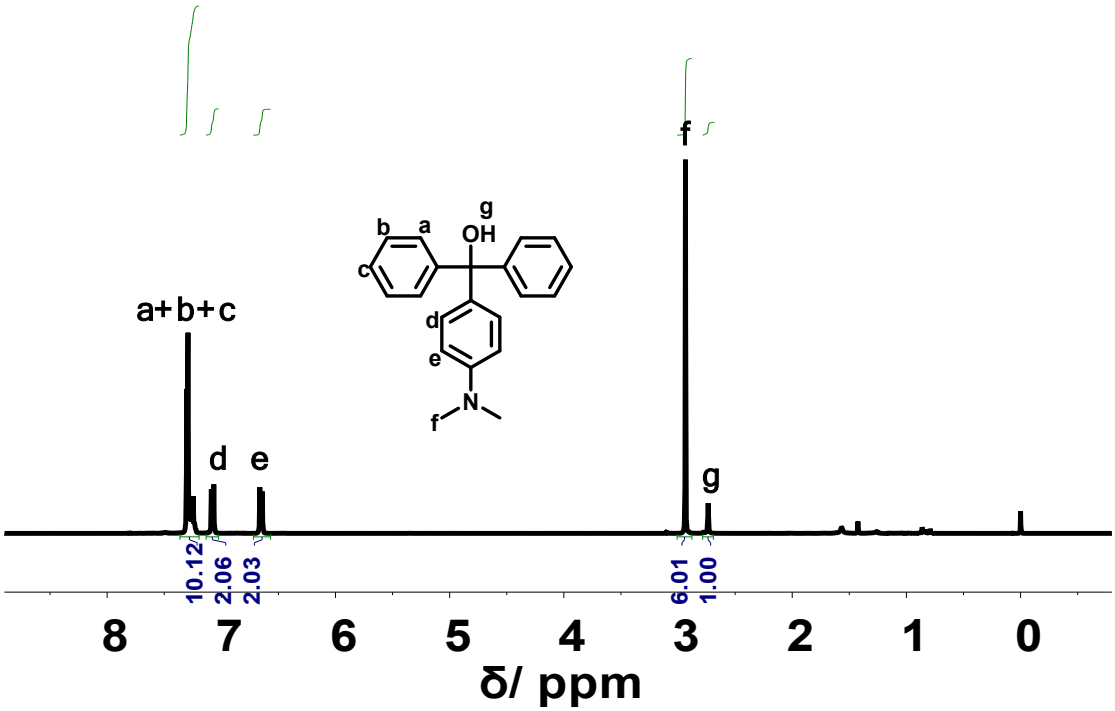


Figure S1. ^{1}H NMR (400 MHz) spectrum of *p*-DMATPM in $CDCl_3$.

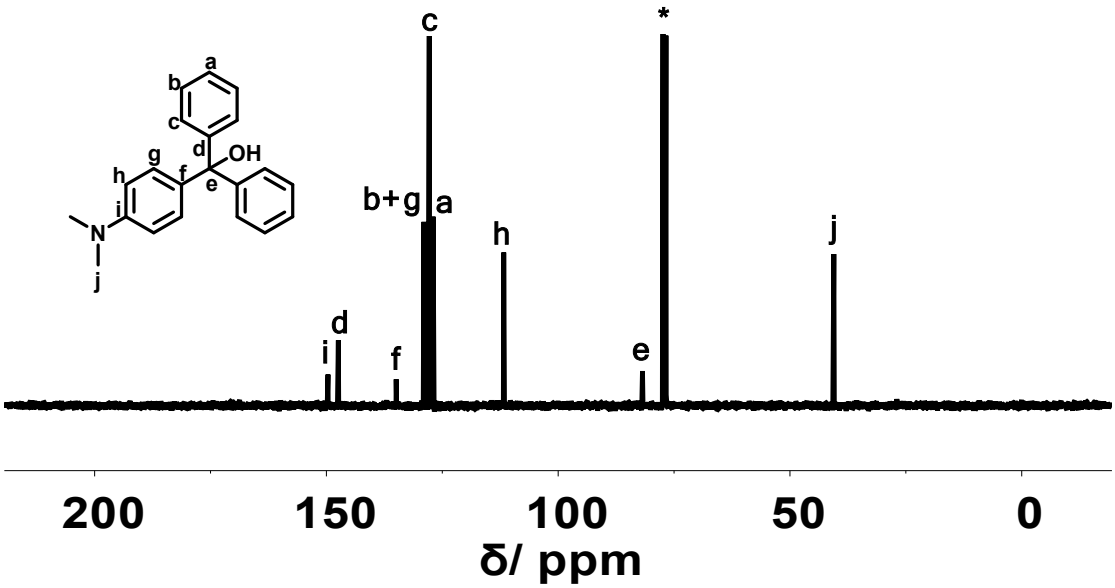


Figure S2. ^{13}C NMR (100 MHz) spectrum of *p*-DMATPM in $CDCl_3$.

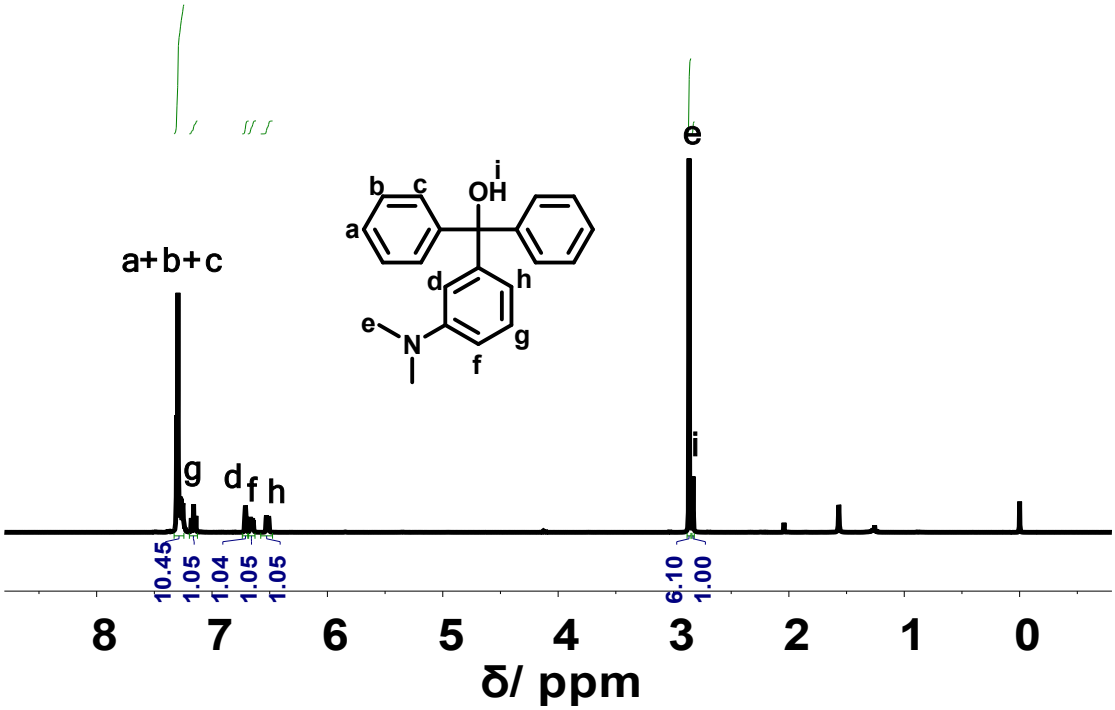


Figure S3. ^{1}H NMR (400 MHz) spectrum of *m*-DMATPM in $CDCl_3$.

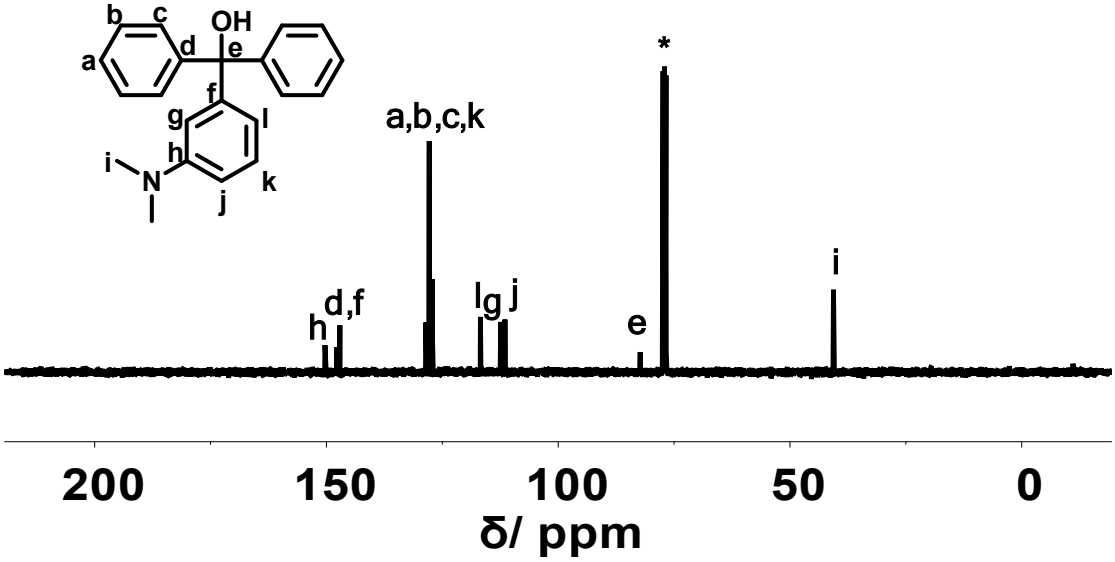


Figure S4. ^{13}C NMR (100 MHz) spectrum of *m*-DMATPM in $CDCl_3$.

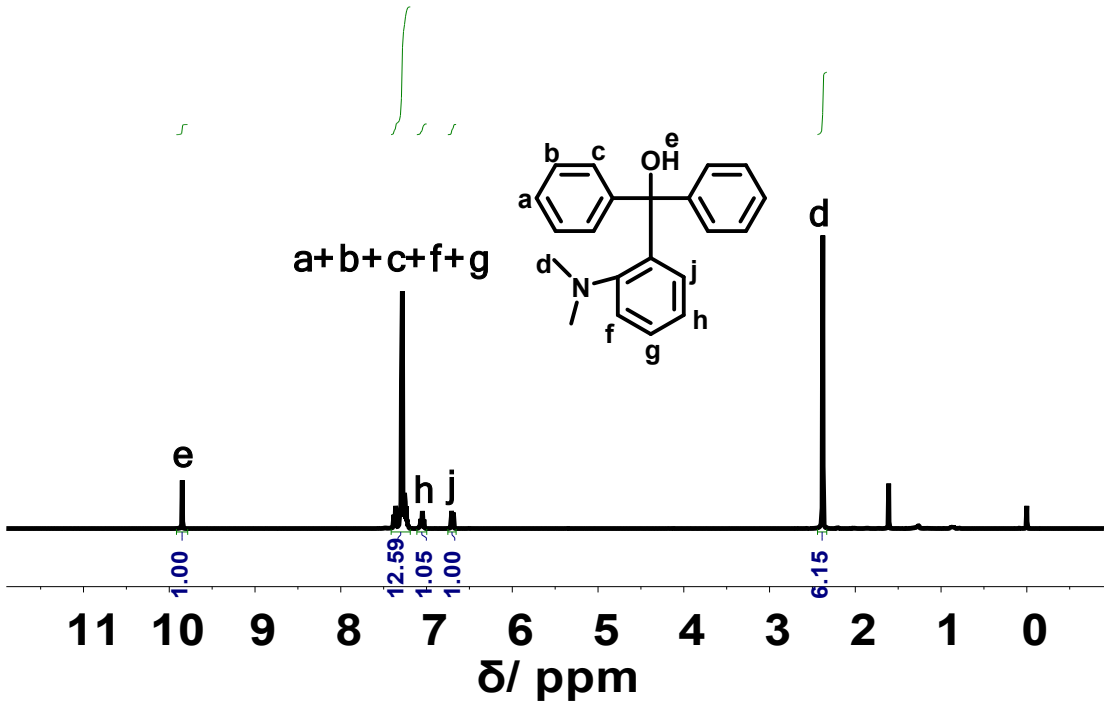


Figure S5. ^{1}H NMR (400 MHz) spectrum of *o*-DMATPM in $CDCl_3$.

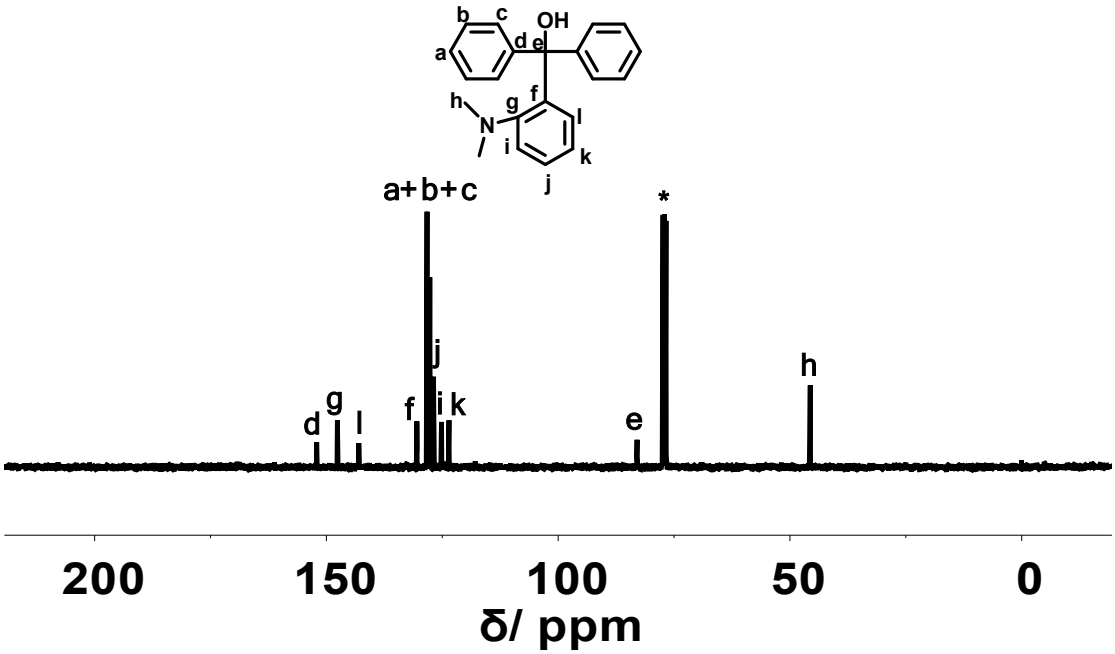


Figure S6. ^{13}C NMR (100 MHz) spectrum of *o*-DMATPM in $CDCl_3$.

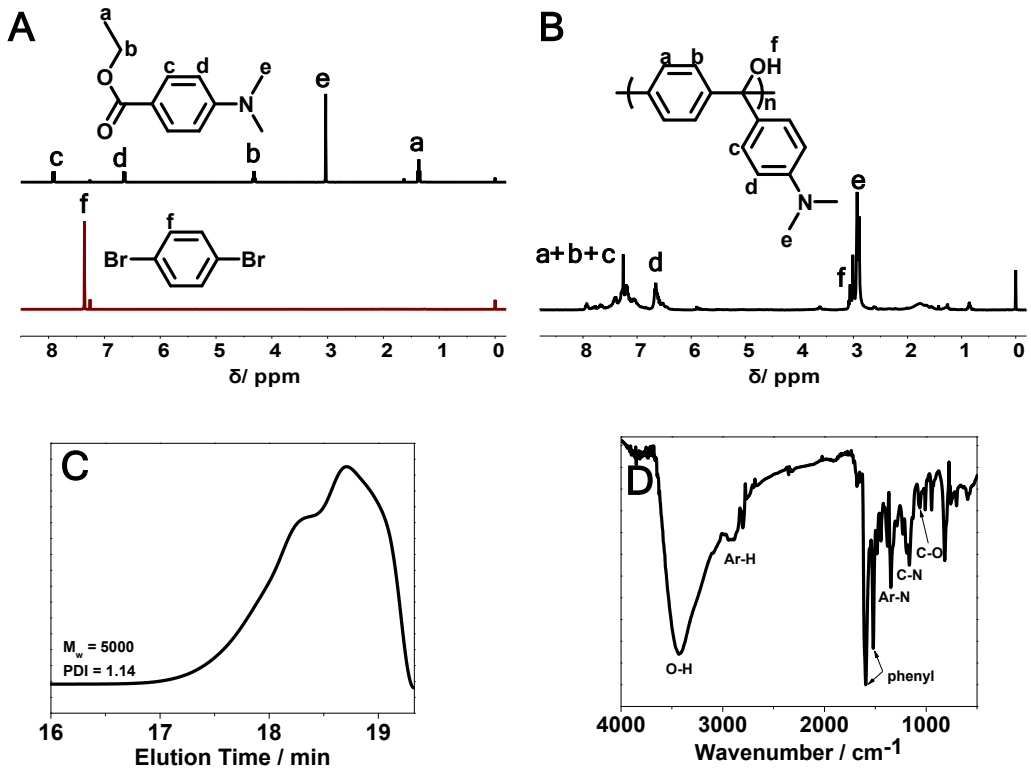


Figure S7. (A) ^{1}H NMR spectra of ethyl 4-dimethylaminobenzoate (top) and 1,4-dibromobenzene (bottom) in $CDCl_3$, ^{1}H NMR spectrum (B), GPC curve (C) and FT-IR spectrum (D) of *p*-P(*p*-DMATPM).

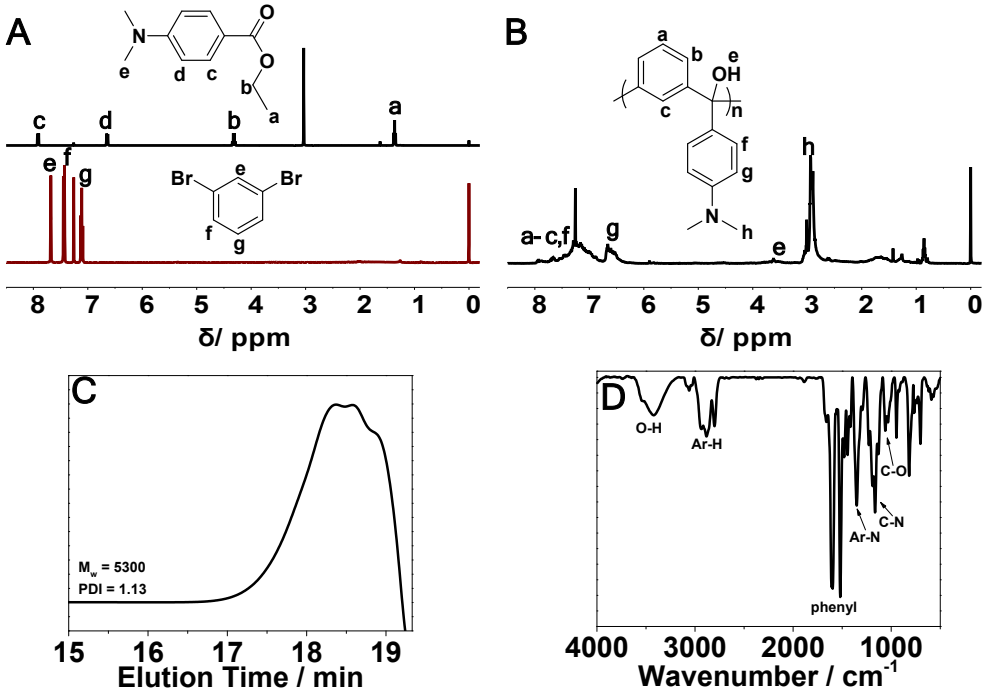


Figure S8. (A) ^{1}H NMR spectra of ethyl 4-dimethylaminobenzoate (top) and 1,3-dibromobenzene (bottom) in $CDCl_3$, ^{1}H NMR spectrum (B), GPC curve (C) and FT-IR spectrum (D) of *m*-P(*p*-DMATPM).

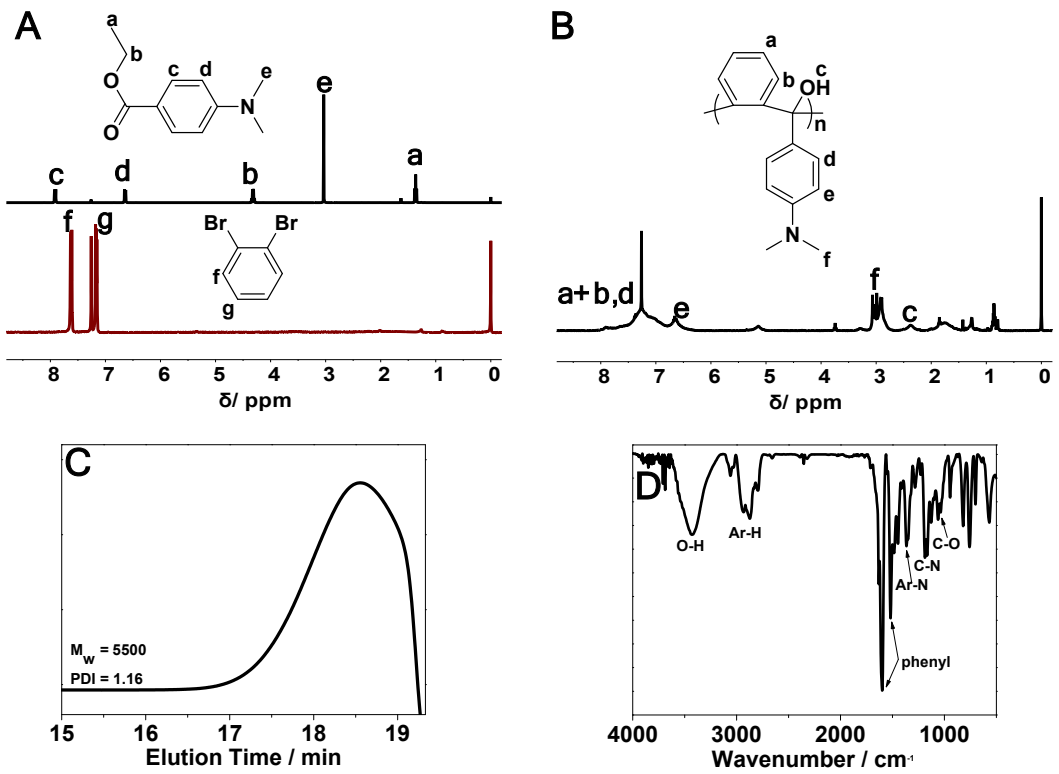


Figure S9. (A) ^{1}H NMR spectra of ethyl 4-dimethylaminobenzoate (top) and 1,2-dibromobenzene (bottom) in $CDCl_3$, ^{1}H NMR spectrum (B), GPC curve (C) and FT-IR spectrum (D) of *o*-P(*p*-DMATPM).

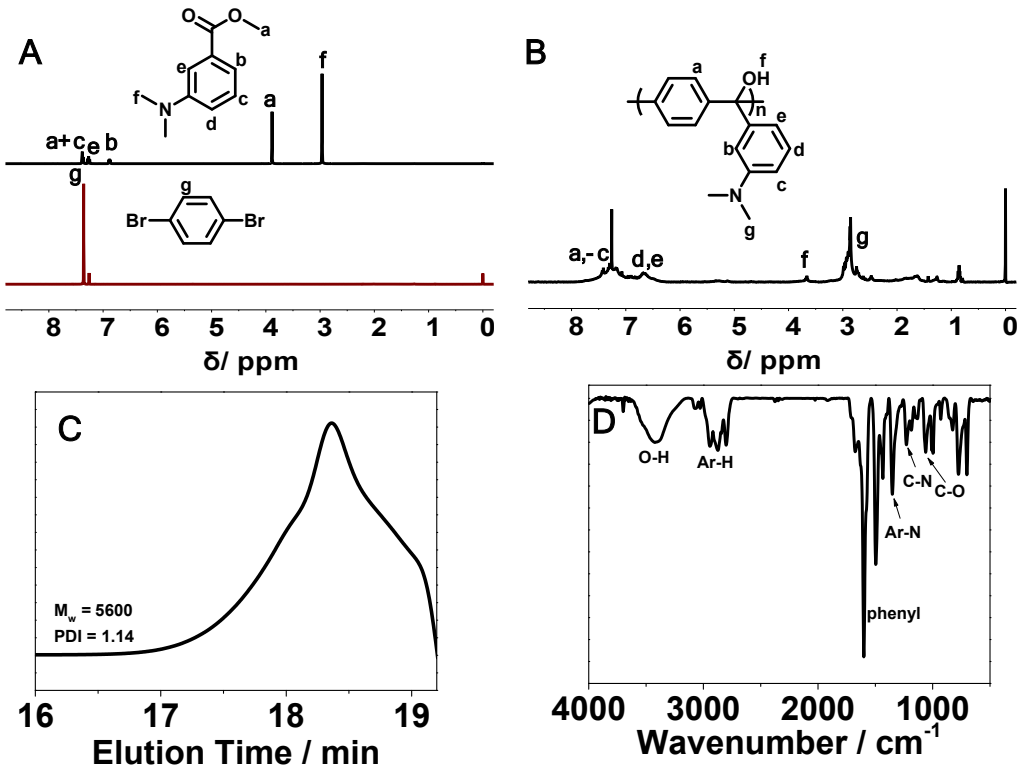


Figure S10. (A) ^{1}H NMR spectra of methyl 3-dimethylaminobenzoate (top) and 1,4-dibromobenzene (bottom) in $CDCl_3$, ^{1}H NMR spectrum (B), GPC curve (C) and FT-IR spectrum (D) of *p*-P(*m*-DMATPM).

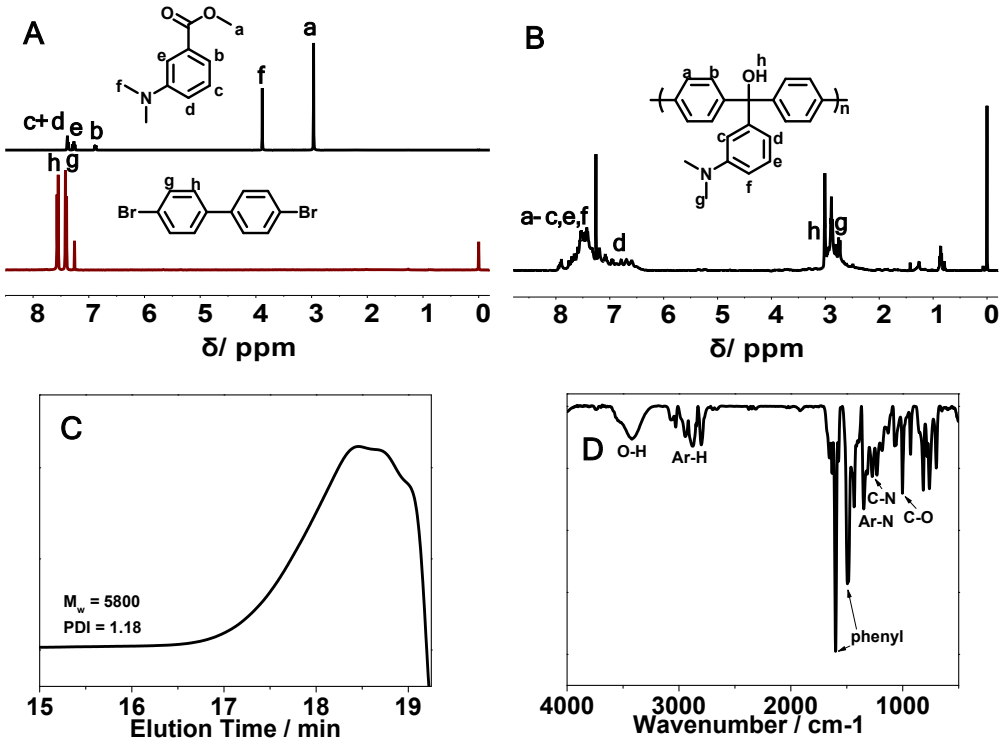


Figure S11. (A) ^{1}H NMR spectra of methyl 3-dimethylaminobenzoate (top) and 4,4'-dibromobiphenyl (bottom) in $CDCl_3$, ^{1}H NMR spectrum (B), GPC curve (C) and FT-IR spectrum (D) of *p*-P(*m*-DMAPTPM).

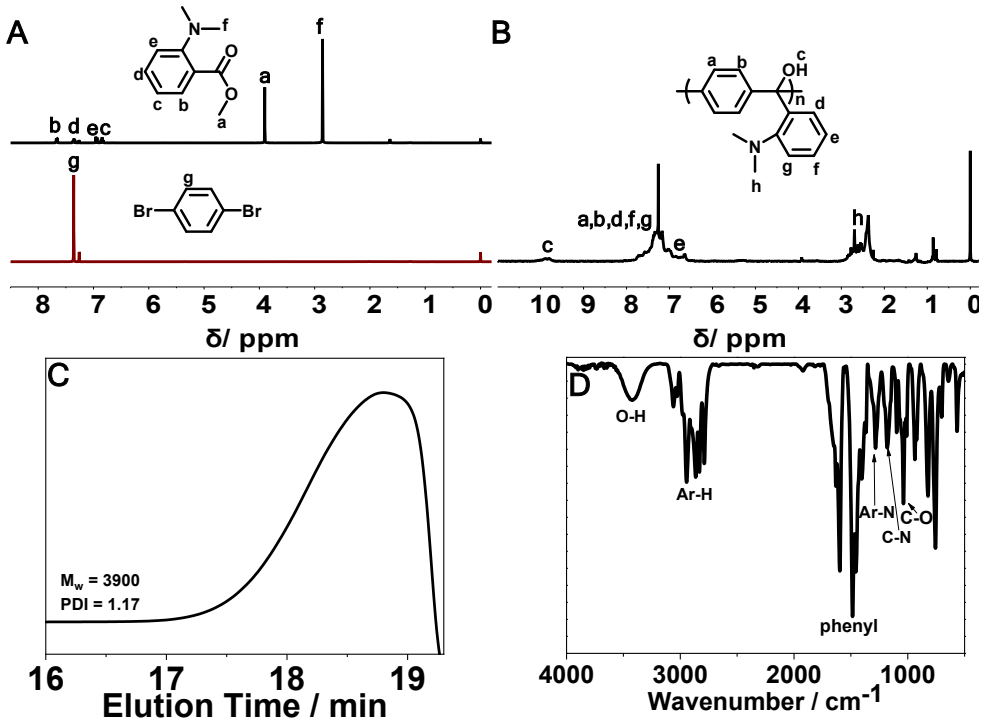


Figure S12. (A) ^{1}H NMR spectra of methyl 2-dimethylaminobenzoate (top) and 1,4-dibromobenzene (bottom) in $CDCl_3$, ^{1}H NMR spectrum (B), GPC curve (C) and FT-IR spectrum (D) of *p*-P(*o*-DMATPM).

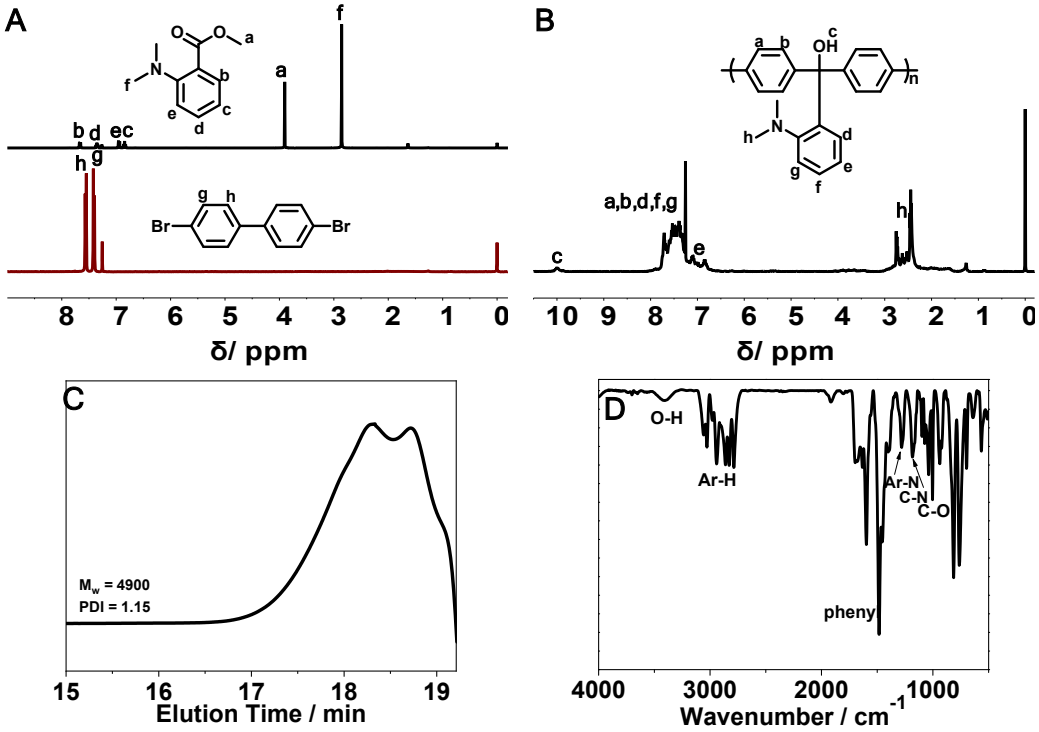
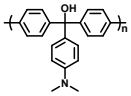
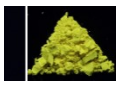
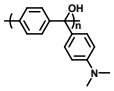
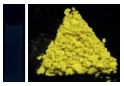
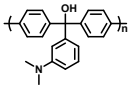
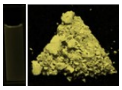
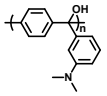
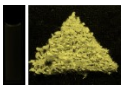
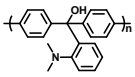
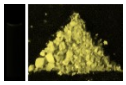
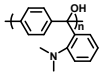
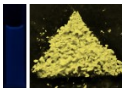
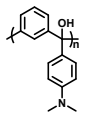
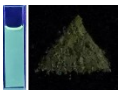
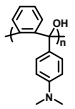
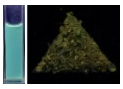


Figure S13. (A) ^{1}H NMR spectra of methyl 2-dimethylaminobenzoate (top) and 4,4'-dibromobiphenyl (bottom) in $CDCl_3$, ^{1}H NMR spectrum(B), GPC curve (C) and FT-IR spectrum (D) of *p*-P(*o*-DMAPTPM).

Characterization of luminescent properties

Table S1. The photophysical data of PDMATPMs.

Entry	Structure	Abbreviation	λ_{abs} (nm)[a]	λ_{em} (nm)		FL[c]
				THF[b]	Solid	
1		*p*-P(*p*-DMAPTPM)	256	-	530	
2		*p*-P(*p*-DMATPM)	262	-	535	
3		*p*-P(*m*-DMAPTPM)	255	-	547	
4		*p*-P(*m*-DMATPM)	250	-	543	
5		*p*-P(*o*-DMAPTPM)	261	-	529	
6		*p*-P(*o*-DMATPM)	238	-	540	
7		*m*-P(*p*-DMATPM)	263	479	-	
8		*o*-P(*p*-DMATPM)	242	476	-	

a. Maximum absorption wavelength;

b. Measured with 0.1 mg/mL solution in THF;

c. Photographs (under irradiation with UV lamp at 365 nm).

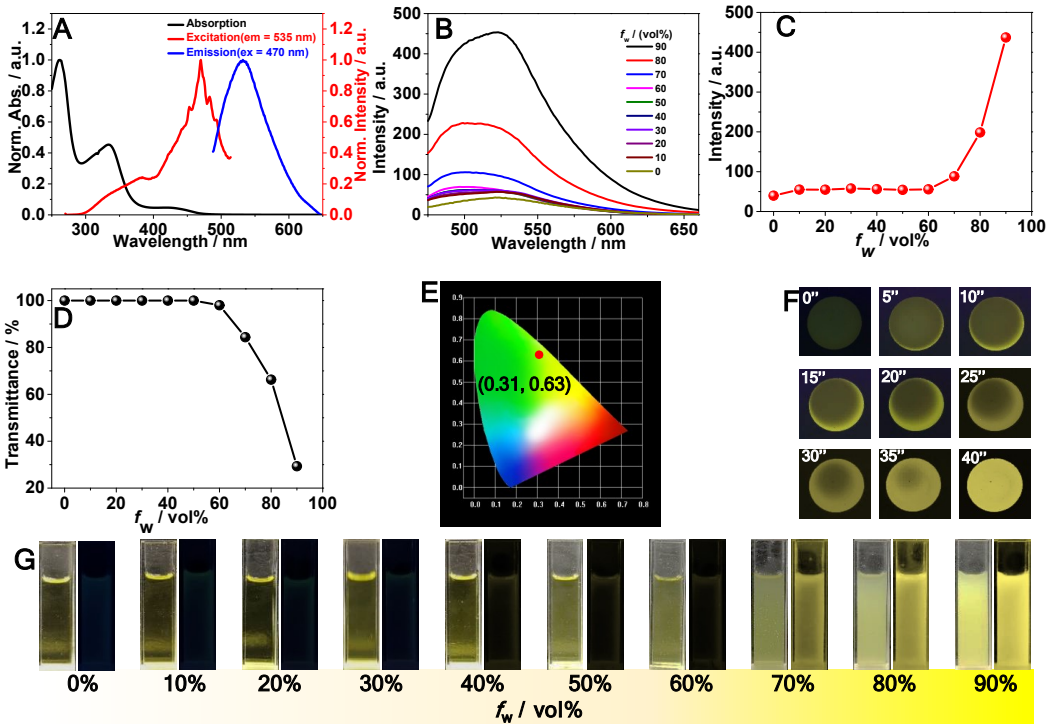


Figure S14. Luminescence properties of *p*-P(*p*-DMATPM). (A) Normalized excitation (red line) and emission (blue line) spectra of *p*-P(*p*-DMATPM) in the solid state and normalized absorption spectra (black line) of *p*-P(*p*-DMATPM) in THF. (B) Emission spectra of *p*-P(*p*-DMATPM) (0.1 mg/mL) in water/THF mixtures with different water volume fractions (f_w, vol %) (excited at 470 nm). (C) Plots of emission intensities of *p*-P(*p*-DMATPM) (0.1 mg/mL) in water/THF mixtures with different water volume fractions (f_w, vol %) (excited at 470 nm). (D) Transmittance of *p*-P(*p*-DMATPM) (0.1 mg/mL) in water/THF mixtures with different water volume fractions (f_w, vol %). (E) CIE coordinate of *p*-P(*p*-DMATPM). (F) Digital photos of one drop of *p*-P(*p*-DMATPM) solution (10 mg/mL in THF) on thin-layer chromatography at different times (time unit is second) of evaporation (under UV irradiation at 365 nm). (G) Digital photos of *p*-P(*p*-DMATPM) (0.1 mg/mL) in water/THF mixtures with different water volume fractions (f_w, vol %) (under sunlight and UV irradiation at 365 nm).

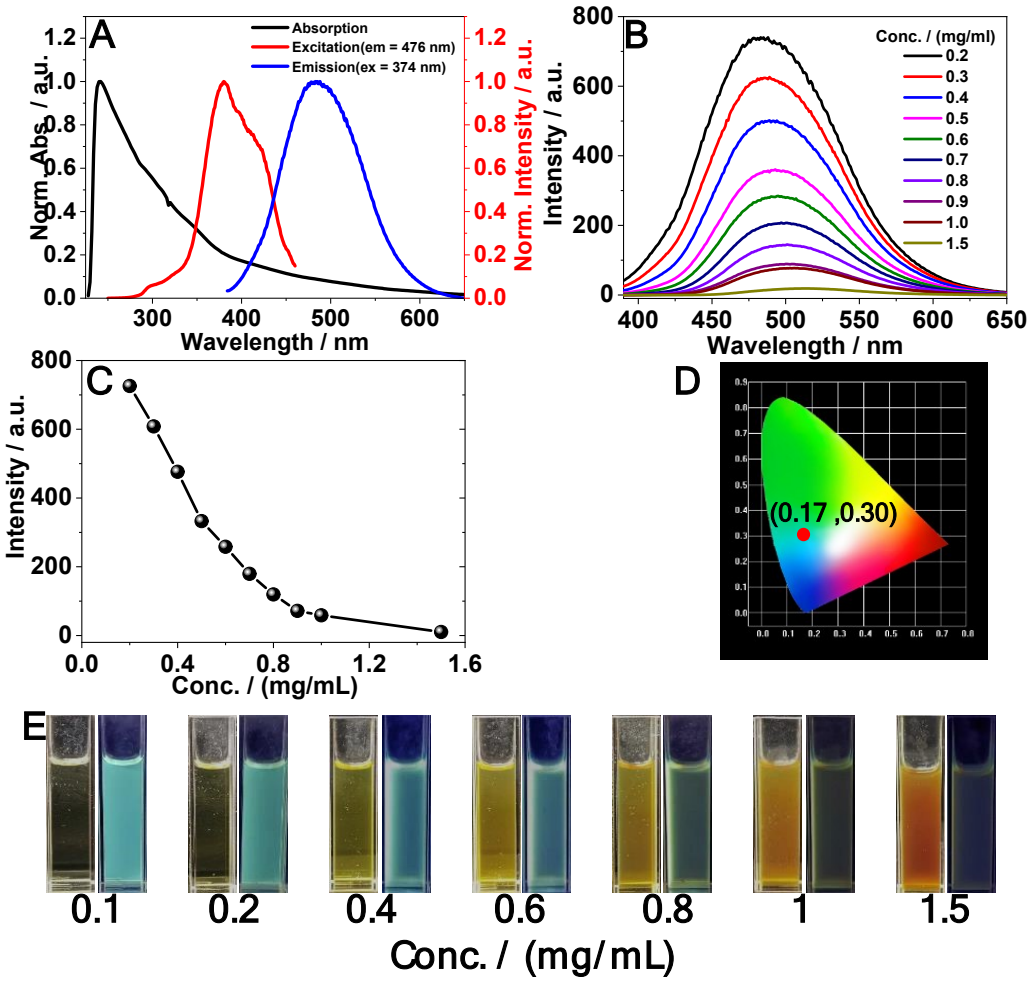


Figure S15. Luminescence properties of *o*-P(*p*-DMATPM). (A) Normalized excitation (red line) and emission (blue line) spectra of *o*-P(*p*-DMATPM) in solution and normalized absorption spectra (black line) of *o*-P(*p*-DMATPM) in THF. (B) The solution luminescence quenching curve (excited at 374 nm), THF was chosen as the solvent used in the measurement. (C) Plots of emission intensities of *o*-P(*p*-DMATPM) with different concentration (excited at 374 nm). (D) CIE coordinate of *o*-P(*p*-DMATPM). (E) Digital photos of *o*-P(*p*-DMATPM) solution with different concentration (under sunlight (left) and UV irradiation at 365 nm(right)).

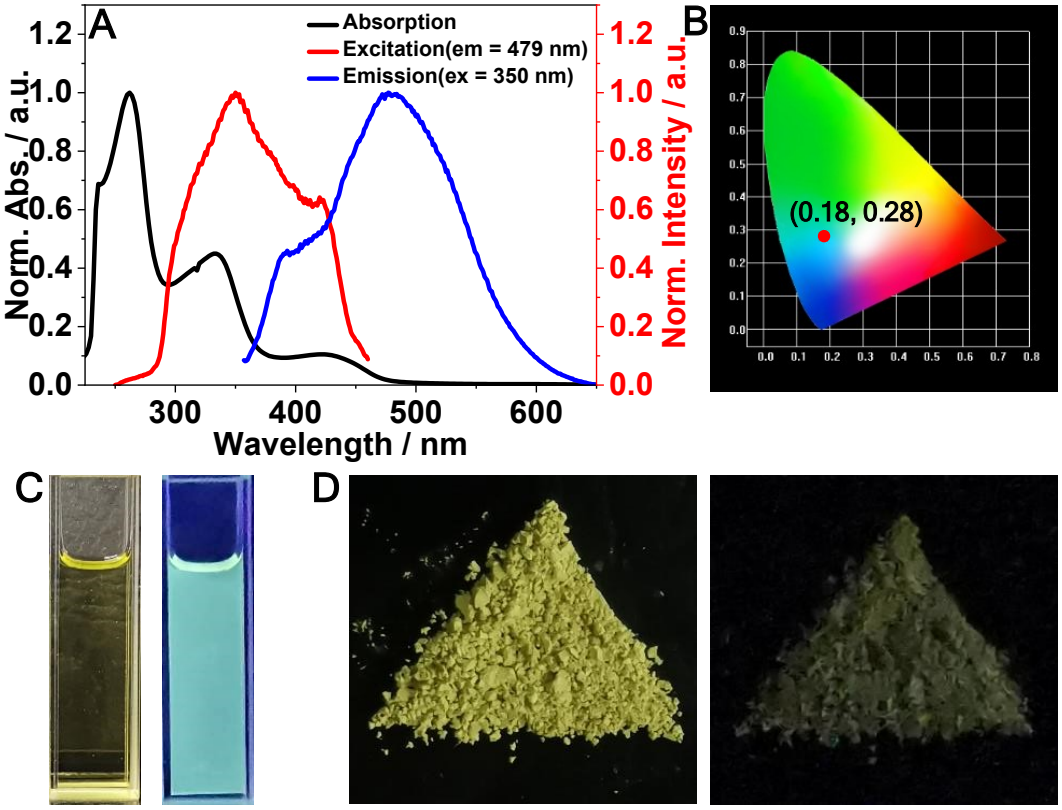


Figure S16. Luminescence properties of *m*-P(*p*-DMATPM). (A) Normalized excitation (red line) and emission (blue line) spectra of *m*-P(*p*-DMATPM) in solution and normalized absorption spectra (black line) of *m*-P(*p*-DMATPM) in THF. (B) CIE coordinate of *m*-P(*p*-DMATPM). (C) Digital photos of *m*-P(*p*-DMATPM) solution in THF with 0.1 mg/mL (under sunlight (left) and UV irradiation at 365 nm (right)). (D) Digital photos of *m*-P(*p*-DMATPM) solid (under sunlight (left) and UV irradiation at 365 nm(right)).

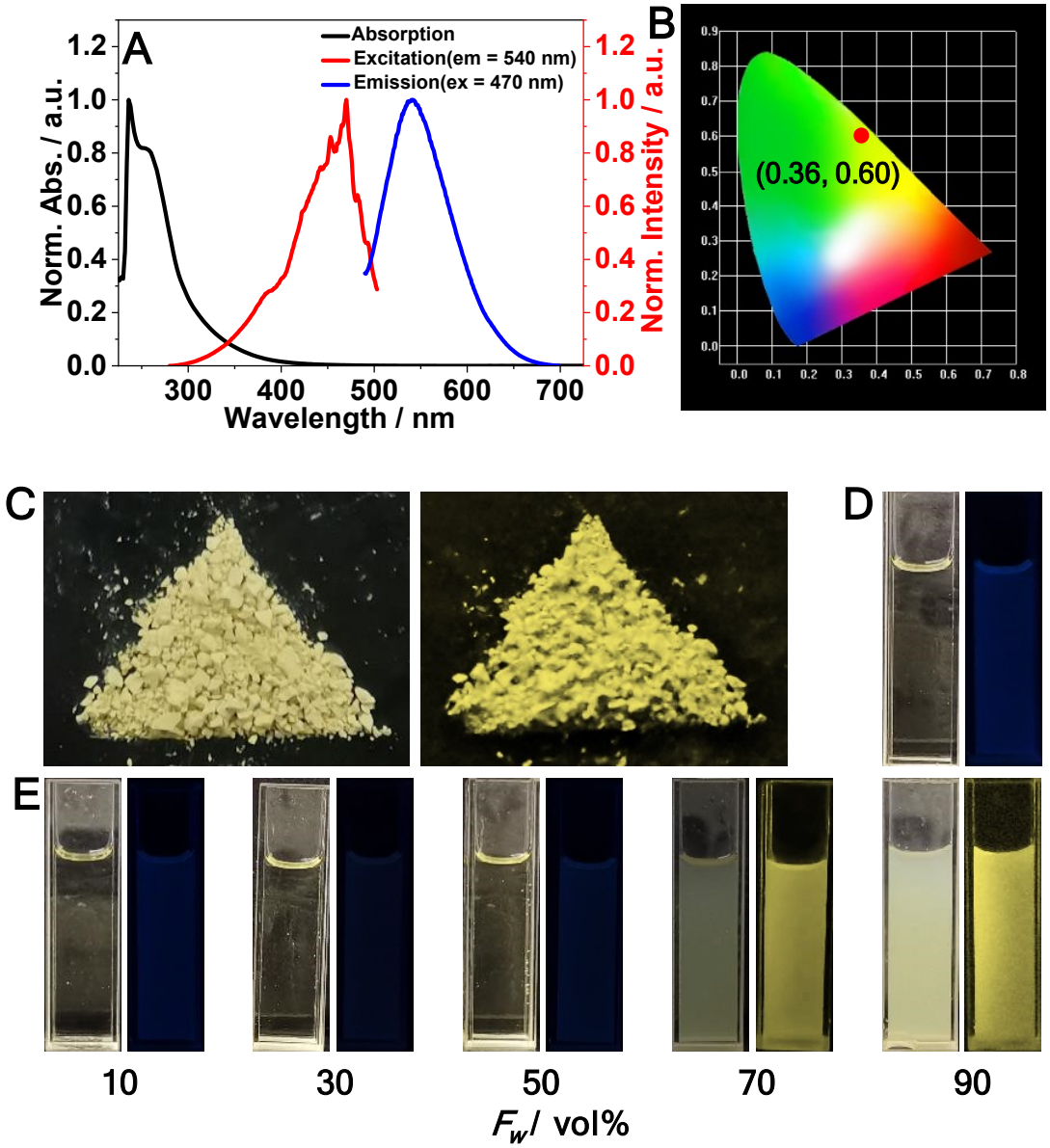


Figure S17. Luminescence properties of *p*-P(*o*-DMATPM). (A) Normalized excitation (red line) and emission (blue line) spectra of *p*-P(*o*-DMATPM) in solution and normalized absorption spectra (black line) of *p*-P(*o*-DMATPM) in THF. (B) CIE coordinate of *p*-P(*o*-DMATPM). (C) Digital photos of *p*-P(*o*-DMATPM) solid (under sunlight (left) and UV irradiation at 365 nm(right)). (D) Digital photos of *p*-P(o-DMATPM) solution in THF with 0.1 mg/ mL (under sunlight (left) and UV irradiation at 365 nm (right)). (E) Digital photos of *p*-P(*o*-DMATPM) (0.1 mg/mL) in water/THF mixtures with different water volume fractions (f_w, vol %) (under sunlight and UV irradiation at 365 nm).

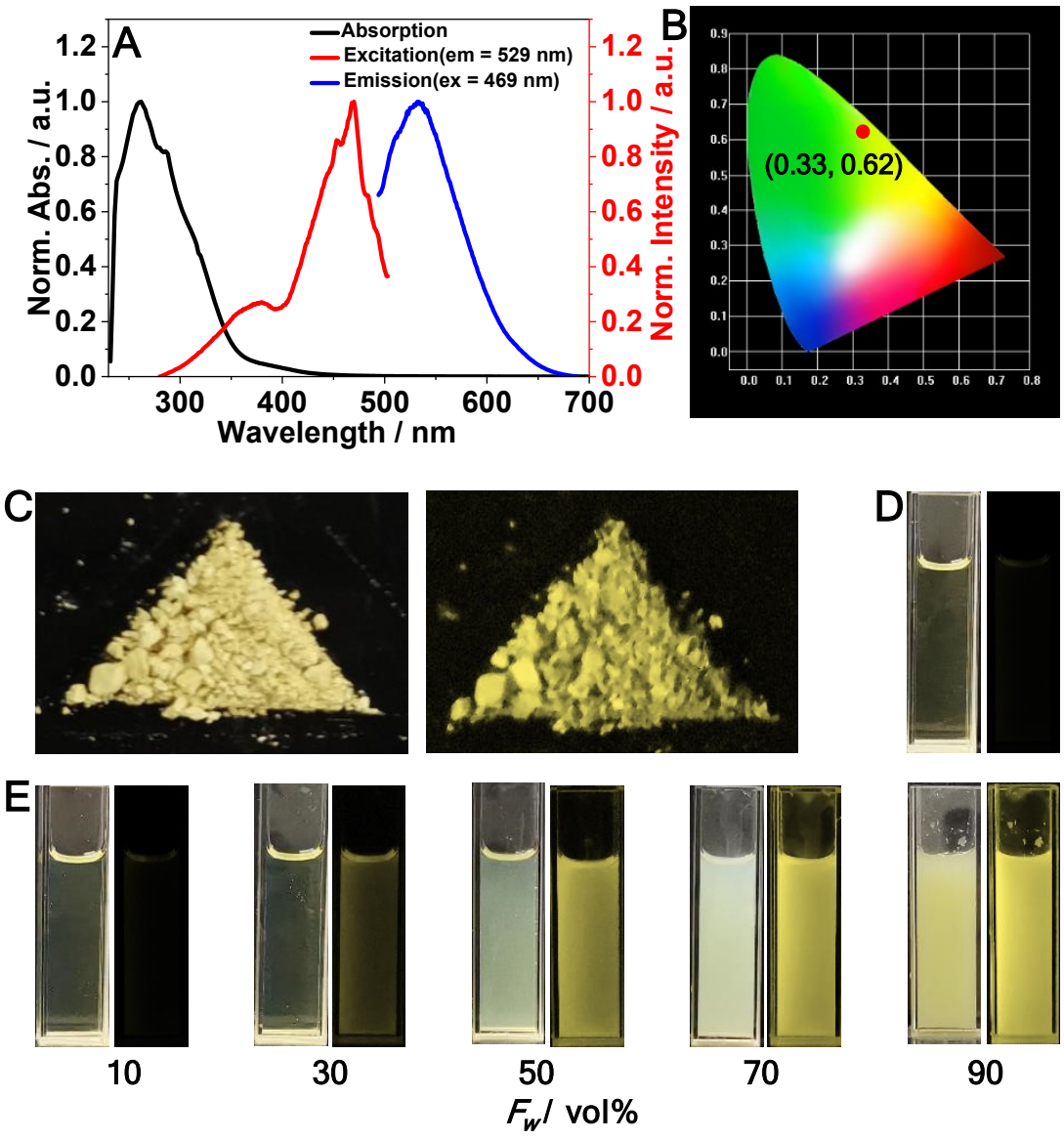


Figure S18. Luminescence properties of *p*-P(*o*-DMAPTPM). (A) Normalized excitation (red line) and emission (blue line) spectra of *p*-P(*o*-DMAPTPM) in solution and normalized absorption spectra (black line) of *p*-P(*o*-DMAPTPM) in THF. (B) CIE coordinate of *p*-P(*o*-DMAPTPM). (C) Digital photos of *p*-P(*o*-DMAPTPM) solid (under sunlight (left) and UV irradiation at 365 nm(right)). (D) Digital photos of *p*-P(o-DMAPTPM) solution in THF with 0.1 mg/ mL (under sunlight (left) and UV irradiation at 365 nm (right)). (E) Digital photos of *p*-P(*o*-DMAPTPM) (0.1 mg/mL) in water/THF mixtures with different water volume fractions (f_w, vol %) (under sunlight and UV irradiation at 365 nm).

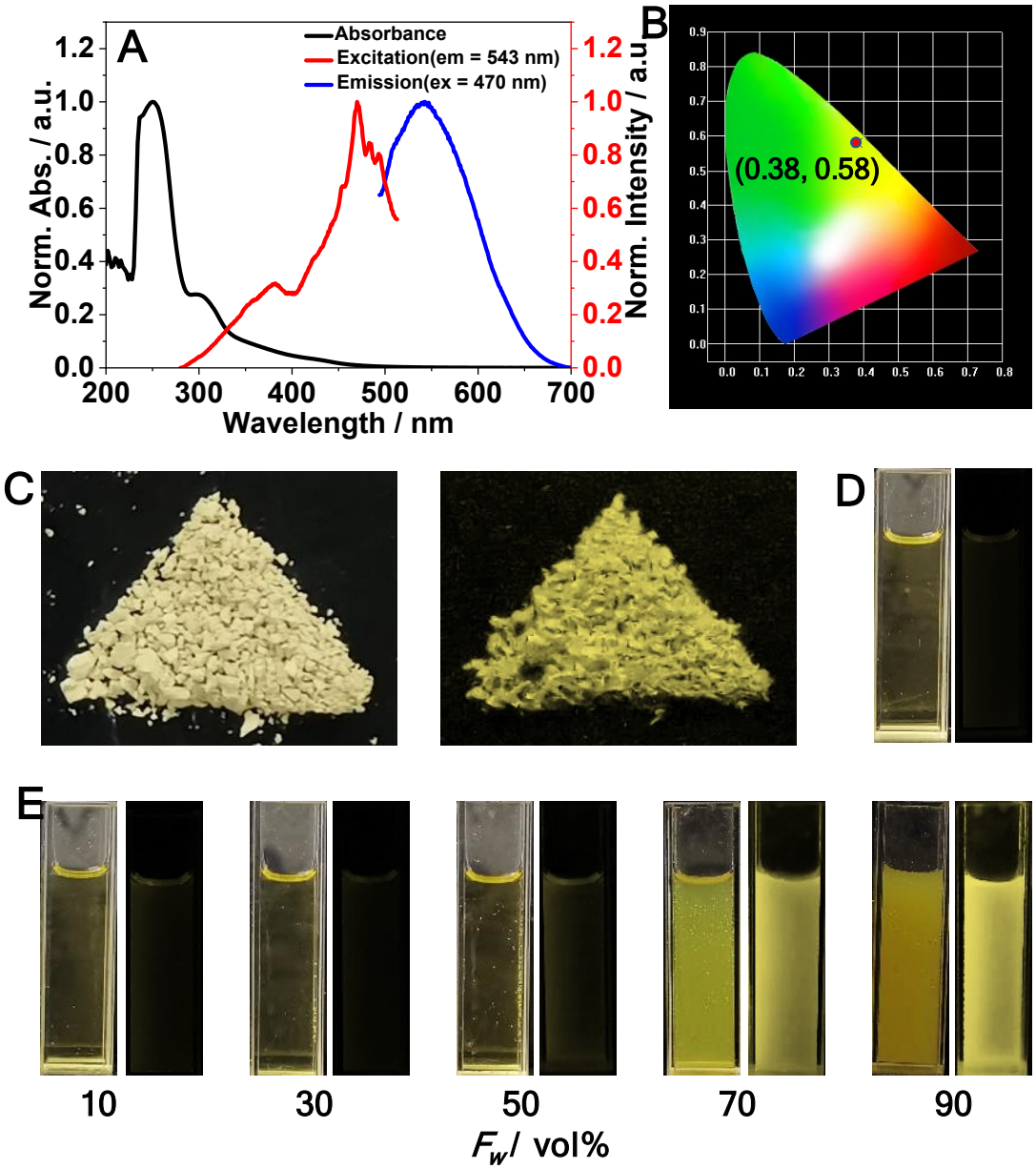


Figure S19. Luminescence properties of *p*-P(*m*-DMATPM). (A) Normalized excitation (red line) and emission (blue line) spectra of *p*-P(*m*-DMATPM) in solution and normalized absorption spectra (black line) of *p*-P(*m*-DMATPM) in THF. (B) CIE coordinate of *p*-P(*m*-DMATPM). (C) Digital photos of *p*-P(*m*-DMATPM) solid (under sunlight (left) and UV irradiation at 365 nm(right)). (D) Digital photos of *p*-P(*m*-DMATPM) solution in THF with 0.1 mg/ mL (under sunlight (left) and UV irradiation at 365 nm (right)). (E) Digital photos of *p*-P(*m*-DMATPM) (0.1 mg/mL) in water/THF mixtures with different water volume fractions (f_w, vol %) (under sunlight and UV irradiation at 365 nm).

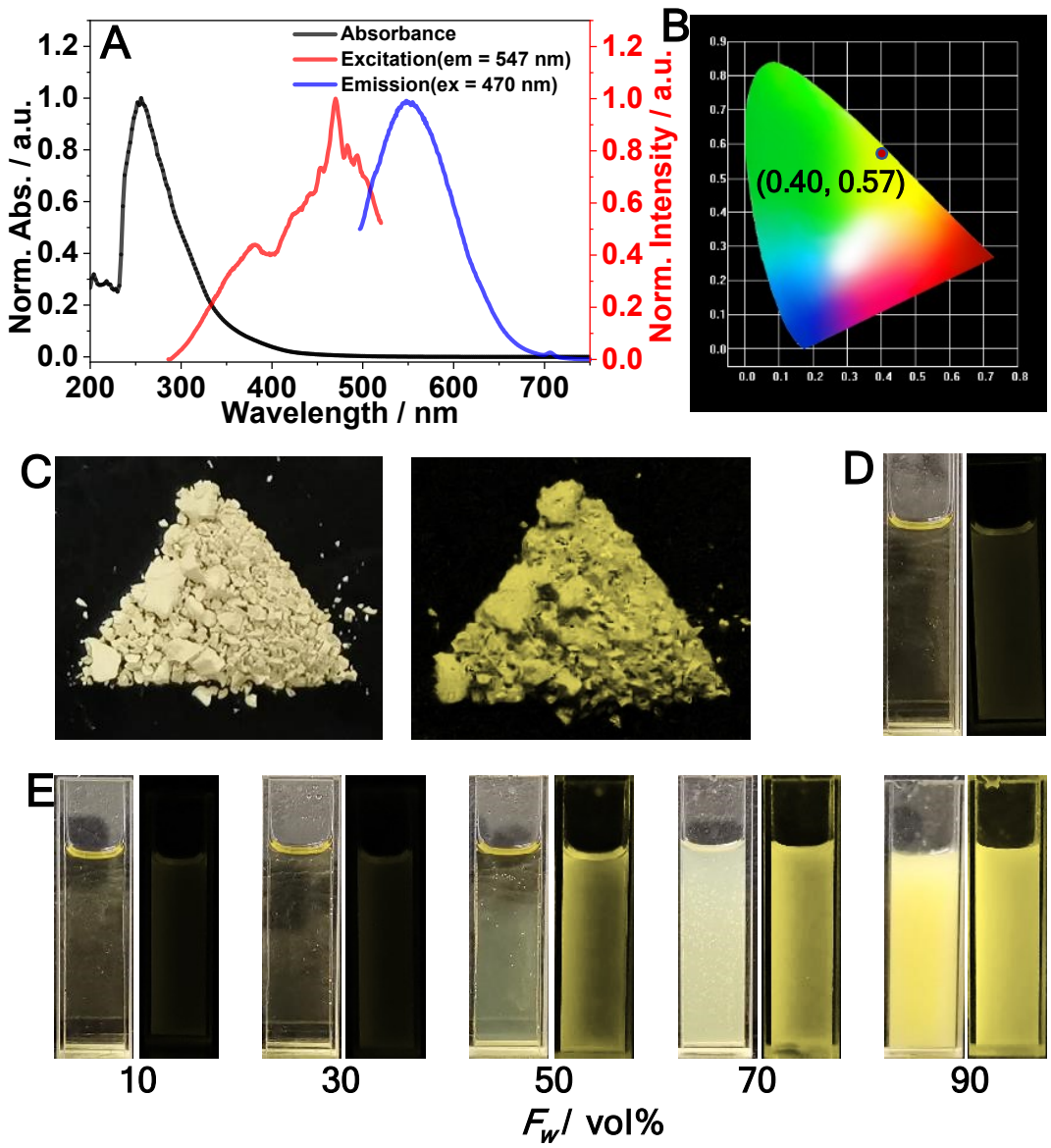


Figure S20. Luminescence properties of *p*-P(*m*-DMAPTPM). (A) Normalized excitation (red line) and emission (blue line) spectra of *p*-P(*m*-DMAPTPM) in solution and normalized absorption spectra (black line) of *p*-P(*m*-DMAPTPM) in THF. (B) CIE coordinate of *p*-P(*m*-DMAPTPM). (C) Digital photos of *p*-P(*m*-DMAPTPM) solid (under sunlight (left) and UV irradiation at 365 nm(right)). (D) Digital photos of *p*-P(*m*-DMAPTPM) solution in THF with 0.1 mg/ mL (under sunlight (left) and UV irradiation at 365 nm (right)). (E) Digital photos of *p*-P(*m*-DMAPTPM) (0.1 mg/mL) in water/THF mixtures with different water volume fractions (f_w, vol %) (under sunlight and UV irradiation at 365 nm).

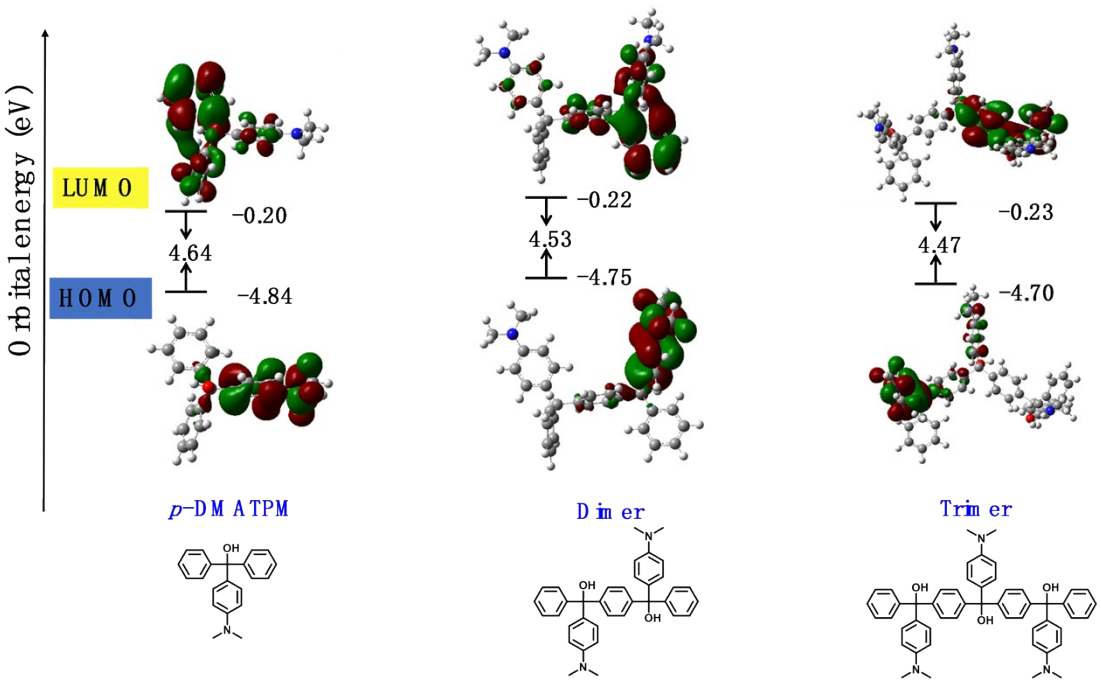


Figure S21. Electron cloud distributions and energy levels (eV) of *p*-DAMTPM, dimer, trimer, in the S1 excited state calculated by TD-DFT B3LYP/6-311G*, Gaussian 09 program.

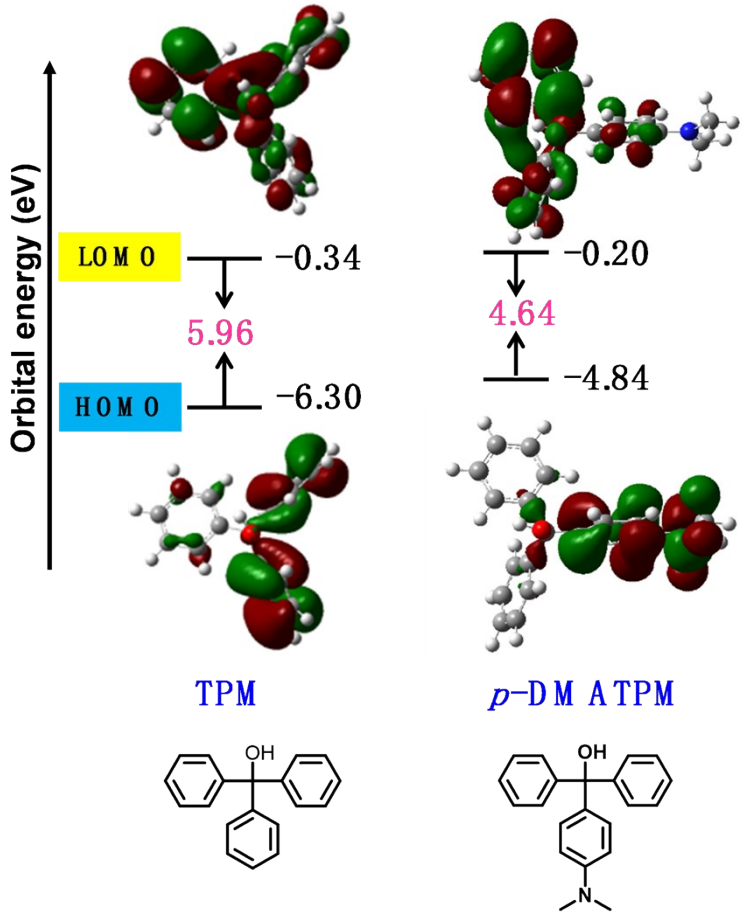


Figure S22. Electron cloud distributions and energy levels (eV) of TPM and *p*-DMATPM in the S1 excited state calculated by TD-DFT B3LYP/6-311G*, Gaussian 09 program.

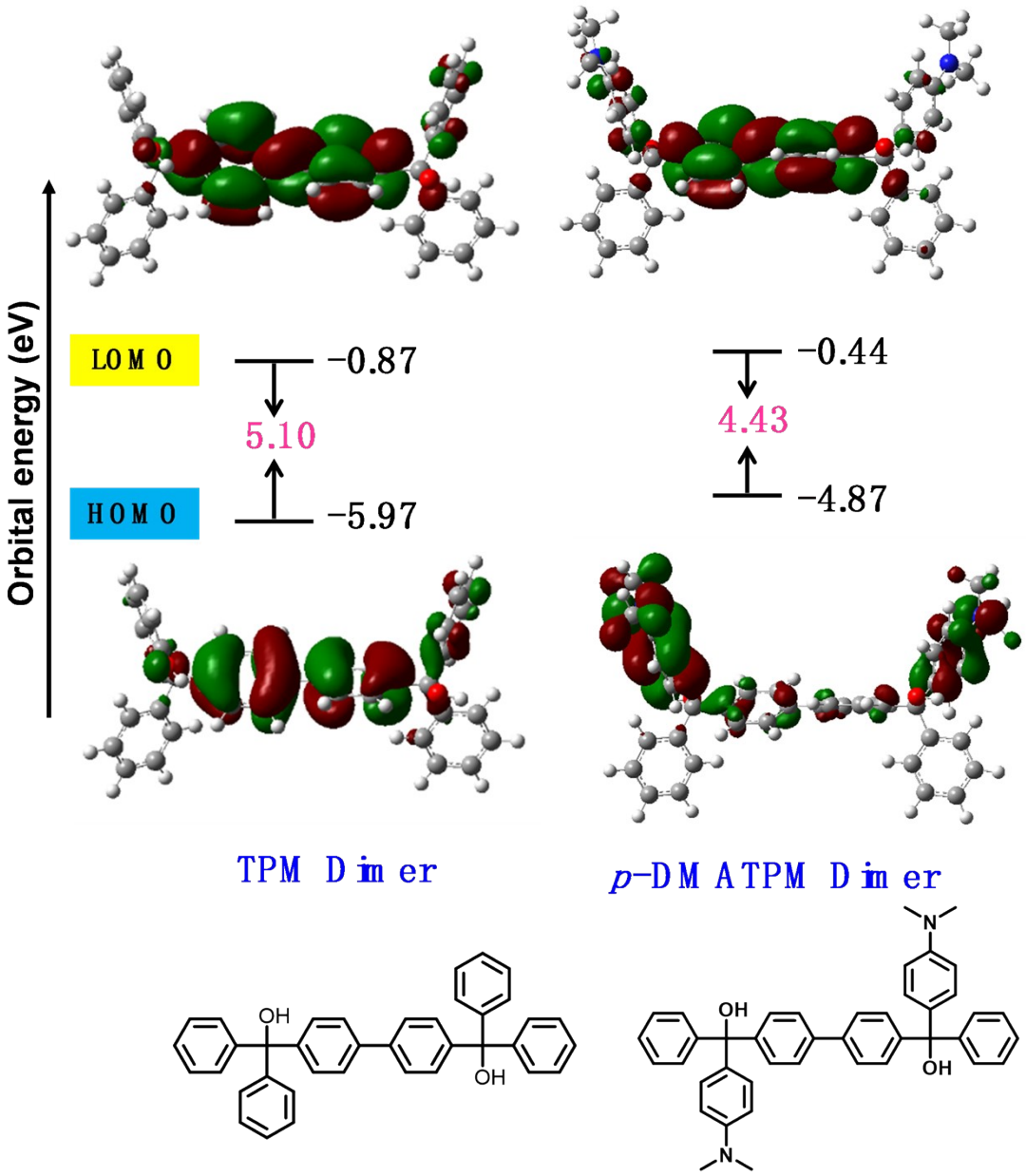


Figure S23. Electron cloud distributions and energy levels (eV) of TPM Dimer and *p*-DMATPM Dimer in the S1 excited state calculated by TD-DFT B3LYP/6-311G*, Gaussian 09 program.

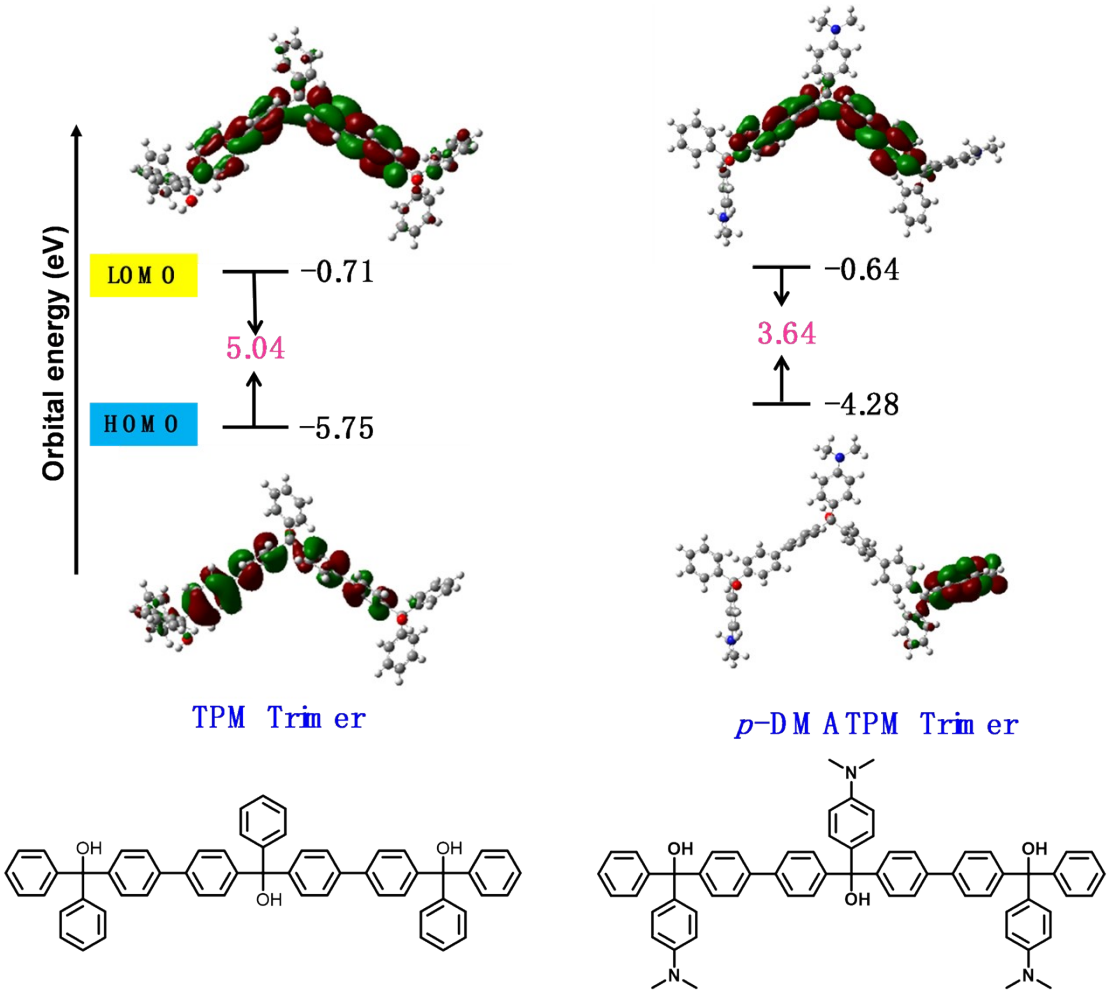


Figure S24. Electron cloud distributions and energy levels (eV) of TPM Trimer and *p*-DMATPM Trimer in the S1 excited state calculated by TD-DFT B3LYP/6-311G*, Gaussian 09 program.

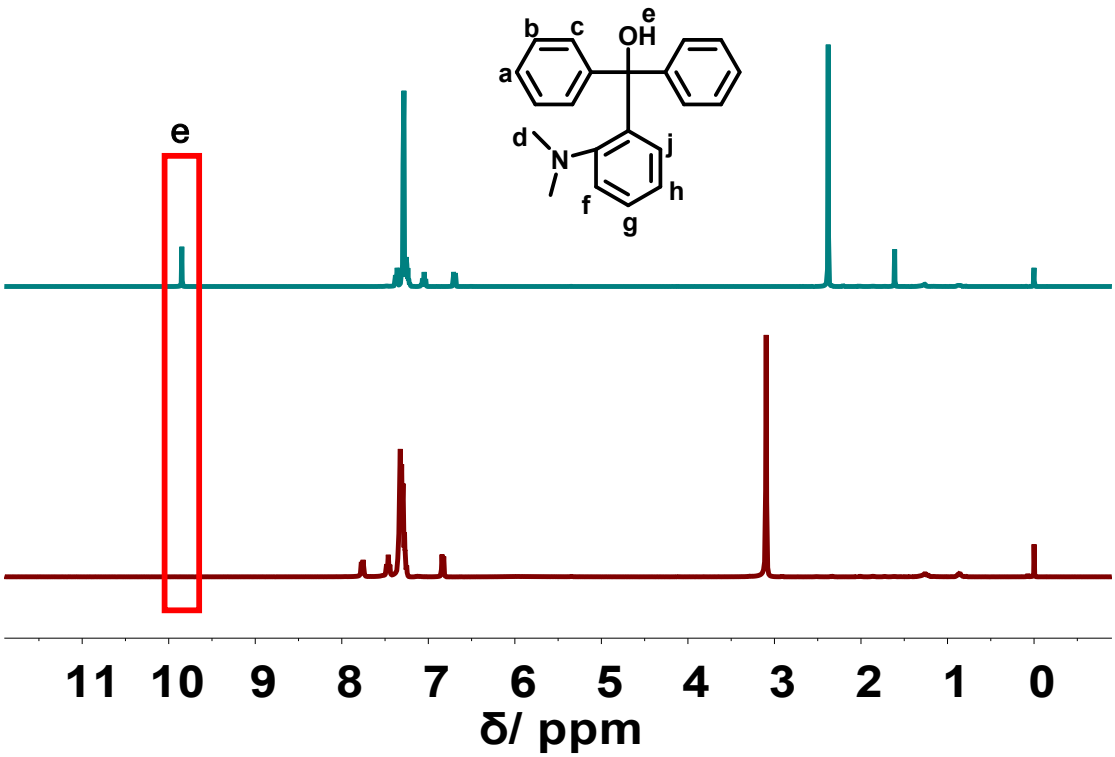


Figure S25. ^{1}H NMR (400 MHz) spectra of *o*-DMATPM (top) and adding 1 eq of DCl (bottom) in $CDCl_3$.

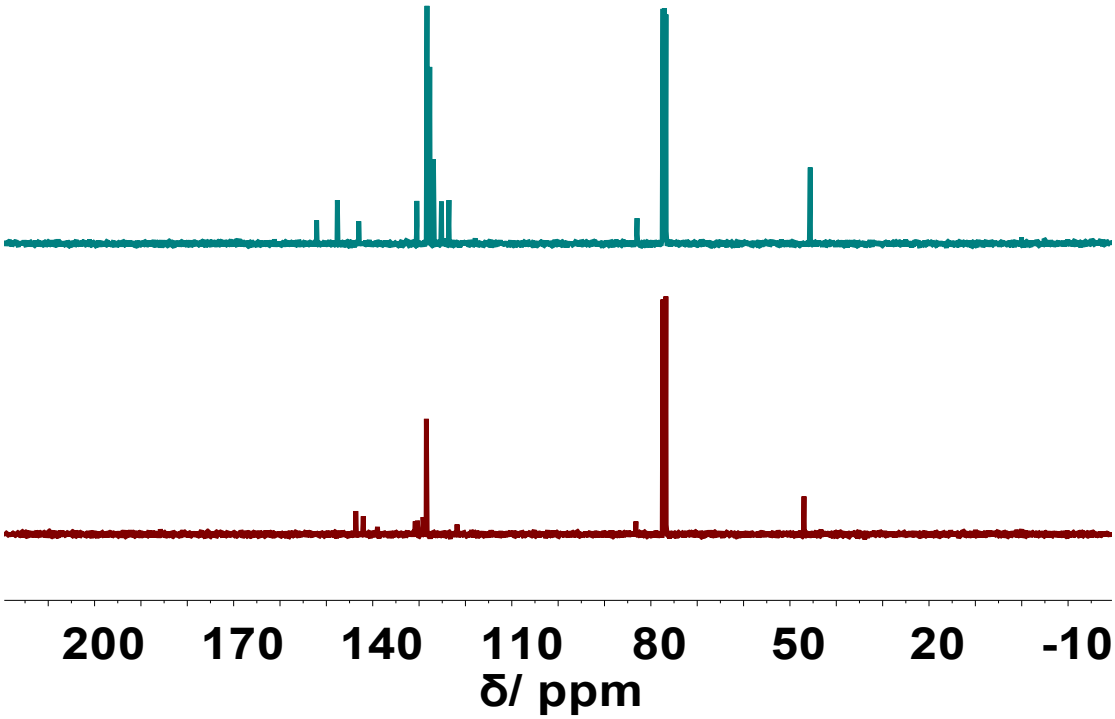


Figure S26. ^{13}C NMR (100 MHz) spectra of *o*-DMATPM (top) and adding 1 eq of DCl (bottom) in $CDCl_3$.

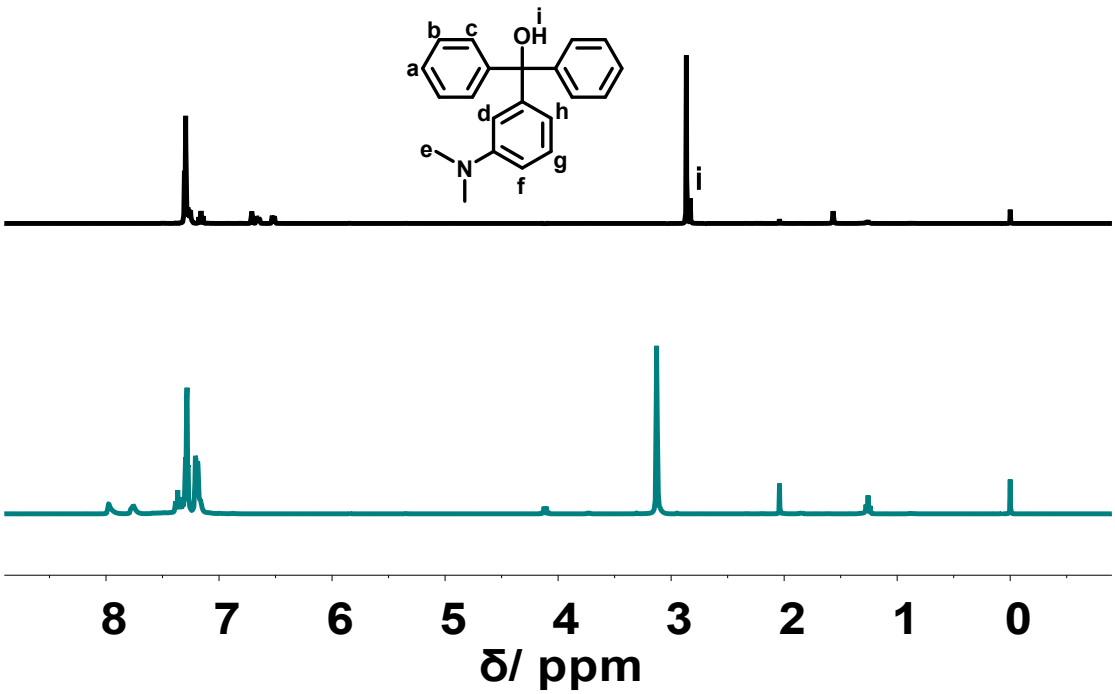


Figure S27. ^{1}H NMR (400 MHz) spectra of *m*-DMATPM (top) and adding 1 eq of DCl (bottom) in $CDCl_3$.

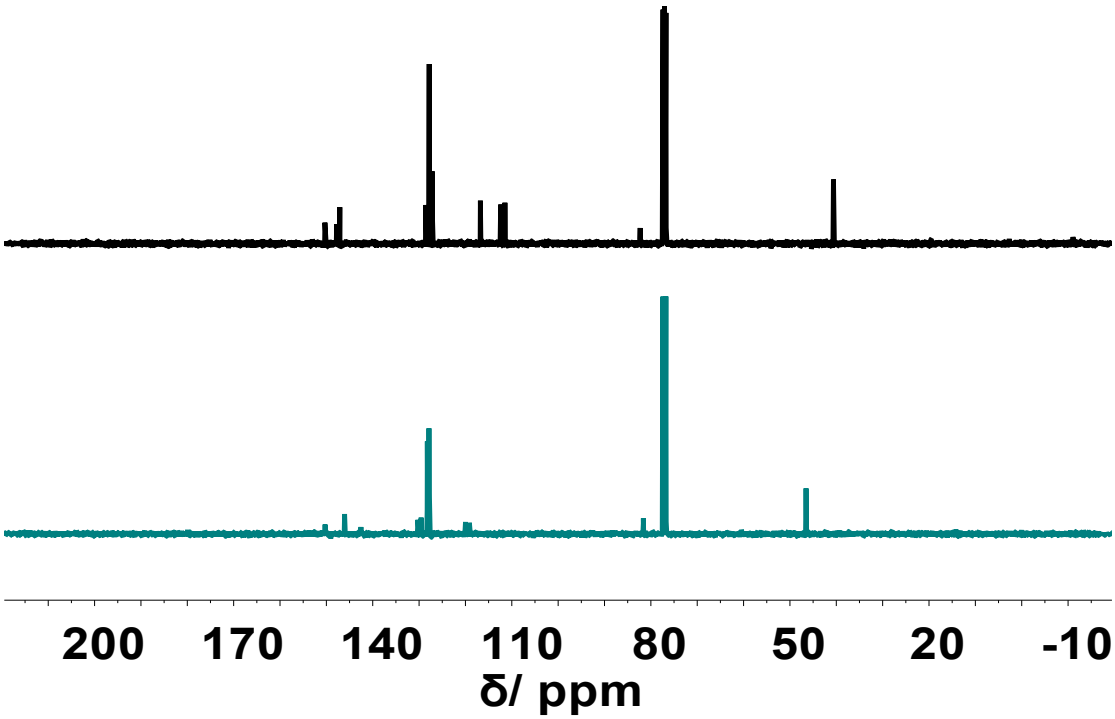


Figure S28. ^{13}C NMR (100 MHz) spectra of *m*-DMATPM (top) and adding 1 eq of DCl (bottom) in $CDCl_3$.

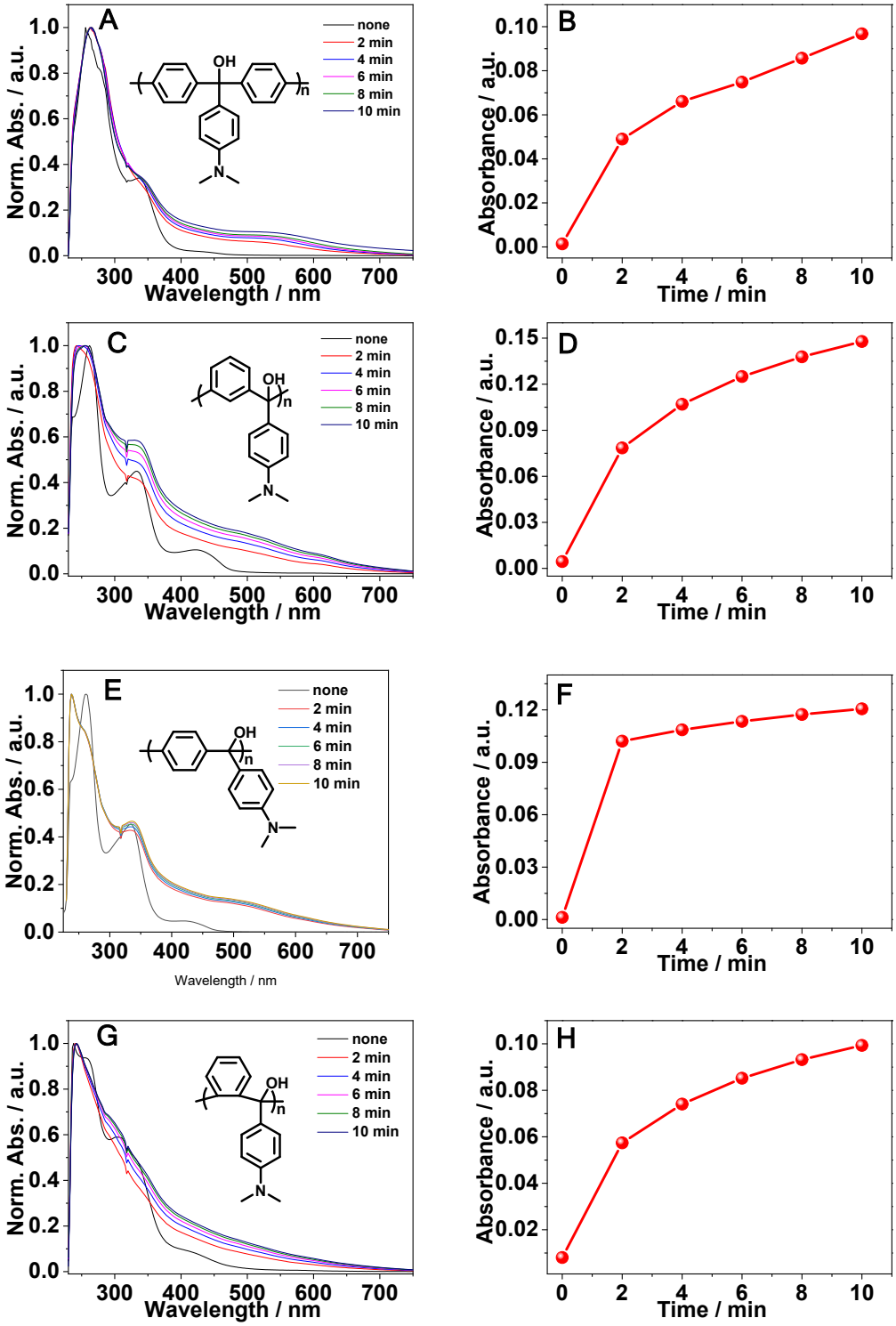


Figure S29. Absorption spectra and intensity of *p*-P(*p*-DMAPTPM) (A), (B), *p*-P(*p*-DMATPM) (C), (D), *m*-P(*p*-DMATPM) (E), (F) and *o*-P(*p*-DNATPM) (G), (H) before and after adding 1 eq HCl.

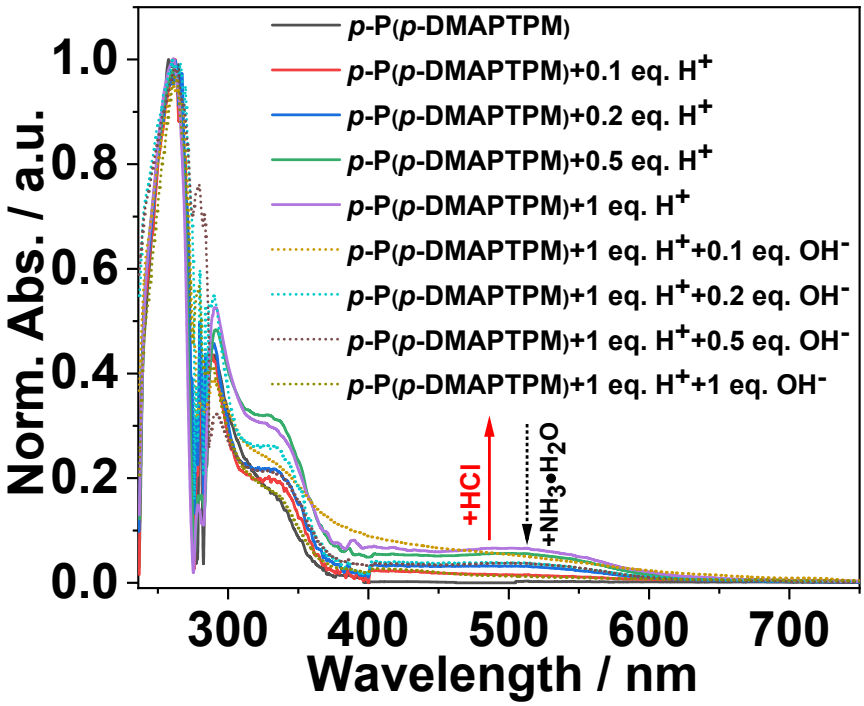


Figure S30. Normalized absorption spectra of *p*-P(*p*-DMAPTPM) with different content of HCl and NH_3.

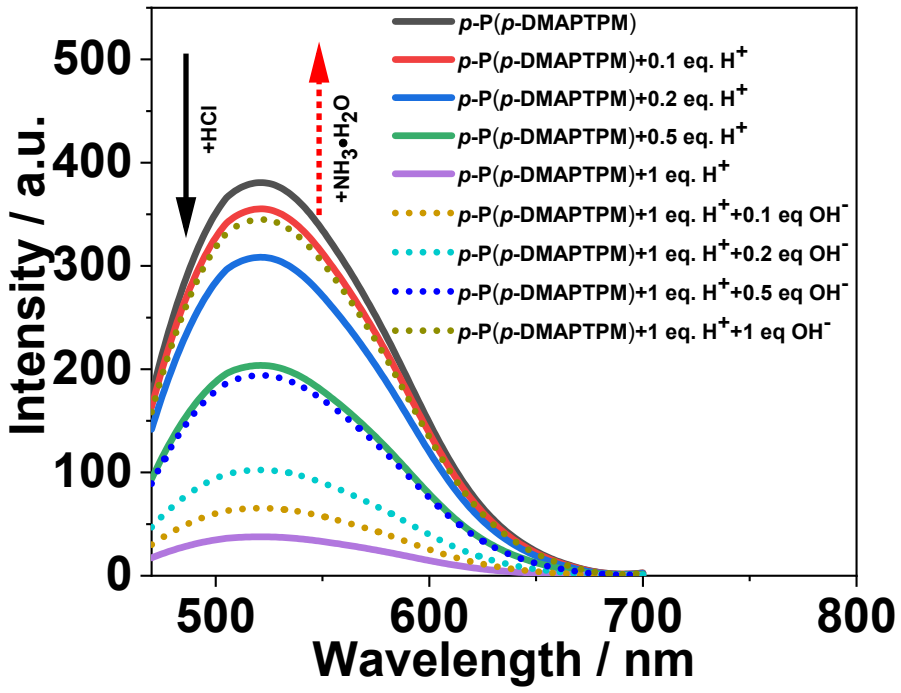
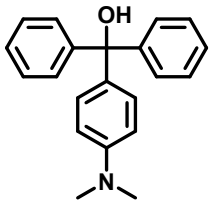


Figure S31. Emission spectra of *p*-P(*p*-DMAPTPM) with different content of HCl and NH_3.

Coordinate of optimized structures

Structure 1：

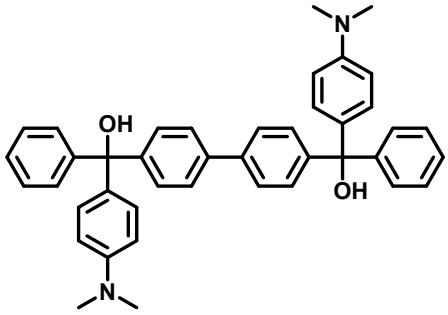


$E(B3LYP)_{S1}$ =-942.60926335

C	2.24305	1.4282	-0.87365
C	0.70305	1.42822	-0.87365
C	0.00552	0.38154	-1.4773
C	0.00556	2.47454	-0.2701
C	-1.38919	0.38161	-1.47793
H	0.5557	-0.44281	-1.95371
C	-1.38958	2.47425	-0.26978
H	0.55517	3.29947	0.20587
C	-2.08701	1.4281	-0.87368
H	-1.93907	-0.44304	-1.95426
H	-1.93925	3.29915	0.20653
H	-3.18669	1.4279	-0.87425
C	2.7564	2.33313	-2.00907
C	3.05922	3.6706	-1.75226
C	2.91871	1.81567	-3.29415
C	3.52362	4.49051	-2.78051
H	2.93042	4.07845	-0.73919
C	3.38418	2.63545	-4.3226
H	2.68025	0.76151	-3.49669
C	3.6865	3.97272	-4.06604
H	3.76173	5.54489	-2.57831
H	3.51245	2.22706	-5.33564
C	2.75637	-0.00758	-1.08964
C	3.54458	-0.62052	-0.11522
C	2.43323	-0.69528	-2.25934
C	4.01006	-1.92062	-0.31083
H	3.7998	-0.0778	0.8065
C	2.89796	-1.99615	-2.45473
H	1.81186	-0.2124	-3.02736
C	3.68638	-2.60883	-1.4808
H	4.63186	-2.40359	0.45689
H	2.64268	-2.53827	-3.37691
H	4.05346	-3.63393	-1.63479
O	2.71972	1.92111	0.38123

H	2.26537	1.46966	1.09632
N	4.17606	4.83713	-5.14956
C	3.36645	6.06297	-5.20219
C	5.58133	5.18841	-4.89917
H	3.89922	6.81948	-5.73954
H	2.4408	5.85803	-5.69826
H	3.17001	6.40366	-4.20708
H	6.17868	4.88633	-5.73393
H	5.66592	6.24651	-4.76437
H	5.9223	4.68808	-4.01694

Structure 2：



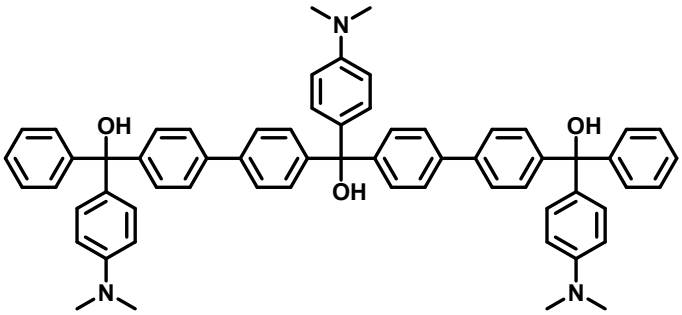
$E(B3LYP)_{S1}$ =-1884.02560790

C	-5.01967	0.94677	-0.87365
C	-6.55967	0.94679	-0.87365
C	-7.25721	-0.09989	-1.4773
C	-7.25716	1.9931	-0.2701
C	-8.65192	-0.09982	-1.47793
H	-6.70702	-0.92424	-1.95371
C	-8.6523	1.99282	-0.26978
H	-6.70756	2.81804	0.20587
C	-9.34974	0.94667	-0.87368
H	-9.20179	-0.92447	-1.95426
H	-9.20198	2.81772	0.20653
H	-10.44942	0.94647	-0.87425
C	-4.50636	-0.48901	-1.08964
C	-4.14694	-0.91633	-2.36819
C	-4.40064	-1.3622	-0.00709
C	-3.68256	-2.21677	-2.56416
H	-4.23113	-0.22792	-3.22156
C	-3.9352	-2.66277	-0.2028
H	-4.6837	-1.02551	1.0007
C	-3.5763	-3.0902	-1.48109
H	-3.39984	-2.55386	-3.572
H	-3.85156	-3.35089	0.65099

C	-4.50633	1.4776	0.47776
C	-3.51038	2.45405	0.51076
C	-5.03711	0.98231	1.66877
C	-3.04489	2.93456	1.73454
H	-3.09158	2.84377	-0.42838
C	-4.57229	1.46357	2.893
H	-5.82221	0.21284	1.64294
C	-3.57624	2.43944	2.92607
H	-2.25943	3.70376	1.76064
H	-4.99127	1.07316	3.83189
O	-4.54299	1.78706	-1.92797
H	-5.25677	2.3499	-2.23674
N	-3.08548	2.94615	4.21576
C	-3.37392	4.38386	4.31917
C	-1.63437	2.72971	4.30711
H	-2.58724	4.93986	3.85345
H	-4.30058	4.59789	3.82886
H	-3.44391	4.66032	5.35046
H	-1.14266	3.66788	4.45864
H	-1.42191	2.07878	5.12934
H	-1.28229	2.28492	3.39986
C	-3.06342	-4.52603	-1.69781
C	-2.95705	-5.39957	-0.61518
C	-2.70535	-4.95325	-2.97641
C	-2.49206	-6.69981	-0.81109
H	-3.2387	-5.06221	0.39284
C	-2.24113	-6.25416	-3.1727
H	-2.78929	-4.26495	-3.82983
C	-2.13431	-7.1274	-2.09031
H	-2.40759	-7.3882	0.0423
H	-1.95927	-6.59086	-4.181
C	-1.62099	-8.56318	-2.3063
C	-1.44989	-8.82578	-3.81406
C	-0.22593	-8.5687	-4.43238
C	-2.51846	-9.32074	-4.56154
C	-0.07087	-8.80591	-5.79799
H	0.61609	-8.17776	-3.84295
C	-2.36322	-9.559	-5.92739
H	-3.48314	-9.52359	-4.07434
C	-1.13973	-9.30156	-6.54571
H	0.89365	-8.6027	-6.28555
H	-3.2058	-9.94965	-6.51641
H	-1.01722	-9.48856	-7.62243
C	-0.26439	-8.73531	-1.59806

C	-0.08612	-9.76428	-0.6729
C	0.78614	-7.86262	-1.88155
C	1.14222	-9.92004	-0.03093
H	-0.91477	-10.45164	-0.44906
C	2.01522	-8.0189	-1.24019
H	0.64586	-7.05169	-2.61082
C	2.19337	-9.04731	-0.31489
H	1.28261	-10.73067	0.69877
H	2.84346	-7.33093	-1.46421
O	-2.56293	-9.49272	-1.76444
H	-2.32065	-10.38393	-2.02642
N	3.48793	-9.21179	0.36185
C	4.37221	-10.04321	-0.46742
C	3.28122	-9.86333	1.66326
H	4.09604	-9.62537	2.31468
H	2.3661	-9.51538	2.09498
H	3.23107	-10.92348	1.52741
H	5.28466	-10.22905	0.05964
H	3.88886	-10.97324	-0.68263
H	4.58676	-9.53253	-1.38288

Structure 3：



$E(B3LYP)_{S1}$ =-2825.44355981

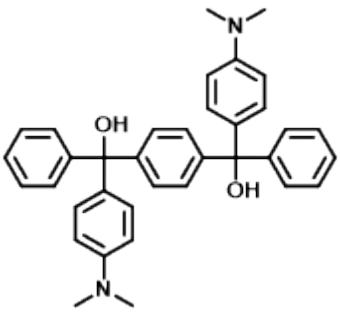
C	3.00428	0.99895	1.14094
C	3.51762	1.72491	2.39834
C	3.72455	1.0121	3.57968
C	3.7758	3.09498	2.3562
C	4.18892	1.66944	4.71876
H	3.52017	-0.06789	3.6128
C	4.24125	3.75248	3.49526
H	3.61293	3.65691	1.42515
C	4.44771	3.04001	4.67648
H	4.35145	1.10778	5.65011

H	4.44513	4.83266	3.46161
C	3.33362	-0.50187	1.24427
C	2.36908	-1.3974	1.70704
C	4.59612	-0.96595	0.87512
C	2.66728	-2.7566	1.80125
H	1.3741	-1.0311	1.99872
C	4.89425	-2.32567	0.96837
H	5.35639	-0.26029	0.5102
C	3.93015	-3.22098	1.43147
H	1.90728	-3.46244	2.1666
H	5.88963	-2.69135	0.67686
H	4.16502	-4.29271	1.50579
C	1.47951	1.18333	1.02828
C	0.89655	1.42852	-0.21531
C	0.68126	1.1051	2.16943
C	-0.48428	1.5961	-0.31753
H	1.52623	1.4909	-1.11467
C	-0.70011	1.27173	2.06721
H	1.14054	0.91168	3.14963
C	-1.28295	1.51734	0.82402
H	-0.94377	1.78999	-1.29762
H	-1.32929	1.20959	2.96707
O	3.63764	1.54726	-0.01799
H	3.53837	0.94006	-0.75492
C	-2.8076	1.70234	0.71079
C	-3.60643	1.62366	1.8519
C	-3.3899	1.94867	-0.53251
C	-4.98733	1.79061	1.74955
H	-3.14714	1.42868	2.83184
C	-4.7711	2.11668	-0.63492
H	-2.76042	2.01089	-1.43196
C	-5.56986	2.03756	0.50581
H	-5.61712	1.72798	2.64885
H	-5.22989	2.31129	-1.61528
C	-7.09462	2.22193	0.39315
N	4.93721	3.73252	5.87719
C	6.37208	3.4625	6.04785
C	4.72515	5.17957	5.72894
H	6.91007	4.38734	6.06003
H	6.53039	2.94562	6.97125
H	6.72023	2.85801	5.2365
H	5.53822	5.60464	5.17835
H	3.80919	5.35389	5.20404
H	4.6737	5.63348	6.69653

C	-7.60288	3.04042	1.59455
C	-8.13142	2.38861	2.70912
C	-7.53474	4.43334	1.5685
C	-8.59231	3.12966	3.79707
H	-8.18571	1.29048	2.72902
C	-7.99482	5.17473	2.65711
H	-7.11803	4.94722	0.6902
C	-8.52368	4.52316	3.77125
H	-9.0095	2.616	4.67536
H	-7.94059	6.27296	2.63647
C	-7.42646	2.96723	-0.913
C	-8.21227	2.35109	-1.88734
C	-6.94153	4.25826	-1.12192
C	-8.51247	3.02564	-3.07059
H	-8.59378	1.33297	-1.72266
C	-7.24255	4.93353	-2.30505
H	-6.32232	4.74409	-0.35401
C	-8.02777	4.31741	-3.27941
H	-9.13132	2.53981	-3.8389
H	-6.86041	5.95159	-2.46932
O	-7.7304	0.94106	0.3858
H	-8.68287	1.05626	0.35224
N	-9.00947	5.30393	4.91812
C	-9.99631	6.29076	4.45637
C	-9.6381	4.40198	5.89394
H	-9.00088	4.29996	6.74743
H	-10.58036	4.80714	6.19871
H	-9.79062	3.44232	5.44596
H	-9.58822	6.84764	3.6389
H	-10.88327	5.7852	4.13604
H	-10.23575	6.95774	5.25805
C	-8.3595	5.06199	-4.58599
C	-7.87508	6.35353	-4.79512
C	-9.14414	4.44518	-5.56039
C	-8.17583	7.02829	-5.97811
H	-7.25715	6.83982	-4.0264
C	-9.44426	5.11964	-6.74421
H	-9.52588	3.42718	-5.3958
C	-8.96038	6.41105	-6.95315
H	-7.79456	8.04653	-6.14274
H	-10.06259	4.63291	-7.51248
C	-9.29221	7.15634	-8.2593
C	-10.63069	6.63996	-8.81914
C	-10.64094	5.63158	-9.78326

C	-11.83274	7.18026	-8.36231
C	-11.85298	5.16413	-10.29087
H	-9.69307	5.20636	-10.14378
C	-13.04528	6.71209	-8.86924
H	-11.82485	7.97491	-7.6023
C	-13.05558	5.70428	-9.83348
H	-11.86112	4.36975	-11.05125
H	-13.9929	7.138	-8.50856
C	-9.40282	8.66585	-7.9751
C	-8.55454	9.56215	-8.6259
C	-10.3511	9.13702	-7.06719
C	-8.65413	10.92924	-8.36828
H	-7.80653	9.19029	-9.34106
C	-10.45151	10.50459	-6.81011
H	-11.01988	8.43076	-6.5543
C	-9.60315	11.40069	-7.46036
H	-7.98512	11.63571	-8.88074
H	-11.19956	10.87584	-6.09451
H	-9.68153	12.47864	-7.25743
O	-8.25476	6.92622	-9.21619
H	-8.51669	7.28784	-10.06603
N	-14.33289	5.21133	-10.36862
C	-15.15741	6.35075	-10.79618
C	-14.0759	4.33336	-11.51928
H	-14.63419	6.90879	-11.54432
H	-16.08075	5.9912	-11.2
H	-15.35747	6.98162	-9.95541
H	-13.15334	3.81199	-11.37107
H	-14.87374	3.62668	-11.61392
H	-14.01354	4.92235	-12.41041

Structure 4：

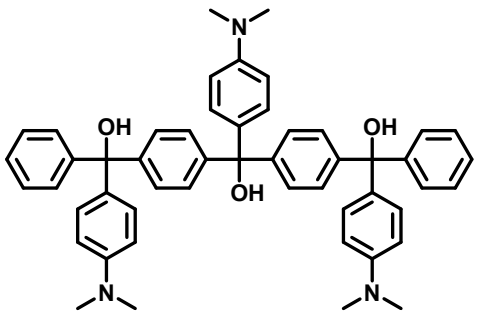


E(B3LYP)S1 =-1653.02074545

C	-1.15447	-0.09862	-0.87365
C	-2.69447	-0.0986	-0.87365
C	-3.39201	-1.14528	-1.4773
C	-3.39196	0.94771	-0.2701
C	-4.78672	-1.14522	-1.47793
H	-2.84182	-1.96964	-1.95371
C	-4.7871	0.94743	-0.26978
H	-2.84236	1.77265	0.20587
C	-5.48454	-0.09873	-0.87368
H	-5.33659	-1.96987	-1.95426
H	-5.33678	1.77233	0.20653
H	-6.58422	-0.09892	-0.87425
C	-0.64116	-1.5344	-1.08964
C	-0.28174	-1.96172	-2.36819
C	-0.53544	-2.40759	-0.00709
C	0.18264	-3.26217	-2.56416
H	-0.36593	-1.27331	-3.22156
C	-0.07	-3.70816	-0.2028
H	-0.8185	-2.0709	1.0007
C	0.2889	-4.13559	-1.48109
H	0.46536	-3.59925	-3.572
H	0.01364	-4.39628	0.65099
C	-0.64113	0.80631	-2.00907
C	0.4525	1.64501	-1.79224
C	-1.26941	0.7874	-3.25424
C	0.91726	2.46508	-2.8202
H	0.94713	1.66025	-0.81022
C	-0.80401	1.60693	-4.28292
H	-2.13126	0.1263	-3.42537
C	0.28906	2.44581	-4.06607
H	1.77888	3.12665	-2.64917
H	-1.29933	1.59151	-5.26471
O	-0.6778	0.39429	0.38123
H	0.24381	0.1496	0.49244
N	0.77919	3.31021	-5.14935
C	0.51259	4.71617	-4.81302
C	2.2261	3.11246	-5.31741
H	1.30707	5.32874	-5.18511
H	-0.41126	5.02055	-5.25884
H	0.44791	4.82259	-3.75029
H	2.7314	3.3931	-4.41696

H	2.42293	2.08257	-5.53071
H	2.57716	3.71776	-6.12689
C	0.80178	-5.57142	-1.69781
C	-0.21289	-6.57244	-1.11471
C	-0.0981	-6.98919	0.21179
C	-1.24672	-7.06238	-1.91265
C	-1.01658	-7.8962	0.73995
H	0.71751	-6.60334	0.84039
C	-2.16614	-7.96892	-1.38419
H	-1.33744	-6.73389	-2.95812
C	-2.05116	-8.38598	-0.05816
H	-0.9258	-8.22522	1.78533
H	-2.9814	-8.35473	-2.01345
H	-2.77526	-9.10107	0.35852
C	0.97273	-5.83333	-3.20571
C	2.24772	-6.01671	-3.74168
C	-0.14703	-5.88734	-4.03564
C	2.40286	-6.25337	-5.10738
H	3.13037	-5.97331	-3.08724
C	0.00792	-6.12505	-5.40161
H	-1.152	-5.74301	-3.61335
C	1.2826	-6.30792	-5.9376
H	3.40783	-6.3973	-5.53001
H	-0.87517	-6.16799	-6.05566
O	2.06146	-5.73196	-1.0403
H	2.32588	-6.65417	-1.07511
N	1.44645	-6.55745	-7.37697
C	2.86857	-6.45191	-7.73381
C	0.95927	-7.90647	-7.69899
H	3.43478	-7.1497	-7.15296
H	2.99246	-6.67028	-8.77394
H	3.21362	-5.45892	-7.53428
H	1.66534	-8.63252	-7.35373
H	0.01678	-8.06926	-7.21928
H	0.84106	-7.99955	-8.75836

Structure 4：



E(B3LYP)S1 =-2363.42972473

C	-3.90895	0.5573	0.
C	-2.51379	0.5573	0.
C	-1.81625	1.76505	0.
C	-2.5139	2.97356	-0.0012
C	-3.90873	2.97348	-0.00168
C	-4.60633	1.76528	-0.00068
H	-4.45871	-0.39502	0.00045
H	-1.96428	-0.39521	0.00132
H	-1.9637	3.9257	-0.00126
H	-4.45885	3.92576	-0.00263
H	-5.70593	1.76546	-0.00086
C	-0.27625	1.76516	0.00089
C	0.23708	0.3247	0.18295
C	0.51607	-0.46282	-0.93439
C	0.42323	-0.19265	1.46484
C	0.98044	-1.76761	-0.76978
H	0.36848	-0.05493	-1.94487
C	0.88868	-1.49748	1.62968
H	0.20356	0.42796	2.34559
C	1.16716	-2.28504	0.51265
H	1.19977	-2.38862	-1.65043
H	1.03574	-1.90498	2.64051
C	0.23635	2.64287	1.15781
C	1.28147	3.54143	0.94153
C	-0.34424	2.53961	2.42185
C	1.74628	4.33604	1.98928
H	1.7395	3.62205	-0.05494
C	0.11993	3.3351	3.46978
H	-1.16809	1.83158	2.59245
C	1.16511	4.23313	3.25374
H	2.57047	5.04387	1.81903
H	-0.33831	3.25377	4.46621
O	0.20109	2.28783	-1.24163
H	-0.47353	2.17812	-1.91576
N	1.65518	5.07083	4.35782
C	1.39074	6.48475	4.05482
C	3.10166	4.86724	4.52264
H	2.18598	6.87578	3.45516
H	0.46718	6.56844	3.52103
H	1.32658	7.03919	4.96771
H	3.60829	5.80338	4.41375

H	3.29694	4.46706	5.49559
H	3.45261	4.18309	3.77856
C	1.68001	-3.72576	0.69406
C	3.03659	-3.69985	1.4225
C	3.09686	-3.94967	2.79378
C	4.20503	-3.42675	0.71137
C	4.32526	-3.92571	3.45384
H	2.17541	-4.16419	3.35428
C	5.43401	-3.40372	1.3713
H	4.15773	-3.23001	-0.36945
C	5.49429	-3.653	2.74234
H	4.37278	-4.122	4.53482
H	6.35516	-3.18877	0.81027
C	1.85095	-4.38739	-0.68602
C	1.04707	-5.46966	-1.04508
C	2.80935	-3.90464	-1.57707
C	1.20207	-6.06941	-2.29468
H	0.29211	-5.85051	-0.34207
C	2.96385	-4.50383	-2.82747
H	3.4429	-3.05153	-1.2943
C	2.16052	-5.58615	-3.18634
H	0.56891	-6.92287	-2.57753
H	3.7193	-4.12272	-3.52999
O	0.7378	-4.47326	1.46762
H	1.04976	-5.37558	1.56806
N	2.32359	-6.21844	-4.50335
C	3.39702	-7.22051	-4.43627
C	1.06592	-6.87286	-4.89181
H	4.25435	-6.79342	-3.95933
H	3.06058	-8.06649	-3.8741
H	3.65746	-7.53103	-5.42654
H	1.21307	-7.93186	-4.93386
H	0.30848	-6.64636	-4.17079
H	0.76077	-6.5167	-5.85355
C	6.8505	-3.6267	3.47144
C	7.89827	-2.93236	2.58168
C	8.61083	-3.67131	1.63685
C	8.13484	-1.56474	2.72025
C	9.5602	-3.04283	0.8313
H	8.42464	-4.74964	1.52838
C	9.08377	-0.93573	1.91385
H	7.57319	-0.98215	3.46475
C	9.79653	-1.67452	0.96956
H	10.12233	-3.62533	0.08699

H	9.26978	0.14267	2.02305
C	7.30258	-5.06892	3.76681
C	7.49858	-5.48236	5.08481
C	7.51597	-5.96188	2.71675
C	7.90855	-6.78829	5.35256
H	7.331	-4.7779	5.91239
C	7.92511	-7.26853	2.98446
H	7.36136	-5.63624	1.67791
C	8.12155	-7.68181	4.30209
H	8.06367	-7.11406	6.39136
H	8.09289	-7.9725	2.15636
H	8.44474	-8.71146	4.51345
O	6.71714	-2.90782	4.70039
H	7.53762	-2.96465	5.19555
N	10.79716	-1.01239	0.12032
C	11.51711	-0.00173	0.90843
C	11.75058	-2.01146	-0.38341
H	12.45349	0.21624	0.43877
H	10.9301	0.89108	0.96501
H	11.6918	-0.37686	1.89517
H	12.64689	-1.97499	0.19987
H	11.31694	-2.98692	-0.31035
H	11.98191	-1.79969	-1.40642