Electronic Supplimentary Information

Organoboron compounds constructed through tautomerization of 1*H*-indole to 3*H*-indole for red OLEDs

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1. General information

1-Bromo-3,6-di-*tert*-butyl-9*H*-carbazole[1] and 2-bromo-4-(*tert*-butyl)-*N*-(4-(*tert*-butyl)phenyl)aniline[2] were synthesized according to literature procedures. Toluene for synthesis was dried and distilled. Other chemicals for organic syntheses were obtained from commercial sources and used as received. All synthetic reactions were carried out by using Schlenk techniques under a nitrogen atmosphere. ^{1}H- and ^{13}C{^{1}H}-NMR spectra were recorded on a Varian Mercury 400 MHz spectrometer (400 MHz for ^{1}H and 100 MHz for ^{13}C) with tetramethylsilane as the internal standard. Mass spectra were measured on a Thermo Fisher ITQ 1100 mass spectrometer. Elemental analyses were done on an elementar Vario micro cube analyser. TGA measurements were performed on a TA Q500 thermogravimeter at a heating rate of 10 °C min^{-1} under nitrogen. DSC measurements were performed on a NETZSCH DSC204 instrument at a heating rate of 10 °C min^{-1} under a nitrogen atmosphere. UV-visible absorption spectra were collected on a Shimadzu UV-2550 spectrophotometer. Emission spectra were recorded on a Shimadzu RF-5301 PC spectrometer. The absolute fluorescence quantum yields of solutions and doped films, as well as fluorescence lifetimes, were measured on an Edinburgh FLS920 spectrometer. Electrochemical measurements were performed with a BAS 100W Bioanalytical electrochemical work station, using a platinum disk as the working electrode, a platinum wire as the counter electrode, and an Ag/Ag^{+} electrode as the reference electrode. A 0.1 M solution of *n*-Bu_4NPF_6 in dry CH_2Cl_2 (for oxidation) or THF (for reduction) was used as the supporting electrolyte. The scan rate of the electrochemical measurements was 100 mV s^{-1}.

2. Theoretical calculations

DFT and TD-DFT calculations were performed using Gaussian 09 program[3] at the B3LYP/6-31G(d,p)[4] level of theory. The molecular structures in single crystals were used as the input for optimizing ground-state geometries of the compounds. Based on these optimized structures, the gas-phase vertical transitions were calculated.

3. Single-crystal X-ray diffraction

Diffraction data were collected on a Rigaku RAXIS-PRID diffractometer using the ω-scan mode with graphite-monochromator Mo•Kα radiation. The structure was solved with direct methods using the SHELXTL programs and refined with full-matrix least-squares on F^2.[5] Non-hydrogen atoms were refined anisotropically. The positions of

hydrogen atoms were calculated and refined isotropically. The structures were deposited at the CCDC under the following numbers: 1893122 (for **1**) and 1893121 (for **2**).

4. Device fabrication

HATCN, NPB, TCTA, 3P-T2T and LiF were electronic grade and obtained from commercial sources. **1** and **2** were purified by vacuum sublimation before device fabrication. Commercial ITO-coated glass was used as the starting substrate. Before device fabrication, the ITO glass was pre-cleaned carefully and treated by UV/O_3 for 5 min. The devices were prepared in vacuum at a pressure of 5×10^{-4} Pa. After the deposition of organic layers, LiF and aluminum were thermally evaporated onto the organic surface. The thicknesses of the organic materials and the cathode layers were monitored using a quartz-crystal thickness monitor. The electrical characteristics of the OLEDs devices were measured with a Keithley 2400 sourcemeter. The EL spectra and luminance of the OLED devices were obtained on a PR655 spectrometer. All measurements were carried out on the devices without encapsulations in ambient atmosphere under dark.

5. Syntheses

3,6-Di-*tert*-butyl-1-(1*H*-indol-2-yl)-9H-carbazole (IDBC). Water (65 mL) and THF (130 mL) were added to a mixture of 1-bromo-3,6-di-*tert*-butyl-9*H*-carbazole (7.8 g, 21.8 mmol), (1*H*-indol-2-yl)boronic acid pinacol ester (5.0 g, 20.7 mmol), $Pd(PPh_3)_4$ (1.2 g, 1.1 mmol) and K_2CO_3 (18.0 g, 130.2 mmol) at r.t. After heated at 60 °C for 13 h, the reaction mixture was extracted by CH_2Cl_2 for three times. The collected organic phase was dried with anhydrous Na_2SO_4 and then filtered. After removal of the solvent under reduced pressure, the residue was purified by silica-gel column chromatography (CH_2Cl_2 : petroleum ether = 2 : 3) to provide the product as a white solid (6.1 g, 71%). ^{1}H-NMR (400 MHz, CD_2Cl_2, ppm): δ 8.59 (s, 1H), 8.53 (s, 1H), 8.15 (s, 2H), 7.71 (d, J = 7.9 Hz, 1H), 7.67 (s, 1H), 7.60 – 7.47 (m, 2H), 7.43 (d, J = 8.5 Hz, 1H), 7.25 (t, J = 7.6 Hz, 1H), 7.18 (t, J = 7.5 Hz, 1H), 6.96 (s, 1H), 1.52 (s, 9H), 1.47 (s, 9H). ^{13}C{^{1}H}-NMR (100 MHz, DMSO-d_6, ppm): δ 141.26, 141.22, 138.86, 136.63, 135.68, 134.85, 128.87, 123.80, 123.33, 122.40, 121.41, 121.09, 119.83, 119.23, 115.95, 115.81, 115.44, 111.20, 100.52, 34.60, 34.42, 31.91. MS (ESI, *m/z*): 394.1 $[M]^+$ (calcd: 394.2). Elem. Anal. Calcd (%) for $C_{28}H_{30}N_2$: C, 85.24; H, 7.66; N, 7.10. Found: C, 85.87; H, 7.91; N, 7.00.

Compound 1. A solution of BPh_3 (2.0 g, 8.3 mmol) in toluene (50 mL) was added to a solution of IDBC (3.1 g, 7.8 mmol) in toluene (30 mL) at r.t. The resulting mixture was gradually heated to 100 °C and stirred at this temperature for 24 h. After removal of the solvent

on rotavapor, the residue was purified by silica-gel column chromatography (CH_2Cl_2 : petroleum ether = 1 : 2) to provide compound **1** as a red solid (1.7 g, 39%). ^{1}H-NMR (400 MHz, CD_2Cl_2, ppm): δ 8.42 (s, 1H), 8.10 (s, 1H), 7.78 (s, 1H), 7.57–7.53 (m, 5H), 7.25–7.11 (m, 10H), 6.86 (d, J = 8.7 Hz, 1H), 4.64 (s, 2H), 1.52 (s, 9H), 1.38 (s, 9H). ^{13}C{^{1}H}-NMR (100 MHz, CD_2Cl_2, ppm): δ 174.16, 149.38, 143.55, 142.41, 141.81, 141.46, 134.27, 133.07, 128.03, 127.78, 126.80, 126.48, 126.27, 125.15, 124.57, 124.42, 124.18, 121.64 120.32, 117.01, 114.17, 109.99, 38.48, 35.20, 34.88, 32.10, 32.07. MS (ESI, *m/z*): 558.0 $[M]^+$ (calcd: 558.3). Elem. Anal. Calcd (%) for $C_{40}H_{39}BN_2$: C, 86.01; H, 7.04; N, 5.02. Found: C, 86.39; H, 7.38; N, 4.84.

4-(*Tert*-butyl)-*N*-(4-(*tert*-butyl)phenyl)-2-(1*H*-indol-2-yl)aniline (IDBA). IDBA was synthesized and purified using the methods described for IDBC, with the starting material 1-bromo-3,6-di-*tert*-butyl-9*H*-carbazole replaced by 2-bromo-4-(*tert*-butyl)-*N*-(4-(*tert*-butyl)phenyl)aniline. The compound was obtained as a white solid in a yield of 60%. ^{1}H-NMR (400 MHz, DMSO-d_6, ppm): δ 11.30 (s, 1H), 7.60 (s, 1H), 7.50 (d, J = 7.8 Hz, 1H), 7.41 (d, J = 8.1 Hz, 1H), 7.26–7.18 (m, 5H), 7.08 (t, J = 7.0 Hz, 1H), 7.00–6.91 (m, 3H), 6.76 (s, 1H), 1.34 (s, 9H), 1.24(s, 9H). ^{13}C{^{1}H}-NMR (100 MHz, DMSO-d_6, ppm): δ 144.04, 142.33, 141.31, 138.29, 136.41, 135.87, 128.53, 126.15, 125.69, 125.09, 123.95, 121.15, 120.31, 129.87, 119.06, 116.14, 111.19, 100.98, 34.07, 33.71, 31.38, 31.27. MS (ESI, *m/z*): 396.1 $[M]^+$ (calcd: 396.3). Elem. Anal. Calcd (%) for $C_{28}H_{32}N_2$: C, 84.80; H, 8.13; N, 7.06. Found: C, 84.62; H, 8.48; N, 6.79.

Compound 2. Compound **2** was synthesized and purified using the methods described for compound **1**, with the starting material IDBC replaced by IDBA. The compound was obtained as a red solid in a yield of 34%. ^{1}H-NMR (400 MHz, CD_2Cl_2, ppm): δ 7.46 (d, J = 7.5 Hz, 1H), 7.44–7.41, (m, 4H), 7.31 (d, J = 2.4 Hz, 1H), 7.23 (dd, J = 9.2, 2.4 Hz, 1H), 7.13–7.07 (m, 7H), 7.03 (d, J = 8.6 Hz, 2H), 6.99 (t, J = 7.5 Hz, 1H), 6.71 (d, J = 8.1 Hz, 1H), 6.61 (d, J = 8.5 Hz, 2H), 6.39 (d, J = 9.2 Hz, 1H), 4.40 (s, 2H), 1.29 (s, 9H), 1.20 (s, 9H). ^{13}C{^{1}H}-NMR (100 MHz, CD_2Cl_2, ppm): δ 171.55, 151.94, 149.37, 147.87, 143.55, 137.62, 135.37, 134.97, 132.72, 129.08, 127.61, 127.01, 126.01, 125.56, 125.49, 124.85, 124.10, 119.51, 117.85, 111.32, 38.78, 34.50, 34.03, 31.47, 31.09. MS (ESI, *m/z*): 559.9 $[M]^+$ (calcd: 560.3). Elem. Anal. Calcd (%) for $C_{40}H_{41}BN_2$: C, 85.70; H, 7.37; N, 5.00. Found: C, 85.58; H, 7.57; N, 4.90.

6. Supplementary figures

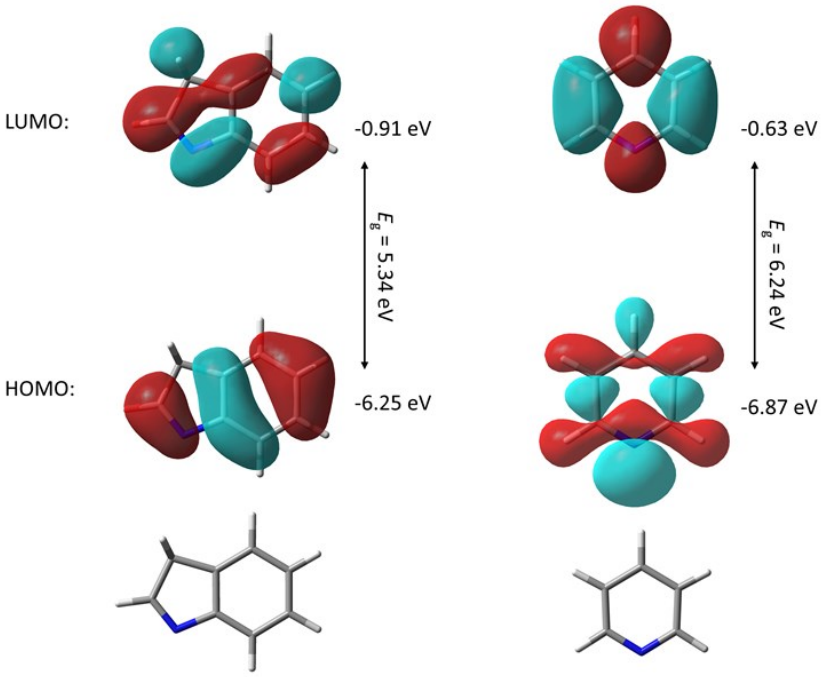


Fig. S1 DFT-calculated frontier molecular orbital distributions and energy levels of 3*H*-indole (left) and pyridine (right).

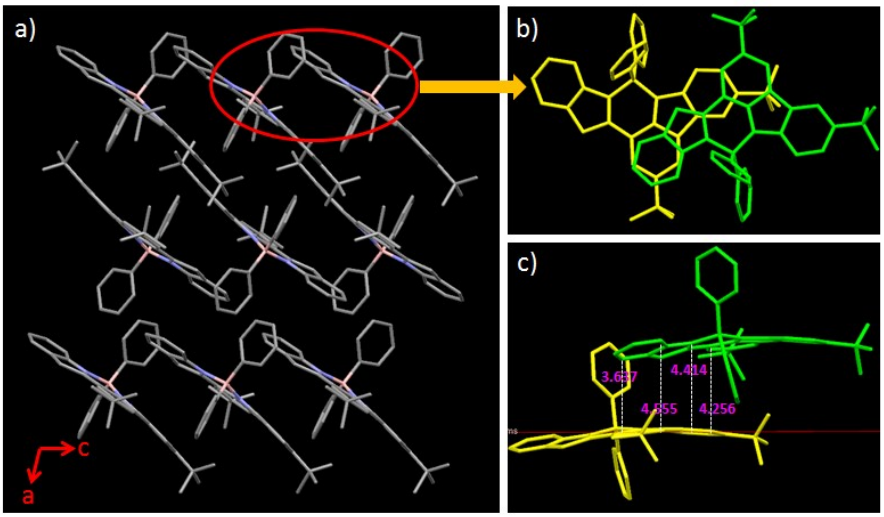


Fig. S2 Molecular packing structure of **1** in the single crystal (solvent molecules and hydrogen atoms are omitted for clarity): a) view along the *b* axis; b) arrangements of neighboring molecules viewed perpendicular to the mean plane of the carbazole moiety; c) distance between the mean plane of the carbazole moiety and the neighboring π-system.

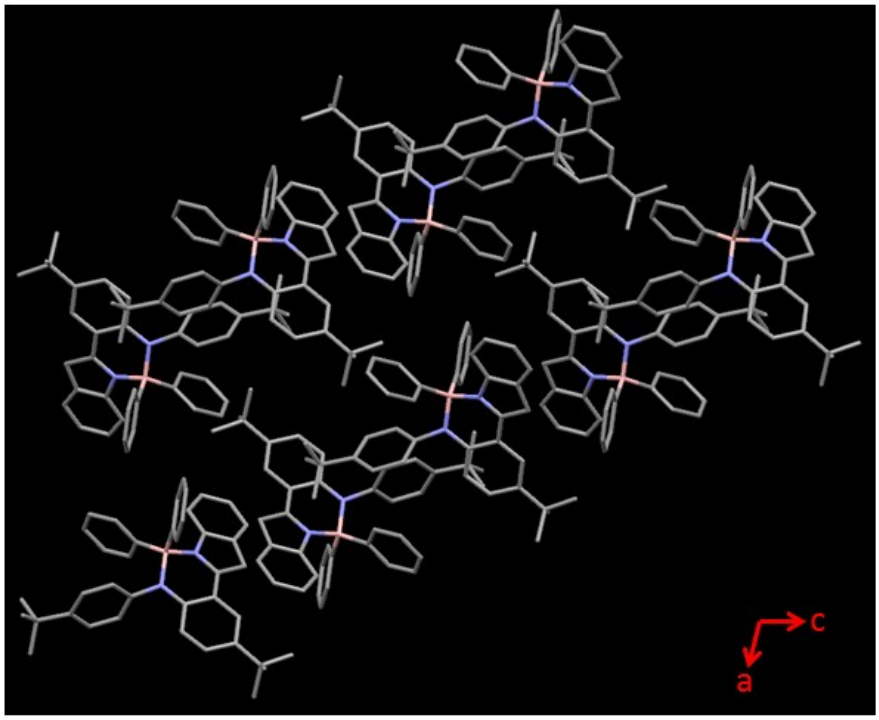


Fig. S3 Molecular packing structure of **2** in the single crystal viewed along the *b* axis (hydrogen atoms are omitted for clarity).

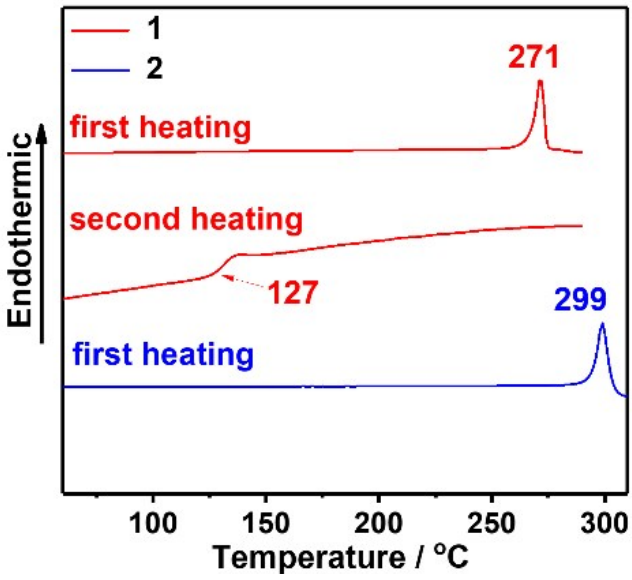


Fig. S4 DSC curves of **1** and **2**.

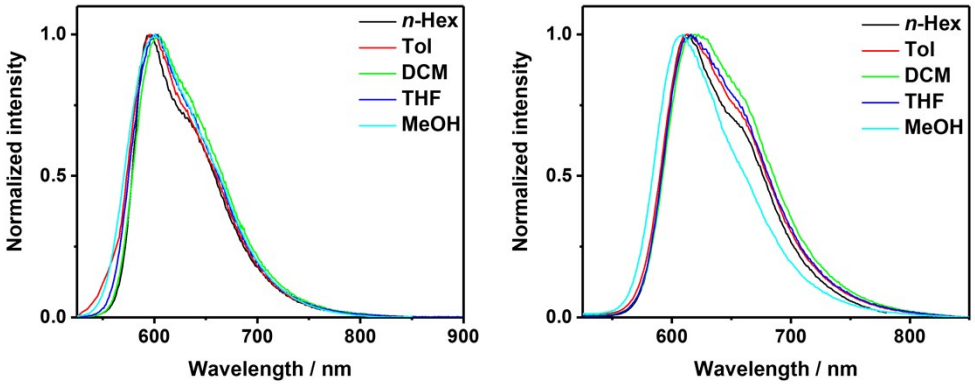
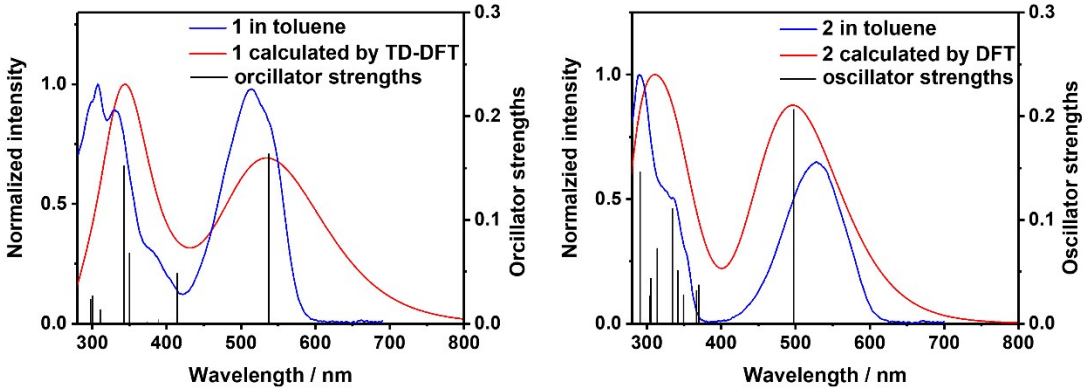


Fig. S5 Luminescence solvatochromism of **1** (left) and **2** (right).



Compound	Transition	*E* / eV	λ / nm	Dominant components
1	$S_1 \leftarrow S_0$	2.31	537	LUMO←HOMO (99%)
2	$S_1 \leftarrow S_0$	2.50	497	LUMO←HOMO (99%)

Fig. S6 Comparison between the calculated (10 singlet states) and experimental absorption spectra and of **1** (left) and **2** (right), as well as the calculated photophysical data of these compounds.

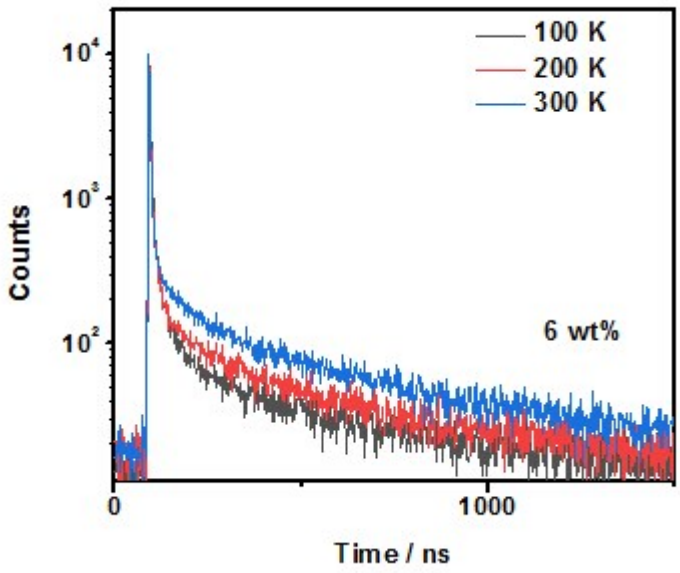


Fig. S7 Temperature-dependent fluorescence decay curves of the doped film with 6 wt% concentration.

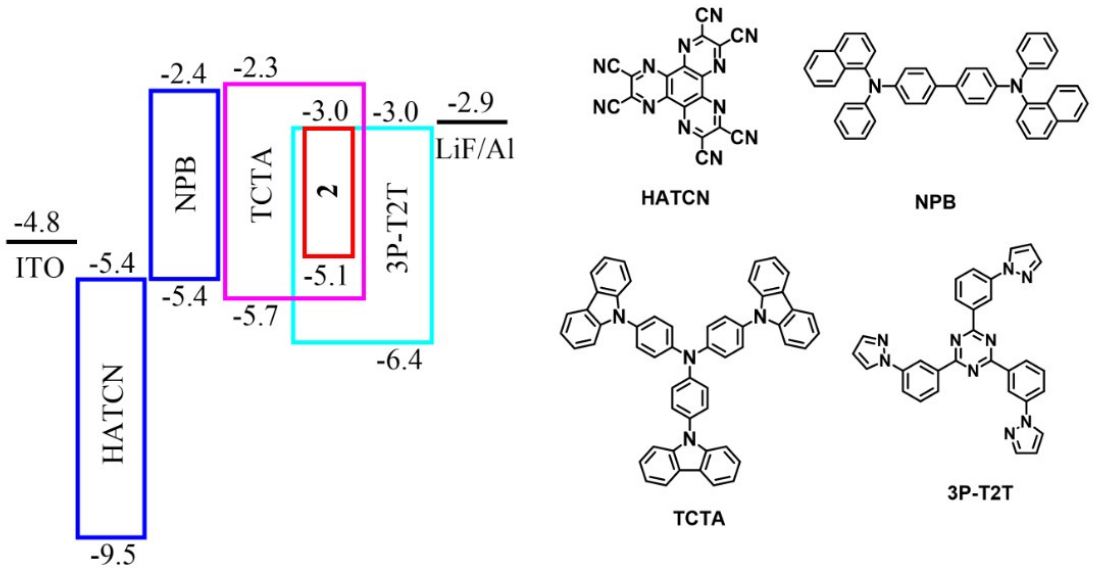


Fig. S8 Structures and energy levels (eV) of the materials adopted in the OLEDs.

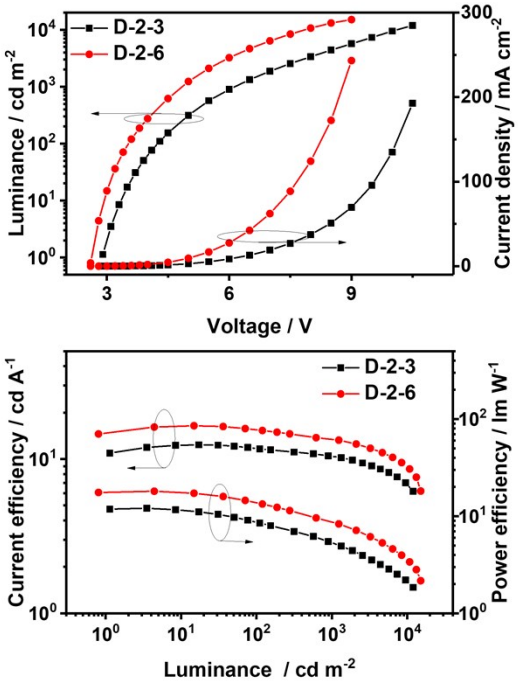


Fig. S9 Current density-voltage-luminance characteristics and the current and power efficiency *vs.* luminance characteristics of the OLED devices.

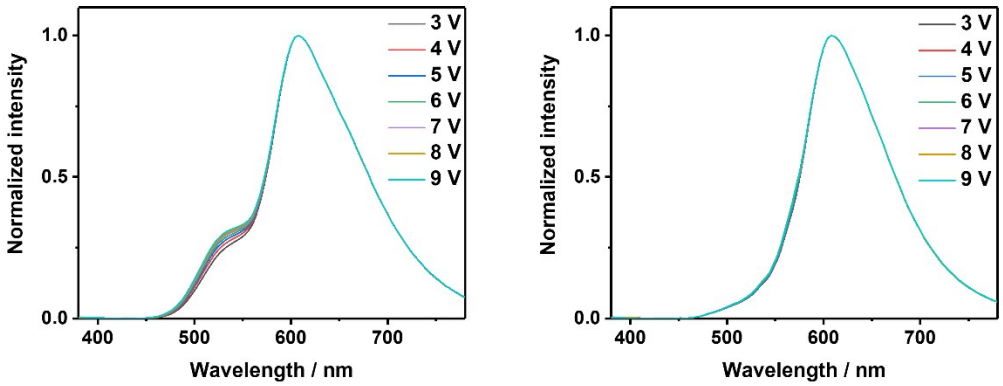


Fig. S10 Electroluminescent spectra of D-2-3 (left) and D-2-6 (right) under a variety of driving voltages.

7. Supplementary tables

Table S1 Summary of the photophysical data of the toluene solutions and doped films of the compounds.

	λ_{abs} / nm	λ_{PL} / nm	PLQY	Lifetime / ns	
				Prompt	Delayed
1 in toluene	514	595	0.40	---	---
2 in toluene	528	611	0.31	---	---
2 in co-host (3 wt%)	---	604	0.56	15	343
2 in co-host (6 wt%)	---	616	0.64	11	229

Table S2 Comparison between the performances of exciplex-hosted red fluorescent OLEDs reported in literatures and in this work.

Emitting layer	Device performance			
	$EQE_{max/100/1000}$[a] [%]	λ_{EL}[b] [nm]	CIE coordinates (x, y)	Ref.
TCTA:3P-T2T:6 wt% **2**	10.2/9.4/8.0	612	(0.620, 0.371)	This work
TCTA:3P-T2T:0.5 wt% DCJTB	7.48/---/7.32	586	---	
TCTA:3P-T2T:1 wt% DCJTB	10.15/---/10.03	605	---	6
TCTA:3P-T2T:1.5 wt% DCJTB	5.63/---/5.13	610	---	
TrisPCz:CN-T2T:1 wt% DCJTB	9.7/---/9.1	---	(0.59, 0.40)	7
TCTA:B4PYMPM:4CzIPN:0.5 wt% DCJTB[c]	12.9/12.4/10.1	---	(0.58, 0.41)	
TCTA:B4PYMPM:4CzPN:0.5 wt% DCJTB[c]	12.3/11.9/9.9	---	(0.58, 0.41)	
TCTA:B4PYMPM:4CzTPN:0.5 wt% DCJTB[c]	8.4/8.0/6.4	---	(0.56, 0.43)	8
TCTA:B4PYMPM:4CzTPN-Ph:0.5 wt% DCJTB[c]	7.5/7.14/5.8	---	(0.59, 0.41)	
TCTA:B4PYMPM:0.5 wt% DCJTB	7.3/7.1/6.0	---	(0.59, 0.41)	
TCTA:B4PYMPM: 0.5 wt% DCJTB	10.6/ ---/ ---	600	---	9
TAPC: 1 wt% DBP/TAPC (3 nm)/TmPyTZ	14.5/---/---	602	(0.527, 0.460)	
TAPC: 1 wt% DBP/mCP (2 nm)/TmPyTZ	14.9/---/---	602	(0.560, 0.429)	10
TAPC: 1%DCJTB/mCP (3 nm)/TmPyTZ	10.4//---/---	584	---	

[a] The maximum EQE and EQEs at 100 and 1000 cd m^{-2}. [b] The EL peak. [c]A sensitizer with thermally-activated delayed fluorescence was adopted for improving device performance.

8. References

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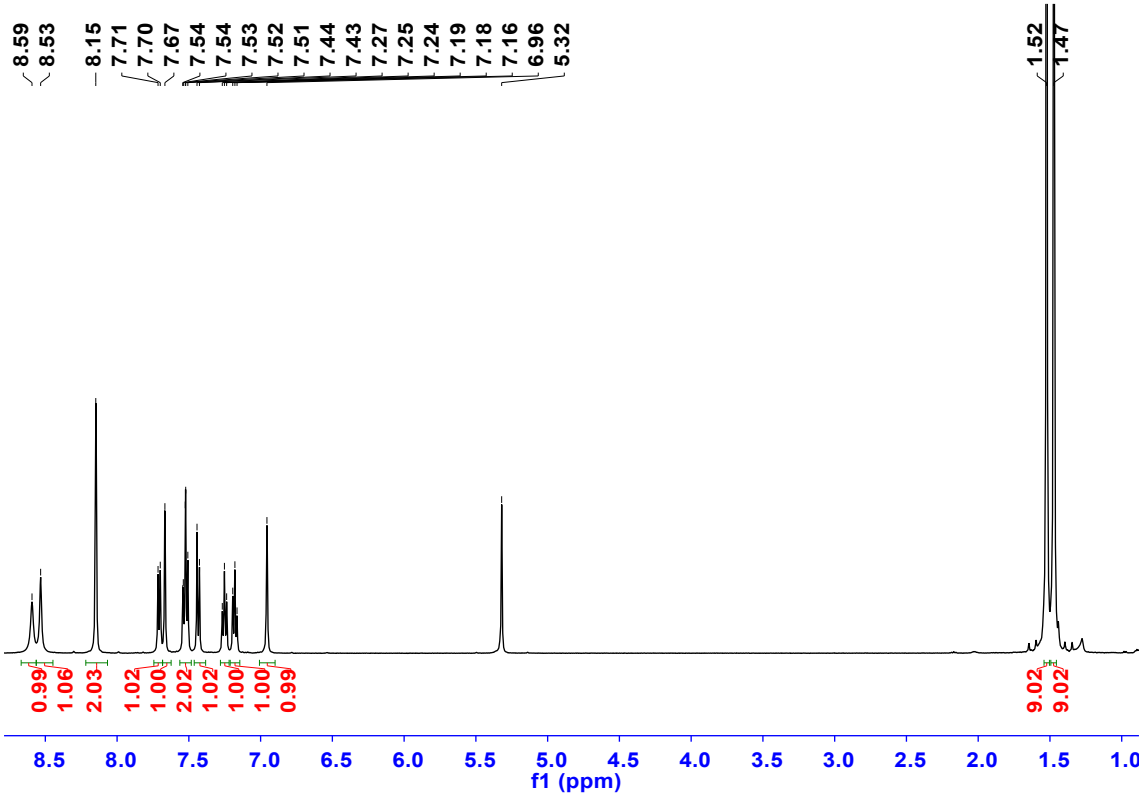
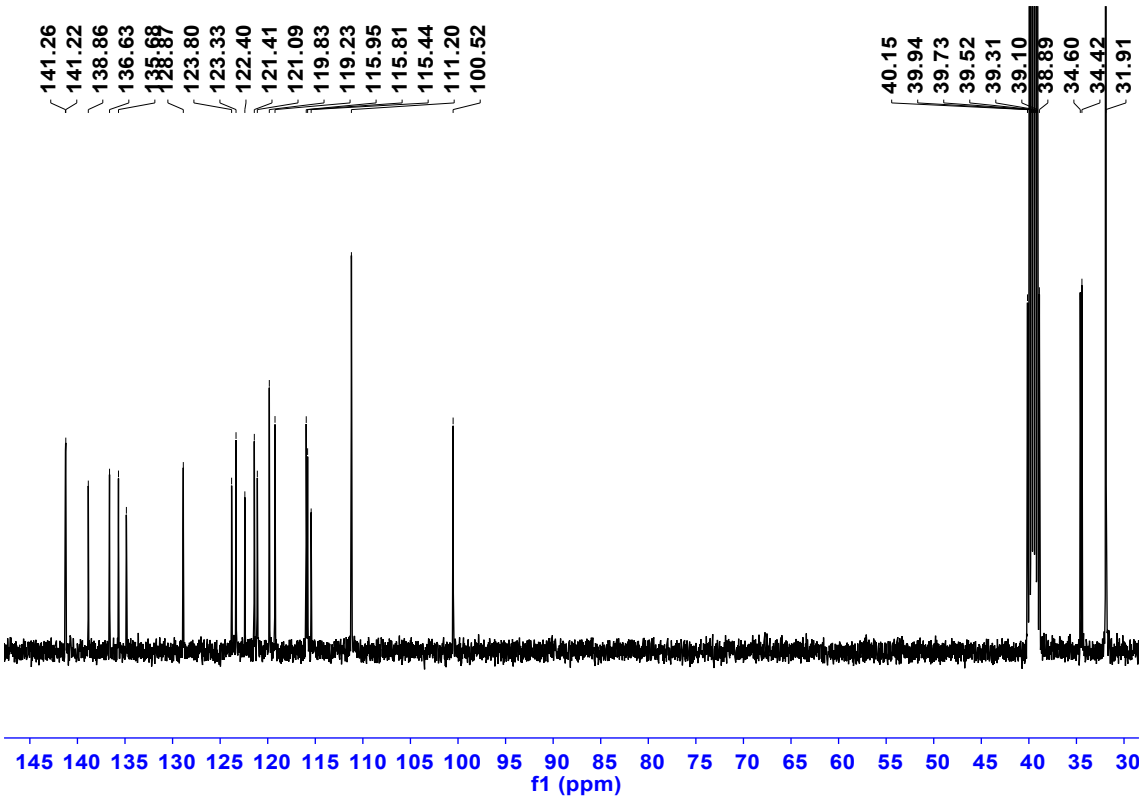
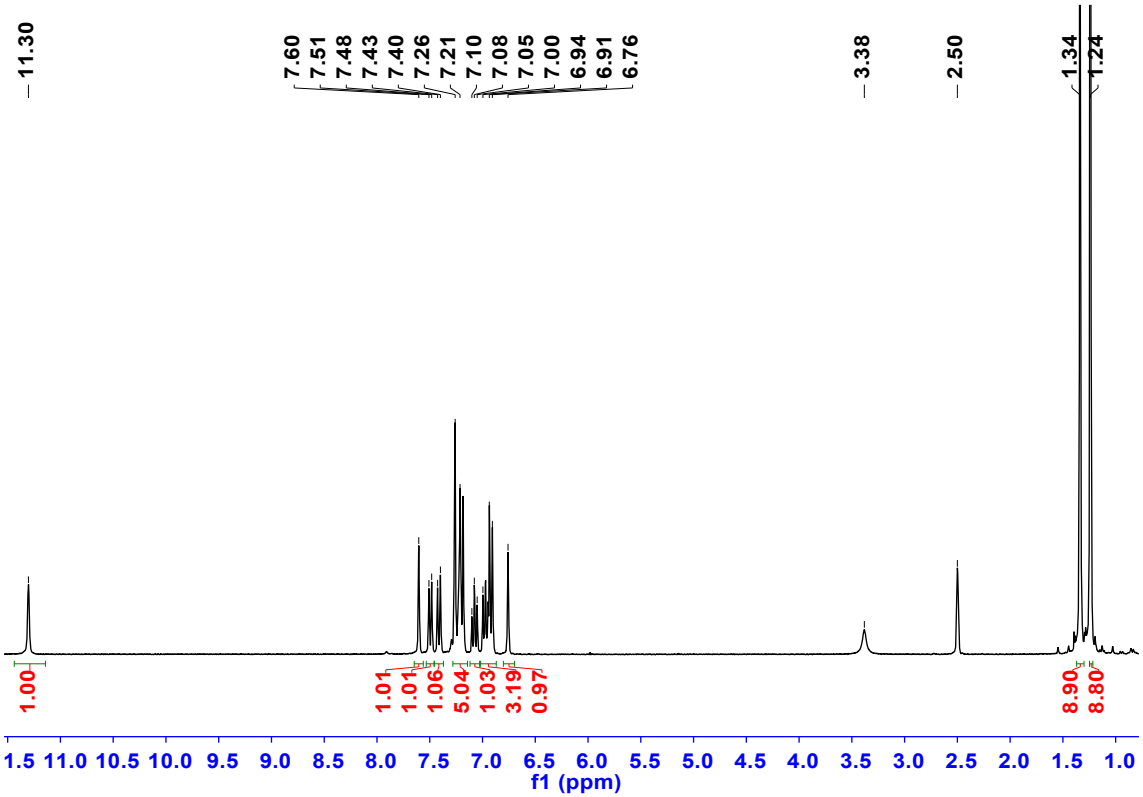
9. NMR spectra



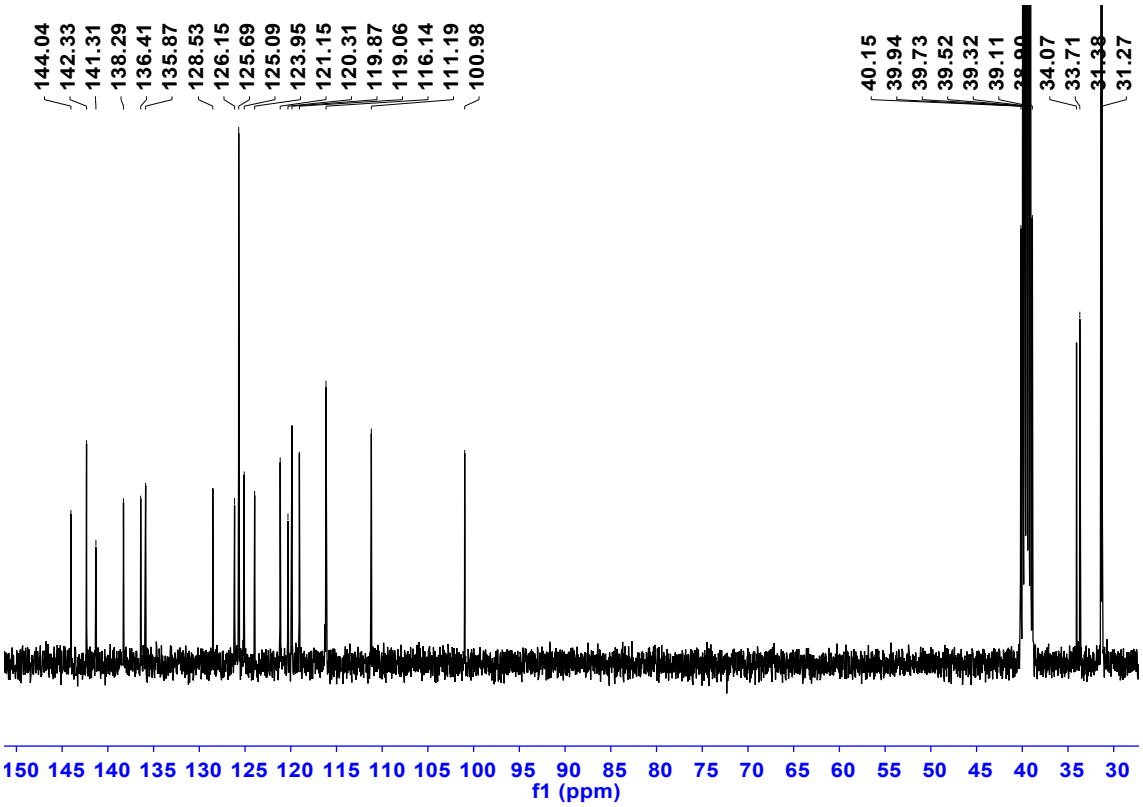
^{1}H-NMR spectrum of **IDBC** in CD_2Cl_2 at 400 MHz.



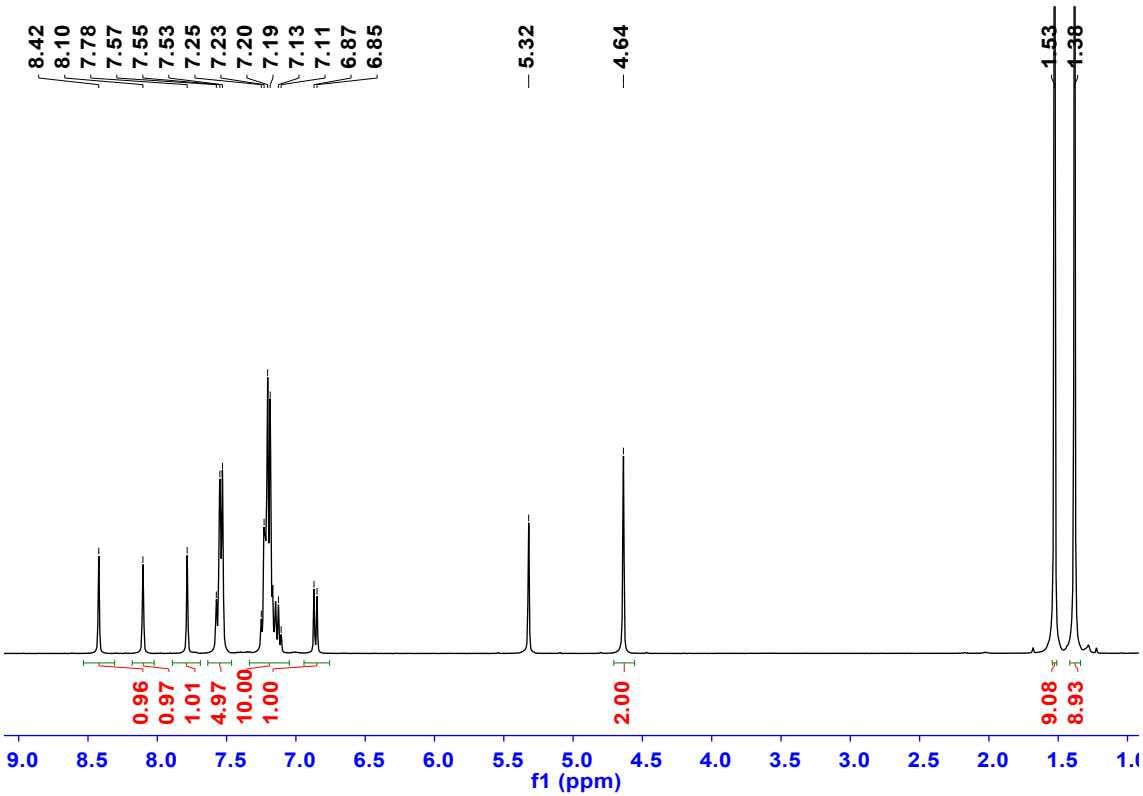
^{13}C{^{1}H}-NMR spectrum of **IDBC** in DMSO-d_6 at 100 MHz.



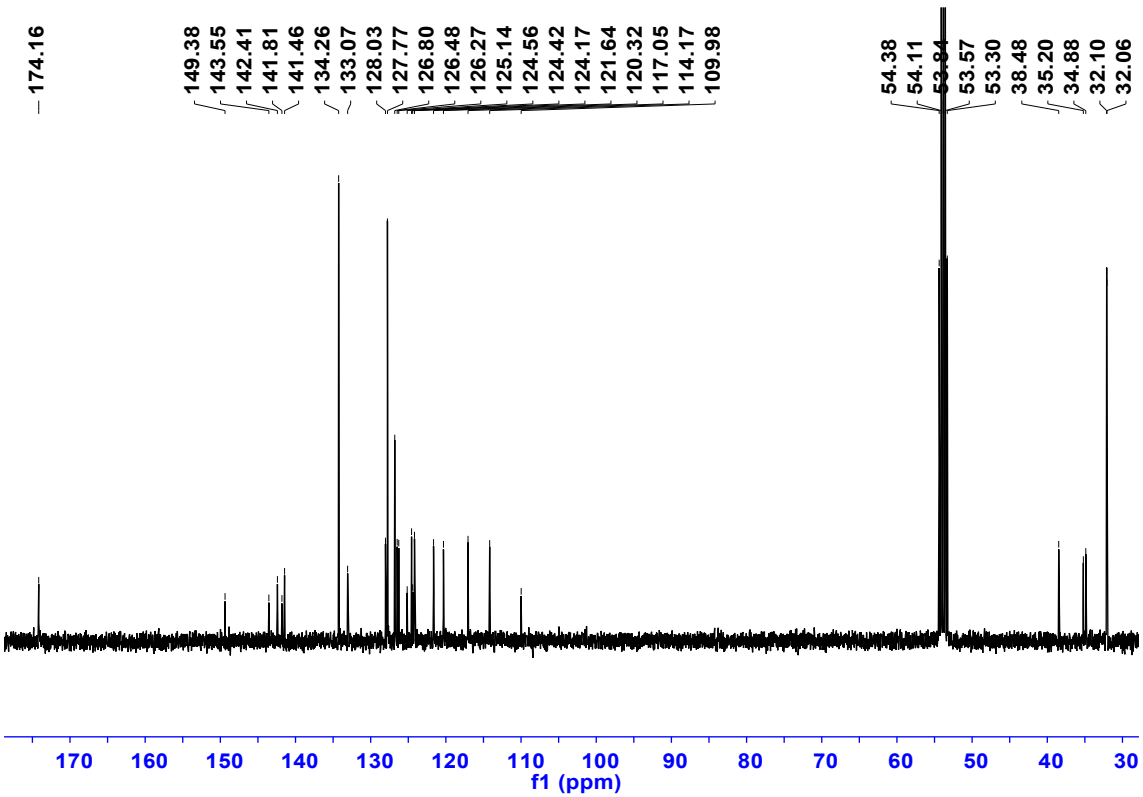
^{1}H-NMR spectrum of **IDBA** in DMSO-d_6 at 400 MHz.



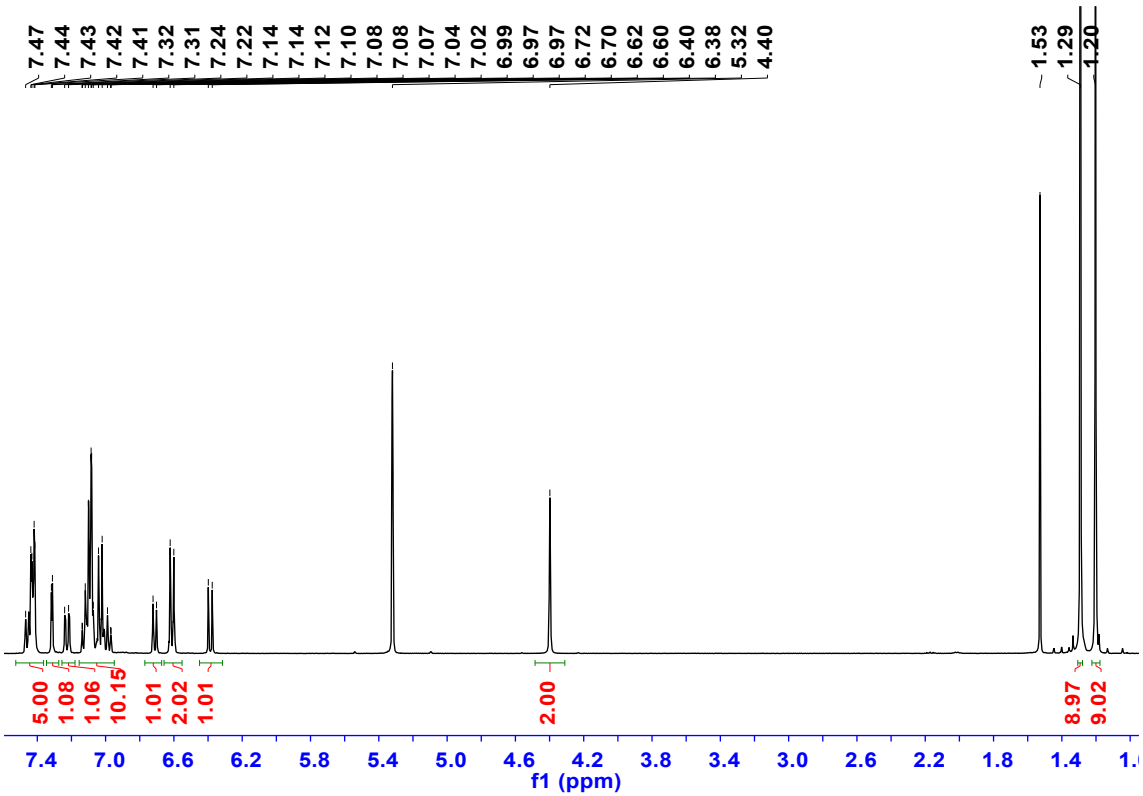
^{13}C{^{1}H}-NMR spectrum of **IDBA** in DMSO-d_6 at 100 MHz.



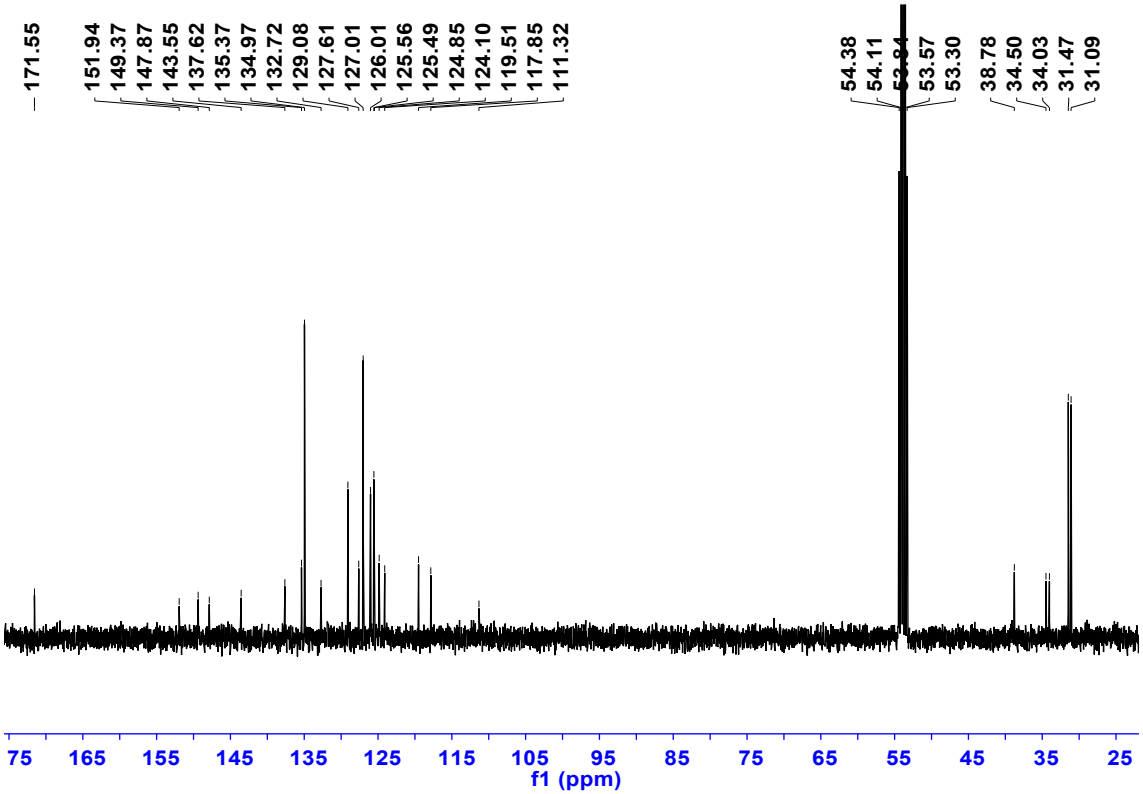
^{1}H-NMR spectrum of **1** in CD_2Cl_2 at 400 MHz.



^{13}C{^{1}H}-NMR spectrum of **1** in CD_2Cl_2 at 100 MHz.



^{1}H-NMR spectrum of **2** in CD_2Cl_2 at 400 MHz.



^{13}C{^{1}H}-NMR spectrum of **2** in CD_2Cl_2 at 100 MHz.

10. Crystallographic data

	1	**2**
Empirical formula	C46 H51 B N2	C40 H41 B N2
Formula weight	642.70	560.56
Temperature	273.15 K	153(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	P 1 21/c 1	$P2_1/n$
Unit cell dimensions	a = 16.3673(10) Å b = 17.2125(11) Å c = 13.2993(7) Å α= 90° β= 95.620(2)° γ = 90°	a = 14.356(3) Å b = 10.988(2) Å c = 21.124(4) Å α= 90° β= 106.05(3)° γ = 90°.
Volume	3728.7(4) $Å^3$	3202.3(12) $Å^3$
Z	4	4
Density (calculated)	1.145 Mg/m^3	1.163 Mg/m^3
Absorption coefficient	0.065 mm^{-1}	0.066 mm^{-1}
F(000)	1384	1200
Theta range for data collection	2.767 to 24.999°.	3.078 to 24.999°.
Index ranges	-19<=h<=19, -20<=k<=20, -15<=l<=13	-16<=h<=16, -11<=k<=12, -24<=l<=25
Reflections collected	44600	14607
Independent reflections	6551 [R(int) = 0.0908]	4710 [R(int) = 0.0596]

Completeness to theta = 24.999°	99.6 %	125.6 %
Absorption correction	Semi-empirical from equivalents	None
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	6551 / 183 / 468	4710 / 0 / 394
Goodness-of-fit on F^2	1.086	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0992, wR2 = 0.2684	R1 = 0.0573, wR2 = 0.1276
R indices (all data)	R1 = 0.1740, wR2 = 0.3304	R1 = 0.1100, wR2 = 0.1444

11. Cartesian coordinates of DFT-optimized geometries

1 optimized by DFT at the B3LYP/6-31G(d,p) level of theory.

	Coordinates (Angstroms)		
Symbol	X	Y	Z
B1	-1.289712	-0.891362	0.189729
C1	-1.510678	-1.153896	1.785898
C2	-2.453111	-0.463259	2.568801
H1	-3.102278	0.275859	2.108151
C3	-2.595551	-0.689207	3.940472
H2	-3.339534	-0.131813	4.504276
C4	-1.786621	-1.623397	4.584211
H3	-1.892060	-1.802857	5.650700
C5	-0.836463	-2.323662	3.838981
H4	-0.192825	-3.052857	4.324570
C6	-0.707363	-2.090216	2.469710
H5	0.047765	-2.647173	1.923628
C7	-1.541373	-2.165511	-0.791077
C8	-1.956946	-3.428805	-0.334339
H6	-2.131054	-3.577282	0.727759
C9	-2.153000	-4.501397	-1.209835
H7	-2.471890	-5.465350	-0.821350
C10	-1.940266	-4.335887	-2.578382
H8	-2.092022	-5.166567	-3.262302
C11	-1.527117	-3.092122	-3.060974
H9	-1.355046	-2.951539	-4.125089
C12	-1.330595	-2.031724	-2.176611
H10	-0.996481	-1.074475	-2.571378
C13	-3.679937	0.226872	-0.508635
C14	-4.478526	-0.914791	-0.518385
H11	-4.061972	-1.895539	-0.338376
C15	-5.841924	-0.748309	-0.777940

H12	-6.483414	-1.624022	-0.793401
C16	-6.391994	0.514061	-1.015869
H13	-7.454505	0.611756	-1.215685
C17	-5.581183	1.654469	-0.993442
H14	-6.005698	2.638600	-1.170434
C18	-4.226672	1.499416	-0.737572
C19	-3.113828	2.501906	-0.626617
H15	-2.943528	3.072871	-1.547377
H16	-3.270997	3.235112	0.174865
C20	-1.929551	1.620533	-0.313441
C21	-0.582435	2.047616	-0.149434
C22	-0.142721	3.391535	-0.165610
H17	-0.889487	4.175439	-0.209792
C23	2.167458	2.676098	-0.108311
H18	3.226191	2.919577	-0.105696
C24	1.778343	1.344636	-0.098306
C25	0.390760	1.036378	-0.084656
C26	1.411691	-0.923074	-0.122153
C27	2.444195	0.057231	-0.120470
C28	3.785390	-0.327088	-0.155818
H19	4.556260	0.438605	-0.151559
C29	3.092978	-2.629930	-0.213432
H20	3.330532	-3.686150	-0.259333
C30	1.743842	-2.277204	-0.177601
H21	0.977997	-3.042115	-0.213153
C31	1.212071	3.726057	-0.128316
C32	1.704724	5.186495	-0.122540
C33	0.542764	6.196845	-0.146606
H22	-0.068092	6.094367	-1.049794
H23	-0.109976	6.087675	0.725836
H24	0.940647	7.216351	-0.134094
C34	2.536254	5.445048	1.156619
H25	2.903420	6.477486	1.172036
H26	1.931500	5.285342	2.055116

H27	3.405528	4.783982	1.219534
C35	2.587123	5.443301	-1.367364
H28	2.019498	5.281543	-2.289566
H29	2.953197	6.476213	-1.369908
H30	3.459775	4.784121	-1.394360
C36	4.137161	-1.681933	-0.199609
C37	5.625049	-2.083967	-0.236676
C38	6.334513	-1.557946	1.033583
H31	7.396944	-1.827701	1.019963
H32	6.268936	-0.468807	1.113993
H33	5.886367	-1.985438	1.936398
C39	5.819769	-3.610853	-0.293509
H34	5.366302	-4.046610	-1.189681
H35	6.888827	-3.846190	-0.317444
H36	5.392657	-4.108983	0.582886
C40	6.296878	-1.469375	-1.487689
H37	5.820938	-1.832068	-2.404570
H38	6.231812	-0.377213	-1.489334
H39	7.358596	-1.739169	-1.525140
N1	-2.277638	0.338614	-0.257240
N2	0.152939	-0.298304	-0.083027

2 optimized by DFT at the B3LYP/6-31G(d,p) level of theory.

Coordinates (Angstroms)			
Symbol	X	Y	Z
B1	0.149442	1.162977	0.391307
C1	2.119502	2.581269	-0.919134
C2	2.376427	0.365426	-0.637885
C3	-0.986501	2.172069	-0.186688
C4	3.404503	2.318150	-1.419582
C5	3.665577	0.847288	-1.264633
H1	3.862437	0.334510	-2.213345

H2	4.518594	0.635514	-0.607000
C6	0.541317	1.351332	1.966926
C7	3.042903	-1.997518	-0.415196
H3	4.060227	-1.687644	-0.622436
C8	3.432253	-5.446077	-1.438088
H4	4.164660	-6.259383	-1.493809
H5	3.408799	-4.942501	-2.410080
H6	2.449161	-5.897183	-1.273145
C9	-2.693717	3.907457	0.093236
H7	-3.243704	4.575117	0.751816
C10	3.852961	-5.209871	1.038931
H8	4.124545	-4.534120	1.856206
H9	4.594674	-6.015626	1.001789
H10	2.887171	-5.660468	1.286490
C11	5.217207	-3.907124	-0.602073
H11	5.553659	-3.215334	0.177309
H12	5.261293	-3.387942	-1.565463
H13	5.934541	-4.732943	-0.641015
C 12	-6.699959	-1.417970	0.858377
H14	-6.689896	-0.335893	1.023931
H15	-6.343274	-1.907152	1.770697
H16	-7.741730	-1.719384	0.708487
C13	-5.969420	-3.350119	-0.549248
H17	-7.017322	-3.649907	-0.664343
H18	-5.560137	-3.874371	0.320608
H29	-5.425519	-3.695759	-1.433286
C14	-6.463692	-1.114627	-1.611582
H20	-7.516806	-1.392097	-1.735158
H21	-5.937590	-1.390268	-2.530216
H22	-6.407351	-0.026207	-1.509414
C15	0.690766	-1.317245	-0.045857
C16	2.054407	-0.982966	-0.326557
C17	2.755569	-3.336880	-0.239463
C18	-1.632012	-0.710066	-0.022988

C19	-4.382692	-1.419708	-0.224179
C20	1.600332	3.875563	-0.917055
H23	0.608979	4.085316	-0.540724
C21	-2.525163	-0.419202	1.010605
H24	-2.165906	0.082687	1.901537
C22	0.442024	0.302182	2.899022
H25	0.080351	-0.667905	2.570718
C23	-1.722578	3.052125	0.623564
H26	-1.532614	3.072881	1.692790
C24	1.028285	2.577646	2.465489
H27	1.131293	3.426079	1.794429
C25	3.807801	-4.454685	-0.310925
C26	-3.873653	-0.766464	0.904640
H28	-4.527898	-0.516662	1.731743
C27	1.271570	1.686766	4.701495
H29	1.548507	1.815448	5.744400
C28	-1.283721	2.184928	-1.563252
H30	-0.743837	1.513159	-2.227553
C29	0.403006	-2.702852	0.108099
H31	-0.612587	-3.007077	0.327191
C30	1.395673	-3.653785	0.024269
H32	1.114146	-4.691055	0.182946
C31	4.192929	3.339498	-1.928534
H33	5.187979	3.134980	-2.313706
C32	0.795443	0.460010	4.242181
H34	0.700712	-0.378757	4.927502
C33	2.402580	4.898129	-1.432915
H35	2.015902	5.912642	-1.442499
C34	1.388296	2.748765	3.802528
H36	1.757725	3.712672	4.143964
C35	-2.129193	-1.354664	-1.165708
H37	-1.454039	-1.573051	-1.987687
C36	3.680788	4.641980	-1.935032
H38	4.280182	5.456014	-2.330661

C37	-5.862436	-1.817013	-0.371036
C38	-3.471185	-1.705685	-1.256038
H39	-3.815053	-2.201234	-2.159471
C39	-2.958741	3.902987	-1.275668
H40	-3.711326	4.566942	-1.692584
C40	-2.248269	3.032457	-2.105921
H41	-2.447438	3.015988	-3.174565
N1	-0.252749	-0.335668	0.055072
N2	1.530770	1.369391	-0.447597