Supporting Information

Experimental Section

Materials. Diphenylamine, paranitrobenzoyl chloride, 4-fluoronitrobenzene, hydrazine hydrate, cesium fluoride, palladium/c catalyst, and pyridine were purchased from Alfa-Aesar company and used as received. Tetrahydrofuran (THF) was distilled from sodium/benzophenone. Dimethyl formamide (DMF) was dehydrated by 4A molecular sieve. All other solvents and reagents as analytical grade were purchased from Guangzhou Dongzheng Company (China) and used without further purification.

Instrumentation. The Two-dimensional NMR spectra of the ITPADA were recorded at room temperature on a Bruker AVANCE AV 400MHz spectrometer, operating at 400.13 MHz for ^{1}H with indirect detection probe and at 100.61 MHz for ^{13}C with broadband probe. Samples were made up as solution of 5-15 mg of each compound in 0.7 mL of deuterated dimethyl sulfoxide (DMSO), using tetramethylsilane (TMS) as the internal reference. Inverse gated decoupling was exploited for quantitative carbon nuclei intensities, using a zgpg30 pulse sequence, 0.45 s acquisition times, and 1.55 s relaxation delays for about 1800 scans. And other NMR spectra were recorded at room temperature on a VARIAN Mercury-Plus 300 spectrometer, operating at 300.08 MHz for ^{1}H with indirect detection probe and at 75.46 MHz for ^{13}C with broadband probe. Mass spectra (MS) were measured on a Thermo MAT95XP-HRMS spectrometer. Elemental analysis (EA) was carried out on a CHNS Elemental Analyzer. Infrared spectra were recorded on a BRUKER TENSOR 27 Fourier-transform infrared (FT-IR) spectrometer. Fluorescence spectra (PL) were determined on a Shimadzu RF-5301PC spectrometer with a slit width of 3 nm and 1.5 nm for emission on 365 nm. The PL quantum yields of ITPADA in the mixed solvent of THF/H_2O were measured according to an absolute method by using a fluoroSENS-fluorimeter that was excited with a Xe lamp. Single crystals of the compound were grown from ethyl acetate/n-hexane. Single-crystal data was collected at 150 K on a single crystal diffractometer (Agilent diffractometer). The X-ray crystallographic intensity data of the powder filter from THF/water with ultrasound treatment and other powder were collected at Bruker D8 ADVANCE X-Ray diffractometer with 10 °/min. The structure was solved by the full-matrix least-squares method against F_0^2 using SHELXTL software. Differential scanning calorimetry (DSC) curves were obtained with a NETZSCH thermal analyzer (DSC 204) at a heating rate of 25 ℃ /min from 50 to 300 ℃ under flowing nitrogen. Thermogravimetric analyses (TGA) were carried out using a thermal analyzer (Shimadzu, TGA-50H) under N_2 gas flow with a heating rate of 20 ℃/min. Molecular simulations of ITPADA were carried out with the Gaussian 09w program package. Equilibrium ground state geometry and electronic properties of the molecule was optimized by means of the density functional theory (DFT) method at the B3LYP level of theory (Beckes-style three-parameter density functional theory using the Lee-Yang-Parr correlation functional) with the 6-31 G(d) basic set.

Synthesis of 4-nitro-N,N-diphenyl-benzamide (IP-NO_2). Diphenylamine (DPA) (3.3846 g, 20 mmol) and pyridine (2.0123ml, 25mmol) were dissolved in the mixture of THF (100 mL), and then stirred for 0.5 h under argon at room temperature followed adding paranitrobenzoyl chloride (NBFC) (4.0825g, 22mmol). After the reaction mixture was stirred at 60 ℃ temperature for 12h, the product was concentrated and purified by silica gel column chromatography using dichloromethane /n-hexane(v/v=3/2). The yield of the product is about 61%. IR (KBr, *v*, cm^{-1}): 1671 (C=O stretching), 1594 (O=C-N stretching), 1083~717 (Ar–H

stretching), 1340 (Ar-C-N stretching). ^{1}H NMR (300 MHz, DMSO-d_6, δ, ppm): 7.15~7.25 (t, 2H), 7.25~7.37 (m, 8H), 7.64~7.72 (dt, 2H), 8.04~8.13 (dt, 2H). ^{13}C NMR (75 MHz, DMSO-d_6, δ, ppm): 123.68, 127.62, 128.43, 129.87, 130.25, 143.48, 148.25, 168.43. MS(EI, m/z): 318 ([M]$^{+}$, calcd for $C_{19}H_{14}N_2O_3$, 318.33). Anal. Calcd for $C_{19}H_{14}N_2O_3$ (318.33, wt %:): C, 71.688; H, 4.432 and N, 8.800; found: C, 71.940; H, 4.420; and N, 8.750.

Synthesis of 4-amino-N,N-diphenyl-benzamide (IP-NH$_2$). IP-NO$_2$ (3.8196g, 12mmol) was dissolved in ethanol (100 ml), and then stirred for about 0.5 h under argon after the temperature was heated for about 80 ℃. Then the palladium/C catalyst (10%Pd) was added, and the hydrazine hydrate (4.8ml) was added drop wise. The reaction mixture was stirred at 80 ℃ for 24 h. After cooling to room temperature, the product was concentrated and purified by silica gel column chromatography using dichloromethane. Yield of the product is about 89%. IR (KBr, *v*, cm^{-1}): 1629 (C=O stretching), 1601 (O=C-N stretching), 1083~717 (Ar–H stretching), 1347 (Ar–C-N stretching), 3366~3466 (-N-H stretching). ^{1}H NMR (300 MHz, DMSO-d_6, δ, ppm) : 5.56 (s, 2H) , 6.33~6.29 (d, 2H), 7.17~7.06 (dt, 8H), 7.32~7.27 (t, 4H). ^{13}C NMR (75 MHz, DMSO-d_6, δ, ppm): 112.93, 122.71, 126.31, 128.04, 129.62, 131.70, 145.49, 151.56, 170.56. MS (EI, m/z): 288 ([M]$^{+}$, calcd for $C_{19}H_{16}N_2O$, 288.3432). Anal. calcd for $C_{19}H_{16}N_2O$ (288.3432, wt %:) C, 79.142; H, 5.593 and N, 9.715; found: C, 78.820; H, 5.619 and N, 9.630.

Synthesis of 4-(bis(4-nitro-phenyl)-amino)-N,N-diphen-ylbenzamide (ITPADN). IP-NH$_2$ (3.0859g, 10.6mmol) and cesium fluoride (6.4448g, 42.4mmol) were dissolved in the mixture of dimethyl formamide (DMF) (75 ml), and then stirred for 0.5 h under argon after the room temperature was heated for 150 ℃ followed adding 4-fluoronitro-benzene (4.5ml, 42.4mmol). After the reaction mixture was stirred for 24h, the product was concentrated and purified by silica gel column chromatography using dichloromethane /n-hexane(v/v=1/1). The yield of the product is about 73%. IR (KBr, *v*, cm^{-1}): 1657 (C=O stretching), 1584(O=C-N stretching), 1083~717 (Ar–H stretching), 1340 (Ar–C-N stretching). ^{1}H NMR (300 MHz, DMSO-d_6, δ, ppm) : 7.06~7.08 (d, 2H), 7.09~7.12 (dt, 4H), 7.20 (s, 2H), 7.22~7.24 (t, 4H), 7.32~7.37 (m, 4H), 7.45~7.48 (d, 4H), 8.13~8.19 (dt, 4H). ^{13}C NMR (75 MHz, DMSO-d_6, δ, ppm): 123.57, 126.17, 126.57, 127.17, 128.31, 129.72, 131.40, 135.04, 143.15, 144.12, 146.16, 151.84, 169.38. MS (EI, m/z): 530 ([M]$^{+}$, calcd for $C_{31}H_{22}N_4O_5$, 530.5303). Anal. calcd for $C_{31}H_{22}N_4O_5$ (530.5303, wt %:) C, 70.181; H, 4.179 and N,10.561; found: C, 70.060; H, 4.187 and N, 10.420.

Synthesis of 4-(bis(4-aminophenyl)amino)-N,N-diphen-ylbenzamide (ITPADA). ITPADN (4.1008g, 7.73mmol) was dissolved in ethanol (100 ml), and then stirred for about 0.5 h under argon after the temperature was heated for about 80 ℃. Then the palladium/c catalyst (10%Pd) was added, then hydrazine hydrate (6.4ml) was added in the mixture slowly. The reaction mixture was stirred at 80 ℃ for 24 h. After cooling to room temperature, the product was concentrated and purified by silica gel column chromatography using dichloromethane. Yield of the product is about 91%. IR (KBr, *v*, cm^{-1}): 1628 (C=O stretching), 1595(O=C-N stretching), 1083~717 (Ar–H stretching), 1330 (Ar–C-N stretching), 3366~3466 (-N-H stretching). ^{1}H NMR (400 MHz, DMSO-d_6, δ, ppm) : 5.04 (s, 4H), 6.30~6.32 (d, 2H), 6.53~6.55 (d, 4H), 6.80~6.82 (d, 4H), 7.10~7.12 (d, 4H), 7.13~7.20 (m, 4H), 7.30~7.34 (m, 4H). ^{13}C NMR (100.61 MHz, DMSO-d_6, δ, ppm): 113.87, 115.26, 123.72, 126.32, 127.89, 128.33, 129.54, 131.02, 134.84, 145.13, 146.99, 151.81, 169.97. MS (EI, m/z): 470 ([M] $^{+}$, calcd for $C_{31}H_{26}N_4O$, 470.5645). Anal. calcd for $C_{31}H_{26}N_4O$ (470.5645, wt %) C, 79.124; H, 5.569 and N, 11.906; found: C, 79.590; H, 5.517 and N, 11.400.

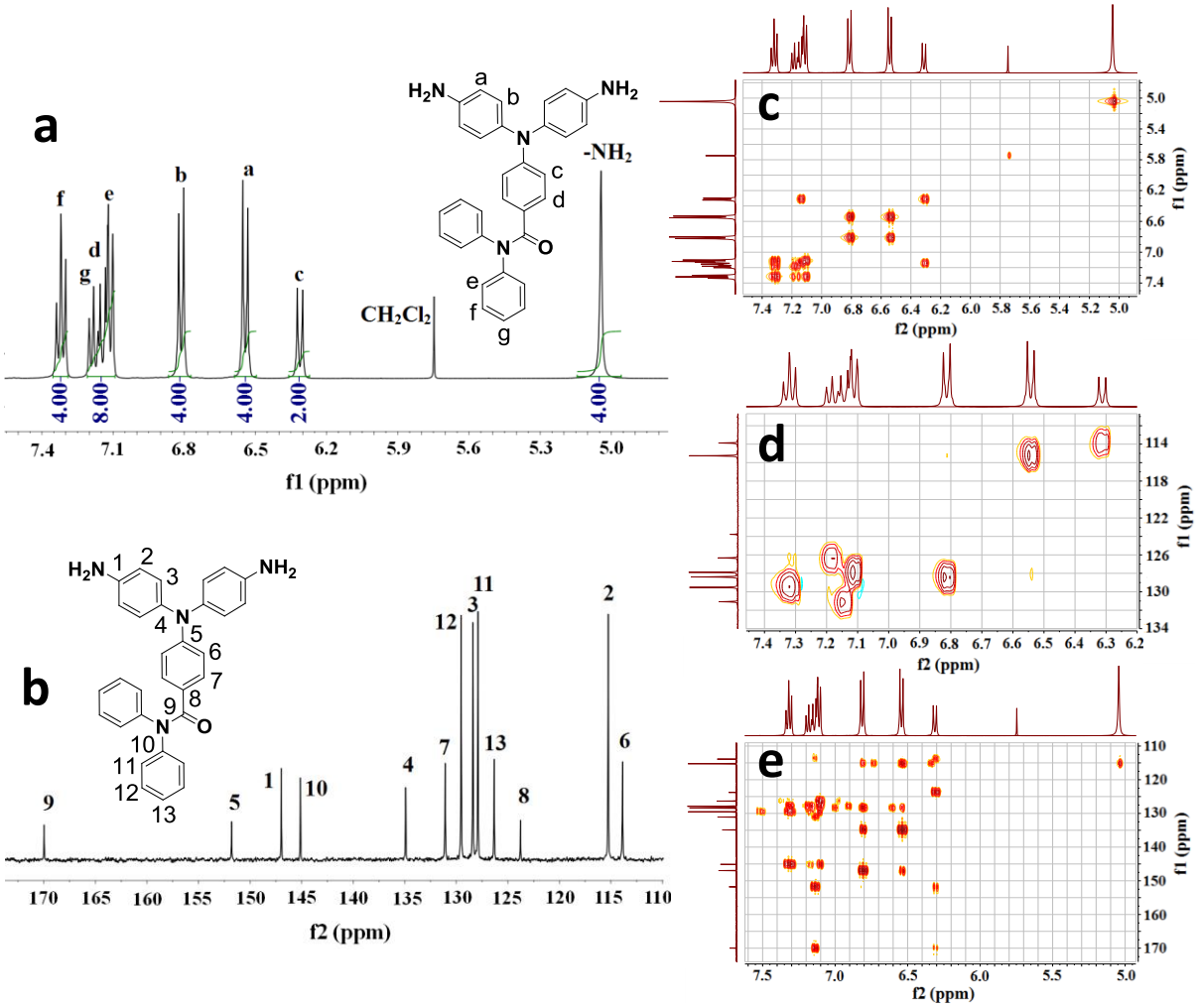


Fig. S1. Characterization of the chemical structure of ITPADA by NMR (400 MHz). a) ^{1}H NMR spectra of ITPADA in DMSO-d_6; b) ^{13}C NMR spectra of ITPADA in DMSO-d_6; c) H–H COSY spectra; d) C–H QC spectra; e) C–H BC spectra.

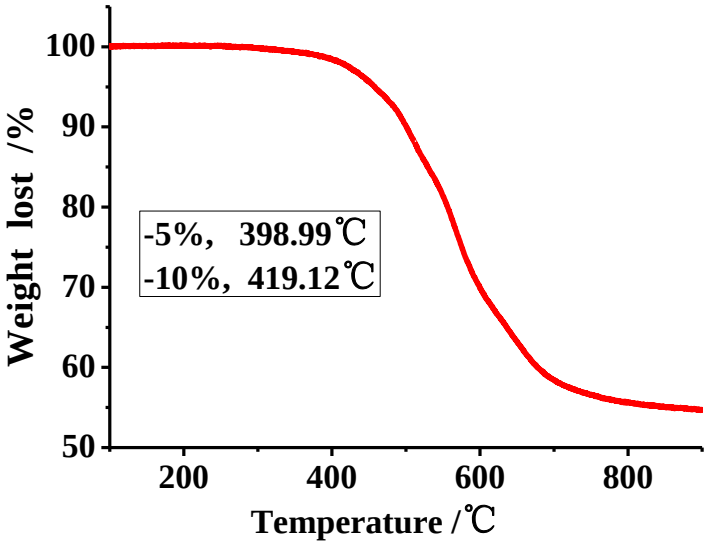


Fig. S2. TGA curve of ITPADA.

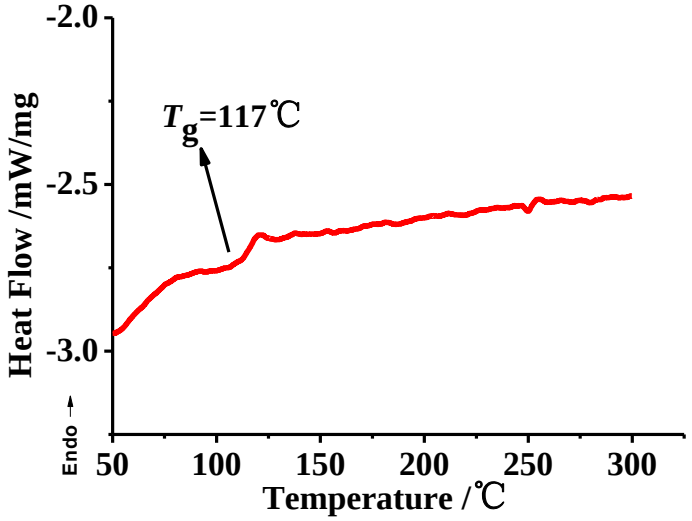
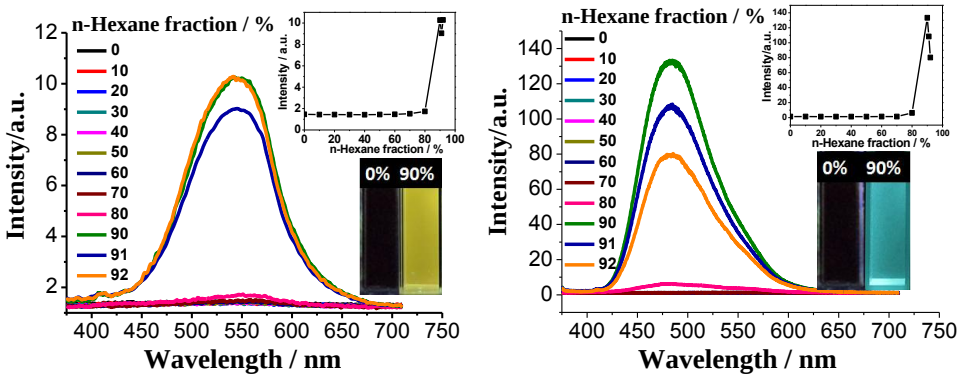
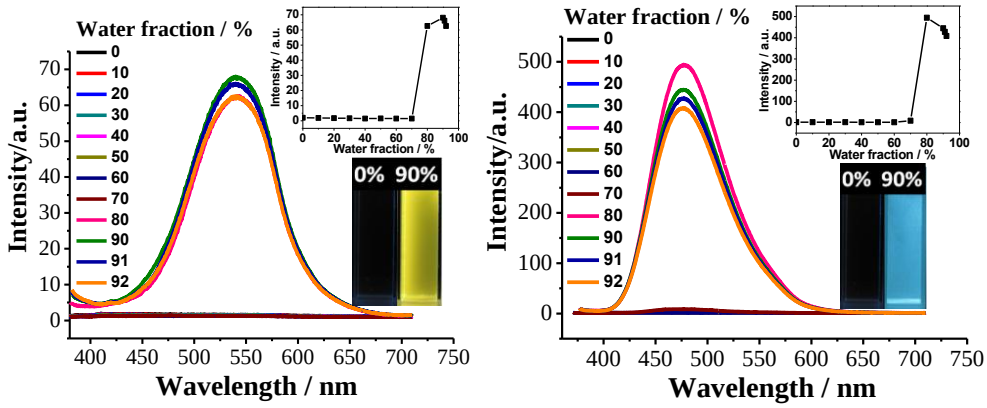


Fig. S3. DSC curve of the ITPADA.



(a) non-ultrasonic (b) ultrasonic

Fig.S4. PL spectra and pictures of ITPADA in the THF/n-hexane mixtures with different n-hexane fractions. (a) non-ultrasonic condition; (b) ultrasonic conduction.



(a) non-ultrasonic (b) ultrasonic

Fig.S5. PL spectra and pictures of ITPADA in the THF/n-hexane mixtures with different n-hexane fractions. (a) non-ultrasonic condition; (b) ultrasonic conduction.

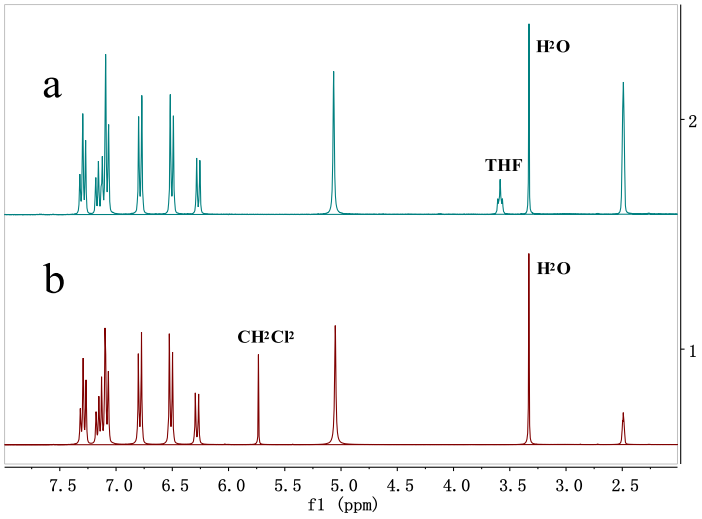


Fig. S6. ^{1}H NMR spectra of ITPADA in DMSO-d_6 (300 MHz) before and after the treatment of ultrasound. a is the compound filter from the THF/H_2O with ultrasound; b is the compound precipitate from the CH_2Cl_2/n-hexane with no ultrasound.

Table S1. Crystallographic Data of ITPADA

empirical formula	C66H60N8O4	
fw	1029.22	
temp.,K	150(2)	
wavelength, Å	1.54184	
cryst syst	triclinic	
spacegroup	P-1	
Unit cell dimensions	a = 13.0465(3) Å	α = 97.5266(16) deg.
	b = 14.1234(3) Å	β= 92.1596(16) deg.
	c = 15.2036(3) Å	γ= 105.3963(17) deg.
Volume, Å3	2669.92(9)	
Z	2	
calculated density, Mg/m3	1.280	
absorption coefficient, mm-1	0.642	
F(000)	1088	
crystal size	0.40 x 0.37 x 0.32 mm	
θ / deg	2.94 - 66.94.	
index ranges	-14≤h≤15, -16≤k≤16, -17≤l≤18	
no. of reflns collected	64083	
no. of in dependent reflns	9446 [R(int) = 0.0435]	
completeness to θ= 66.94	99.3 %	
no. of data / restraints / parameters	9446 / 0 / 705	
goodness-of-fit on F2	1.017	
final R indices [I>2δ(I)]	R1 = 0.0482, wR2 = 0.1298	
R indices (all data)	R1 = 0.0542, wR2 = 0.1366	
largest diff. peak and hole	0.495 and -0.465 e.A-3	

Table S2. Hydrogen bonds of ITPADA [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3B)...N(7)#1	0.91	2.37	3.246(2)	162.7
N(3)-H(3A)...O(2)#2	0.91	2.14	3.0068(19)	157.7
N(4)-H(4B)...N(8)#1	0.91	2.21	3.073(2)	158.2
N(4)-H(4A)...O(1)#3	0.91	2.54	3.1787(19)	127.5
N(7)-H(7A)...N(3)#4	0.91	2.45	3.345(3)	168.7
N(8)-H(8B)...O(1)#5	0.91	2.48	3.179(2)	133.5

Table S3. Short contact of ITPADA [Å and deg.]

Short contact		length (Å)		Angle(deg)
C47-C48…H54	H-π	C47…H54 2.882 C48…H54 2.776		28.35
C5-H4A…O1		C5…H4A O1…H4A	2.828 2.542	62.95
C31-H8B…H31		C31…H8B 2.619 H31…H8B	2.39	21.24
C3-H25		2.858		
C30-H2		2.886		
C31-H3		2.795		
C18-H8A…H18		H8A…H18 2.216 H8A…C18 2.784		17.64
C12-H7A-N3		C12-H7A 2.871 N3-H7A 2.448		
H53-H41		2.375		