

**Electronic Supplementary Information (ESI) for**  
**Intramolecular charge transfer induced emission from triphenylamine-*o*-**  
**carborane dyads**

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**Table of contents**

<b>1</b>	<b>NMR spectra &amp; MALDI-TOF spectra .....</b>	<b>2</b>
<b>2</b>	<b>Thermo-gravimetric analysis .....</b>	<b>6</b>
<b>3</b>	<b>Solvatochromism .....</b>	<b>6</b>
<b>4</b>	<b>Time-resolved emission decay .....</b>	<b>7</b>
<b>5</b>	<b>Density functional calculations.....</b>	<b>8</b>
<b>6</b>	<b>Electrochemistry.....</b>	<b>8</b>
<b>7</b>	<b>Emission spectra .....</b>	<b>错误！未定义书签。</b>
<b>8</b>	<b>Emission spectra and Time-resolved emission decay.....</b>	<b>9</b>

# 1 NMR Spectra & MALDI-TOF spectra

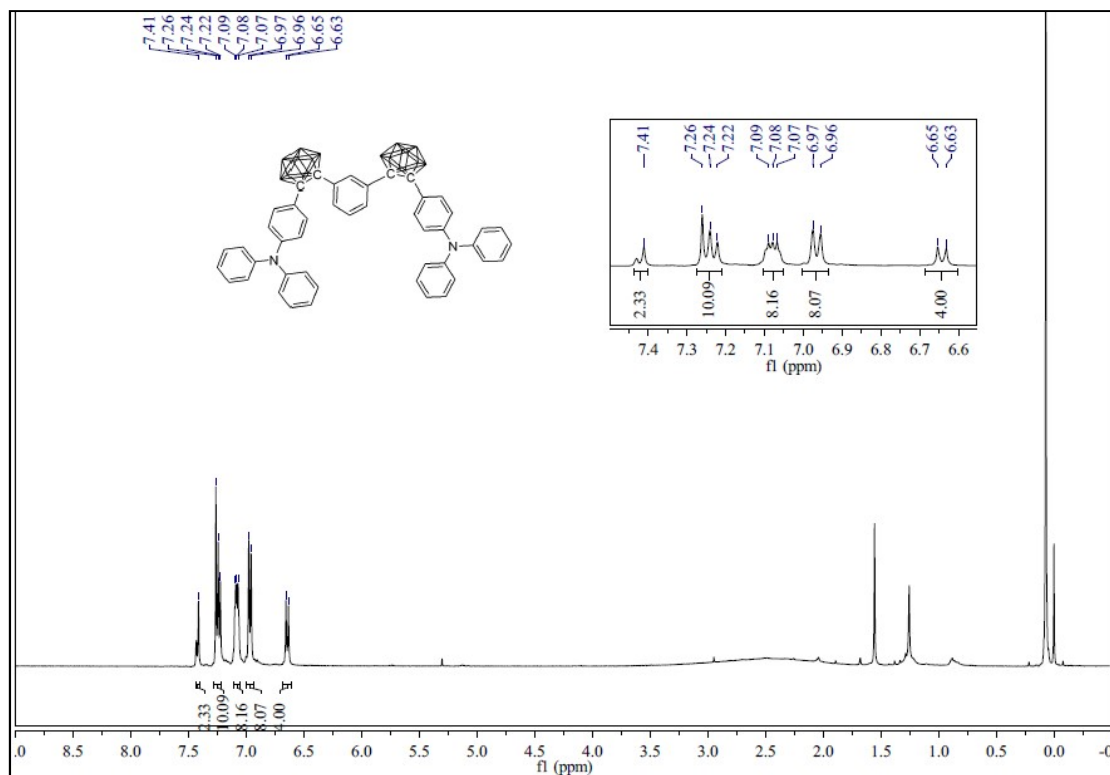


Fig. S1  $^1\text{H}$  NMR spectrum of **o-1** in  $\text{CDCl}_3$ .

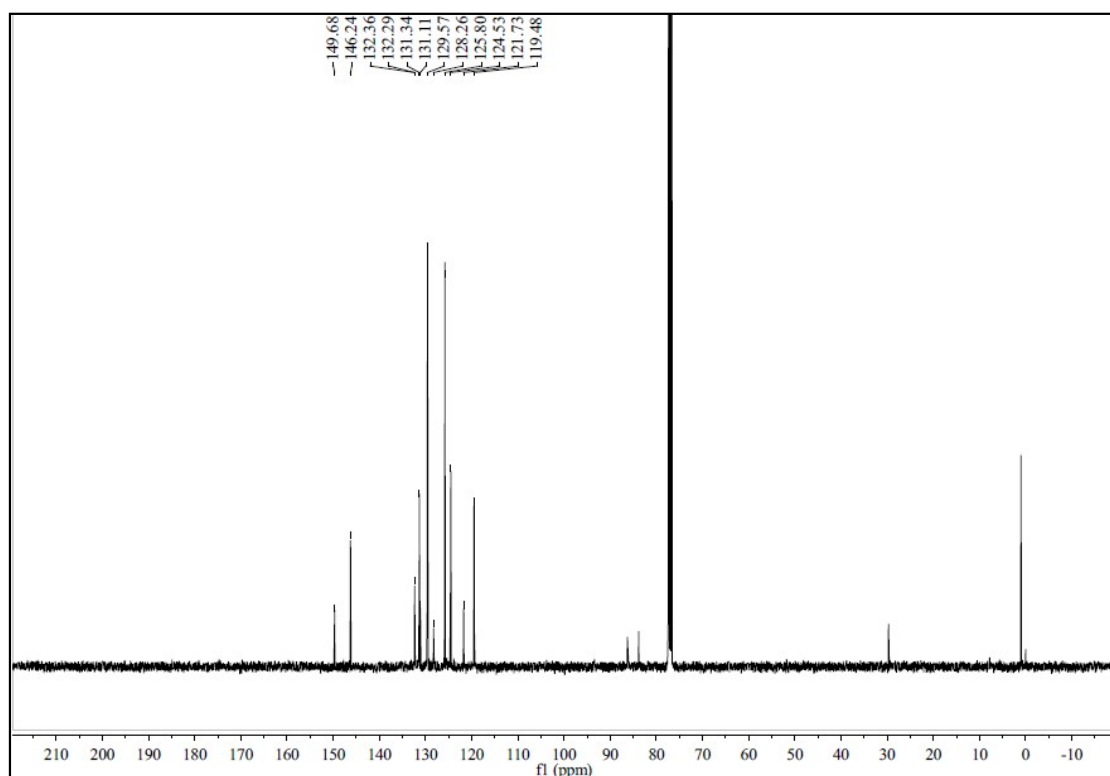
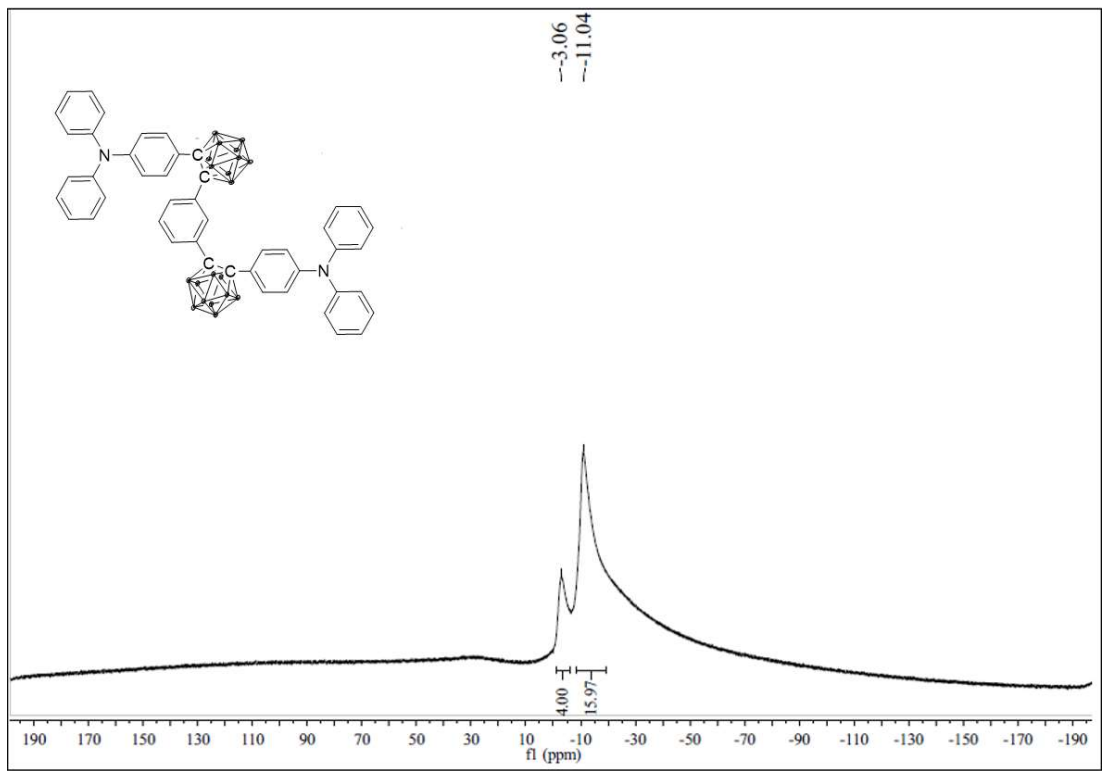
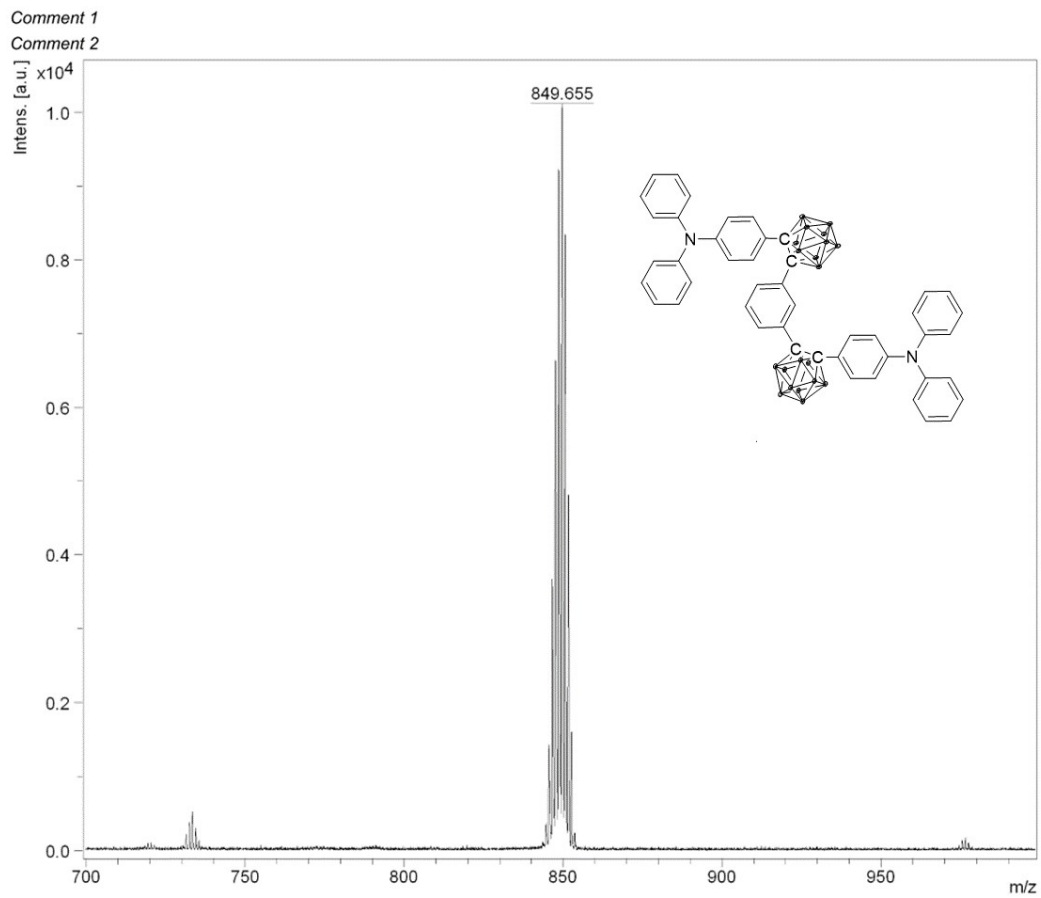


Fig. S2  $^{13}\text{C}$  NMR spectrum of **o-1** in  $\text{CDCl}_3$ .



**Fig. S3**  $^{11}\text{B}$  NMR spectrum of *o*-1 in  $\text{CDCl}_3$ .



**Fig. S4** MALDI-TOF mass spectrum of *o*-1.

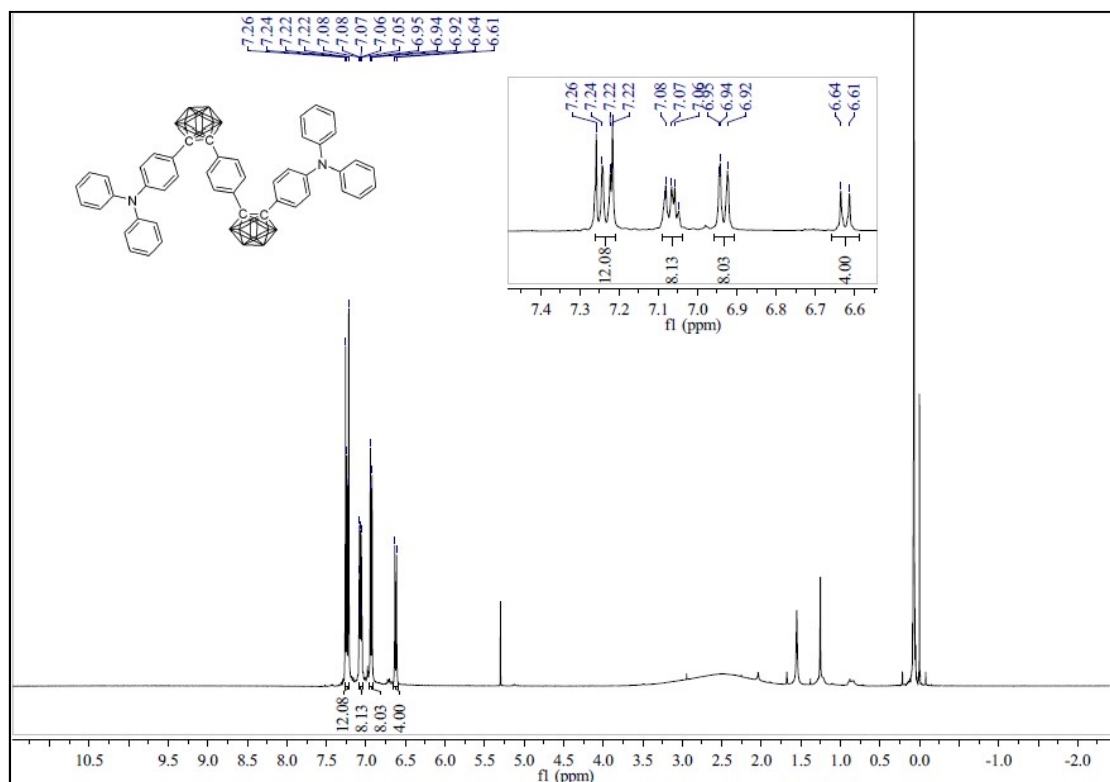


Fig. S5  $^1\text{H}$  NMR spectrum of *o-2* in  $\text{CDCl}_3$ .

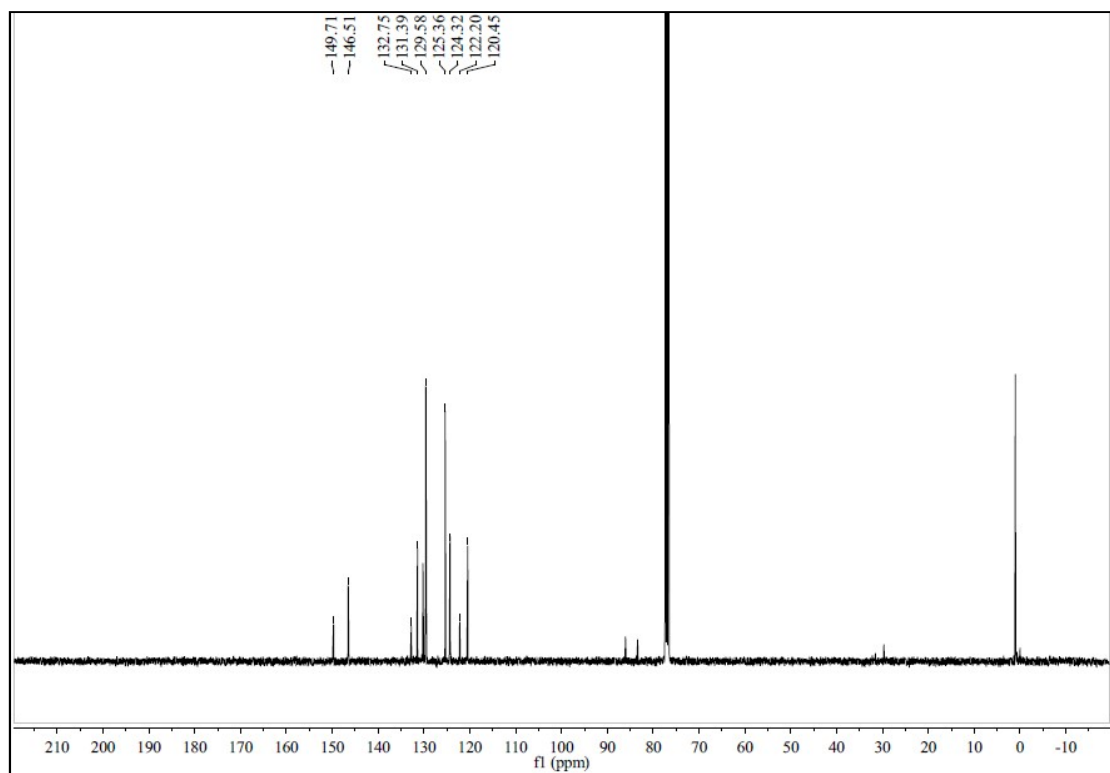
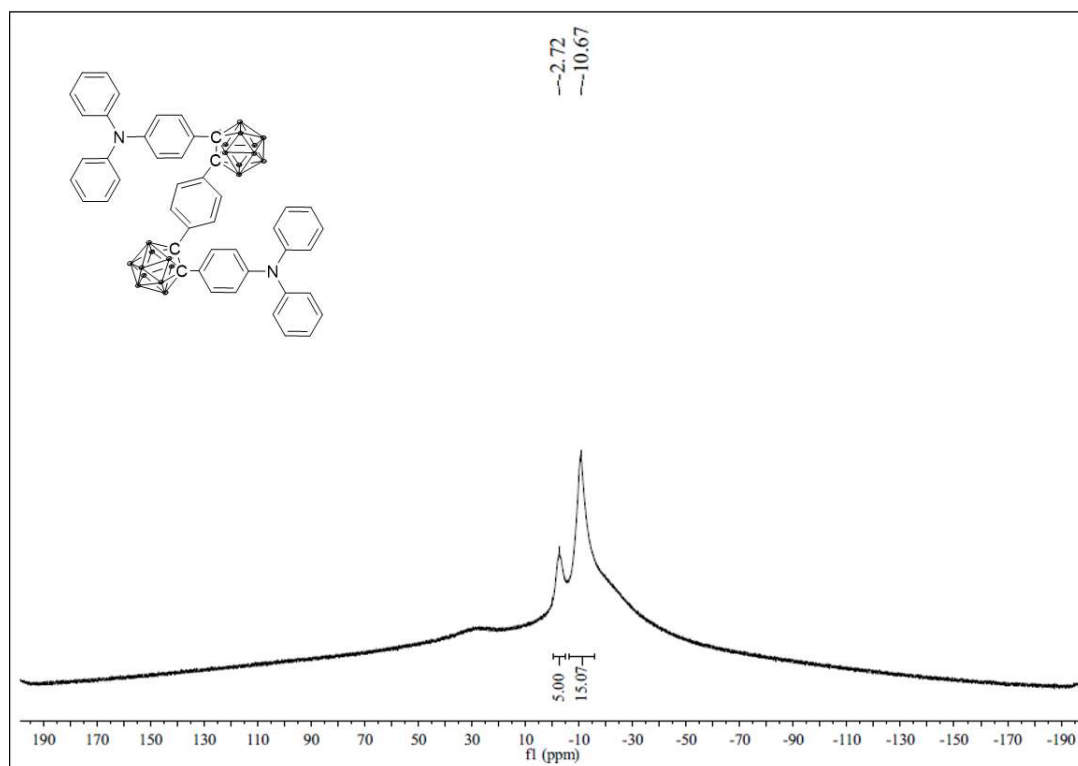
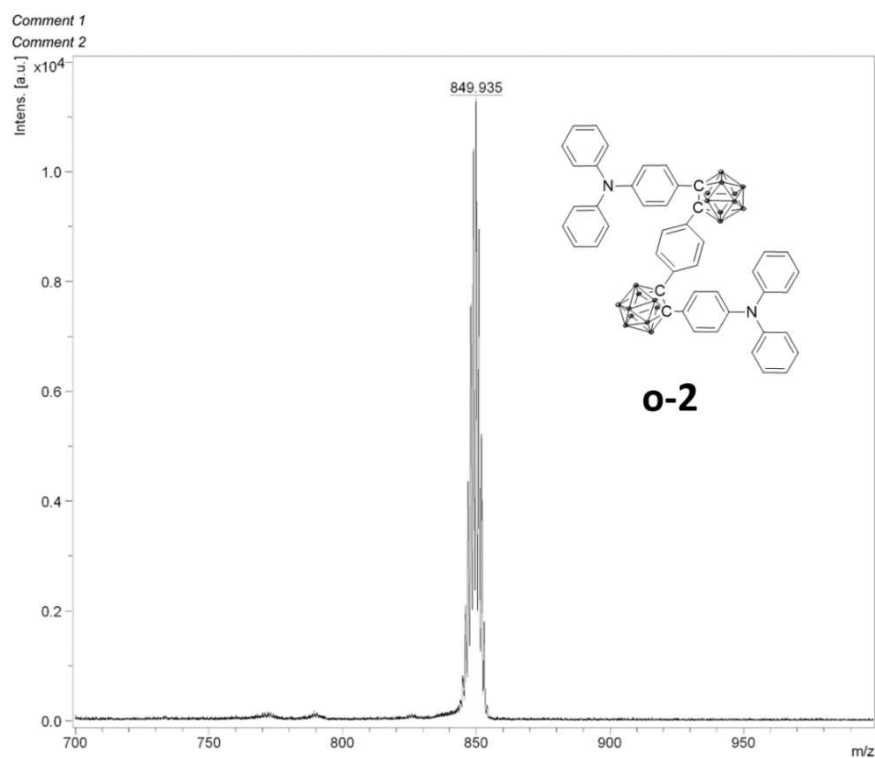


Fig. S6  $^{13}\text{C}$  NMR spectrum of *o-2* in  $\text{CDCl}_3$ .



**Fig. S7**  $^{11}\text{B}$  NMR spectrum of **o-2** in  $\text{CDCl}_3$ .



**Fig. S8** MALDI-TOF mass spectra of **o-2**.

## 2 Thermo-gravimetric analysis

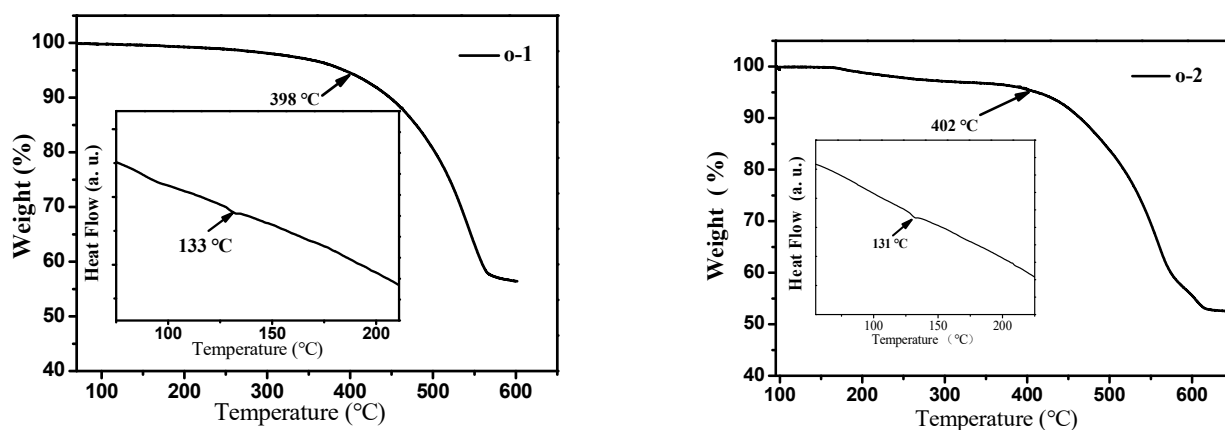


Fig. S9 TGA and DSC curves of *o-1*, *o-2* at a heating rate of  $10^{\circ}\text{C min}^{-1}$ .

## 3 Solvatochromism

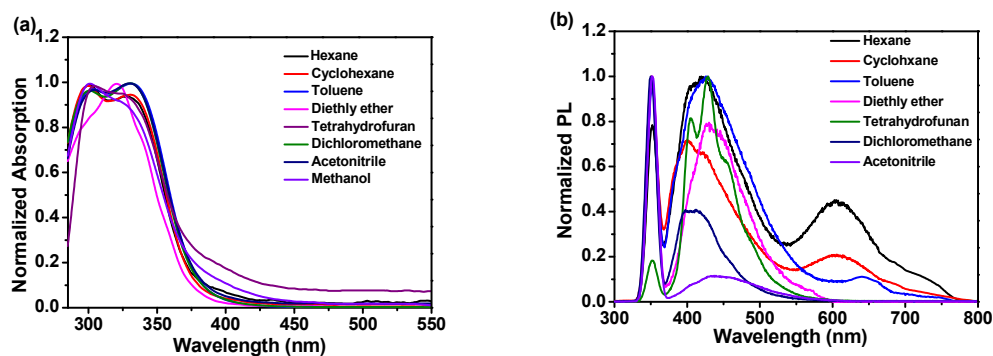


Fig. S10 (a) UV-vis absorption and (b) emission spectra of *o-2* in various solvents at room temperature.

#### 4 Time-resolved emission decay

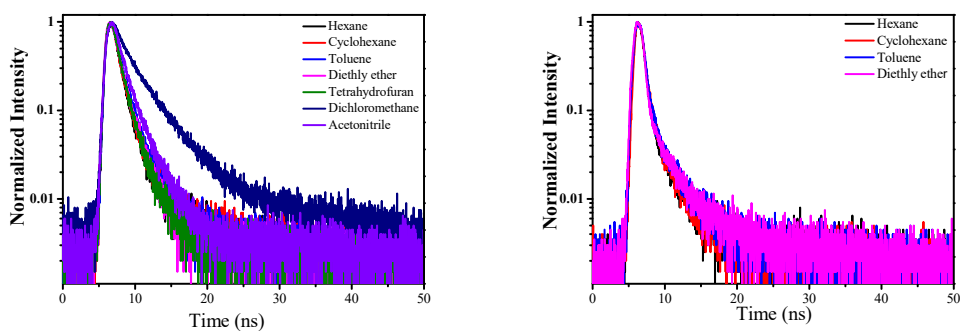


Fig. S11 Emission decay profiles for *o-1* in various solvents.

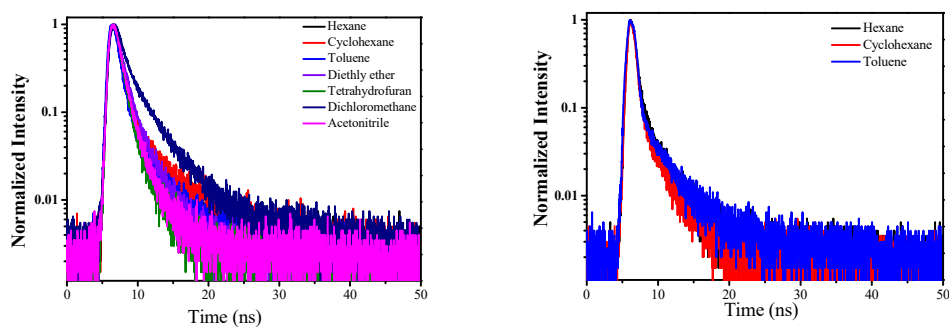
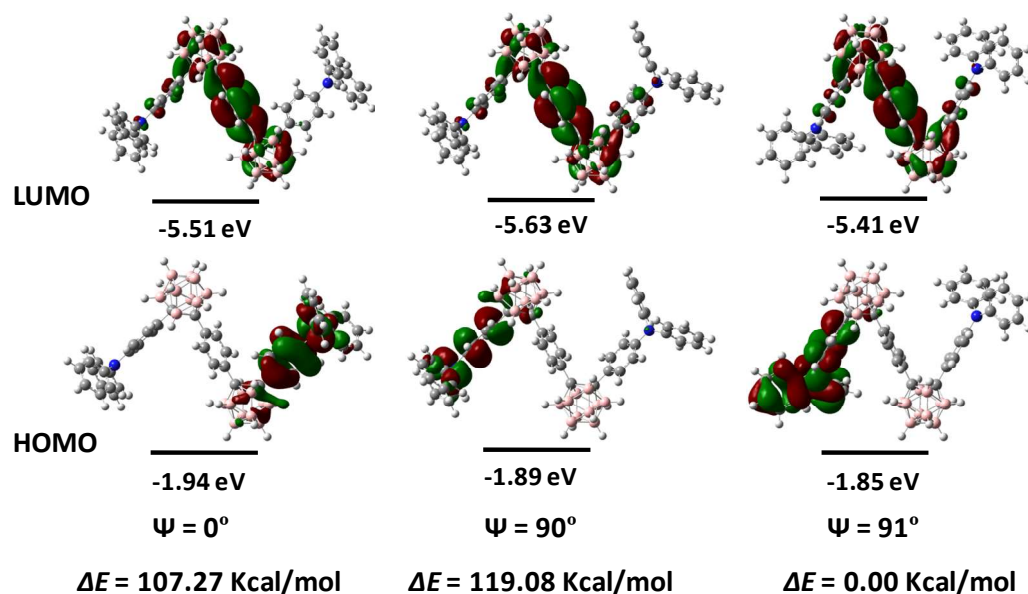


Fig. S12 Emission decay profiles for *o-2* in various solvents.

Table S1 Emission Lifetimes ( $\tau_{em}$ 's) of *o-1* and *o-2*

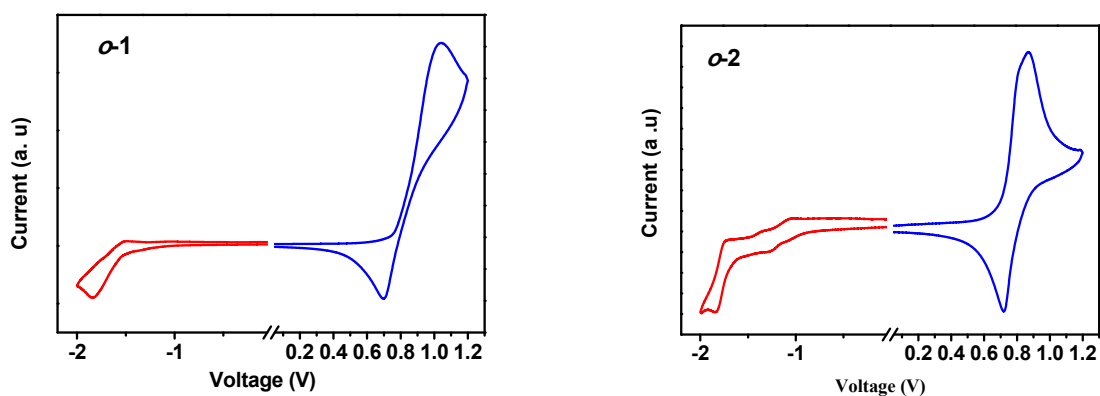
Solvent	<i>o-1</i> (ns)				<i>o-2</i> (ns)			
	TICT		TICT		TICT		TICT	
	$\tau_1$	$\tau_2$	$\tau_1$	$\tau_2$	$\tau_1$	$\tau_2$	$\tau_1$	$\tau_2$
Hex	0.93	2.78	0.46	2.78	0.86	3.56	0.42	2.48
Cyhex	0.96	2.89	0.58	2.91	0.85	4.32	0.44	2.75
Tol	1.13	2.89	0.64	2.98	0.83	3.40	0.47	3.13
Et <sub>2</sub> O	1.02	2.13	--	--	0.98	3.24	--	--
THF	0.99	2.69	--	--	0.94	4.68	--	--
CH <sub>2</sub> Cl <sub>2</sub>	1.64	4.00	--	--	1.21	3.83	--	--
ACN	1.28	3.25	--	--	1.03	3.06	--	--
<b>Film</b>	0.60	2.26	3.09	9.88	0.46	1.99	1.11	8.68

## 5 Density functional calculations



**Fig. S13** Calculated HOMO and LUMO distributions of *o*-1 with the dihedral angles ( $\psi$ ) between the TPA and the phenyl ring of  $0^\circ$ ,  $90^\circ$  and  $91^\circ$ . The difference of total energy and energy levels of each orbital were calculated at the B3LYP/6-31G(d) level by TD-DFT.

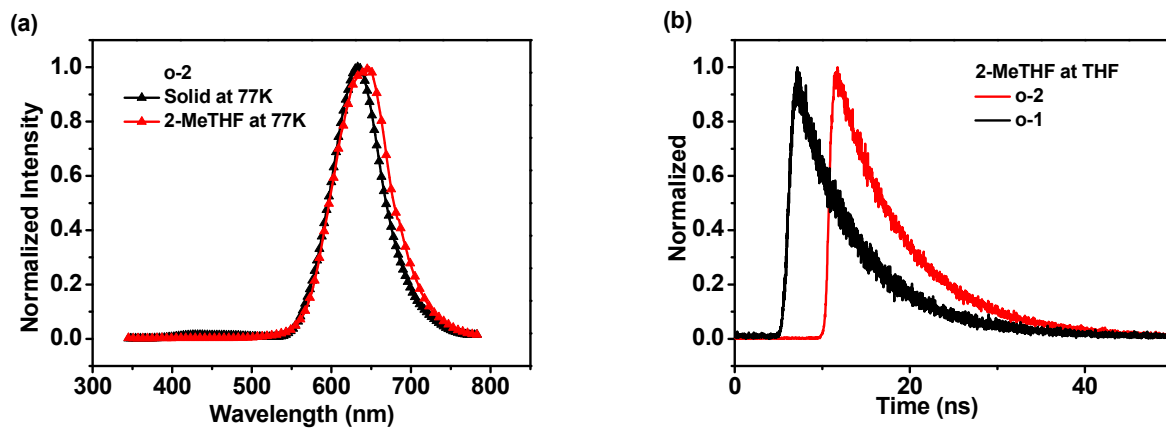
## 6 Electrochemistry



**Fig. S14** Cyclic voltammograms of *o*-1 and *o*-2.



## 7 Emission spectra and Time-resolved emission decay



**Fig. S15** (a) Emission spectra of *o*-2 in solid state and in 2-MeTHF solution at 77 K; (b) Decay time of *o*-1, *o*-2 ( $1 \times 10^{-5}$  M) in 2-MeTHF at 77 K.