Exploring the Sensing Properties of pH-sensitive Carbazole-Based AIE Emitters and its Applications

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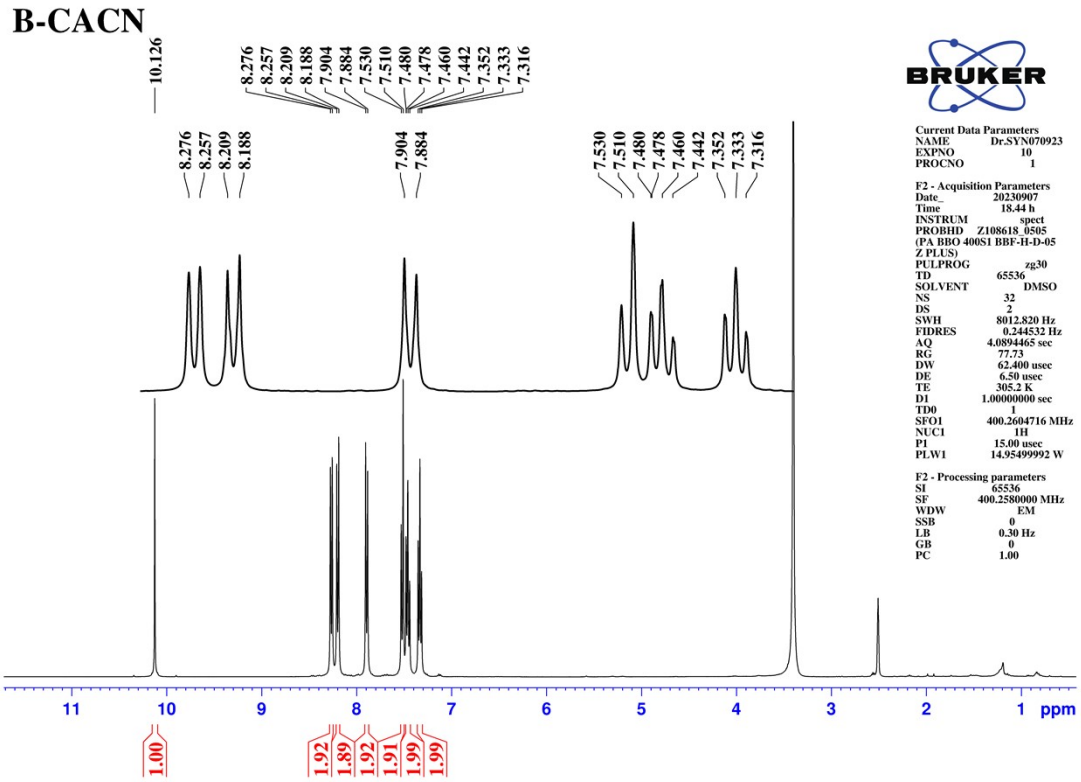
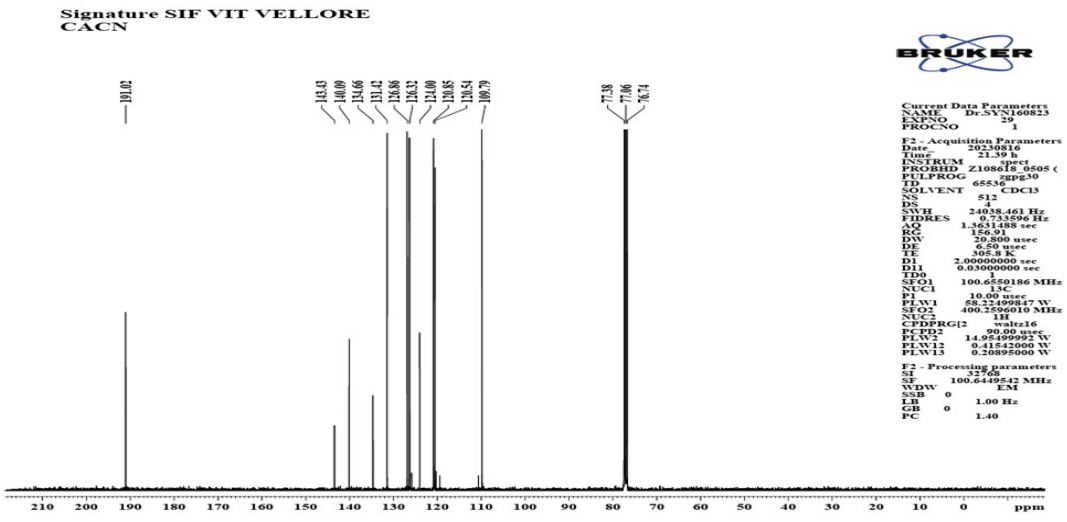
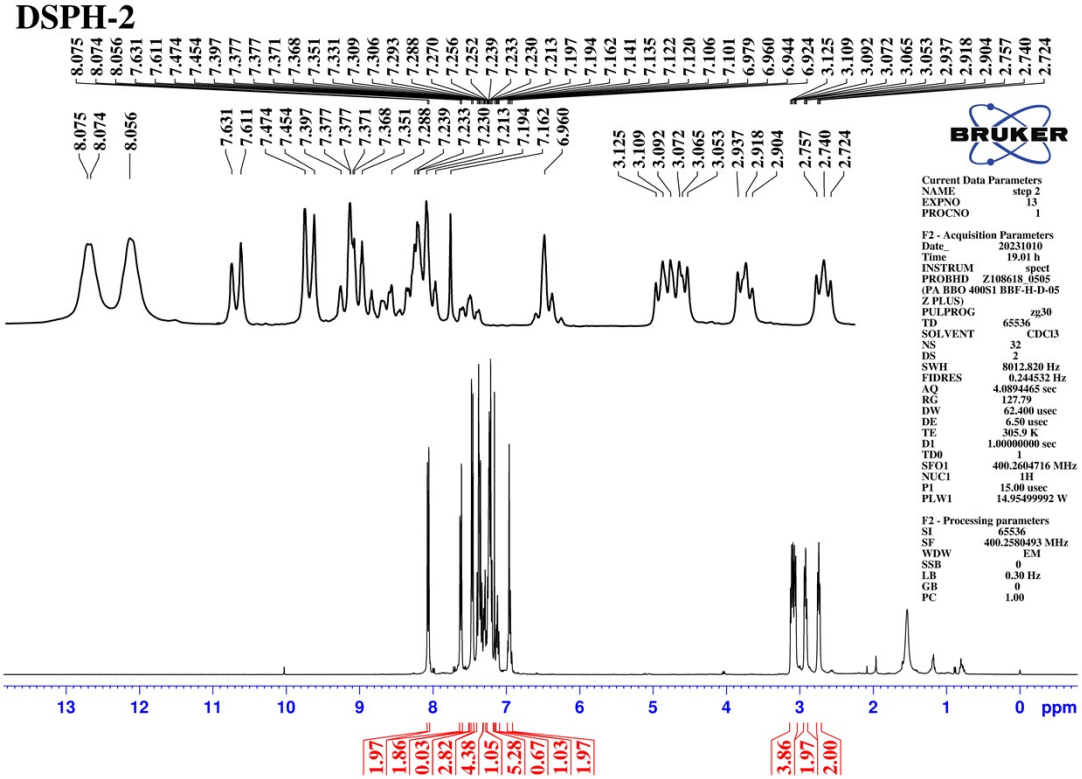


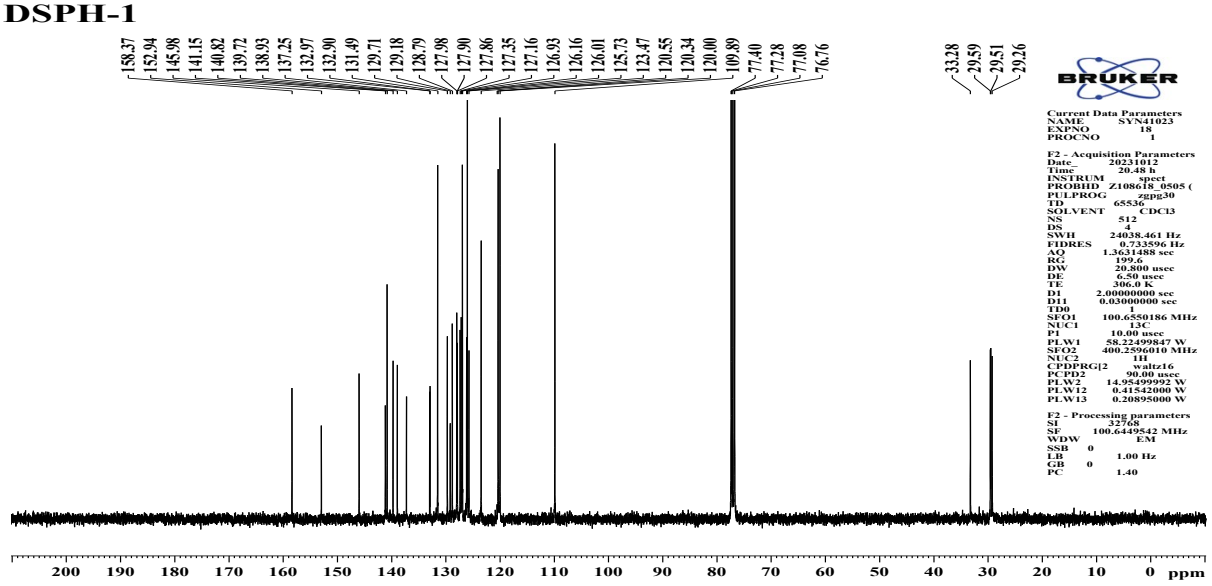
SI Figure S1 ^{1}H NMR spectra of CACN



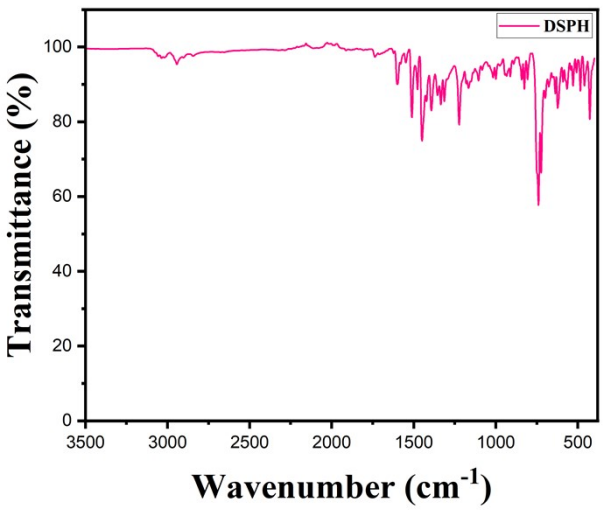
SI Figure S2 ^{13}C NMR spectra of CACN



SI Figure S3 ^{1}H NMR spectra of DSPH

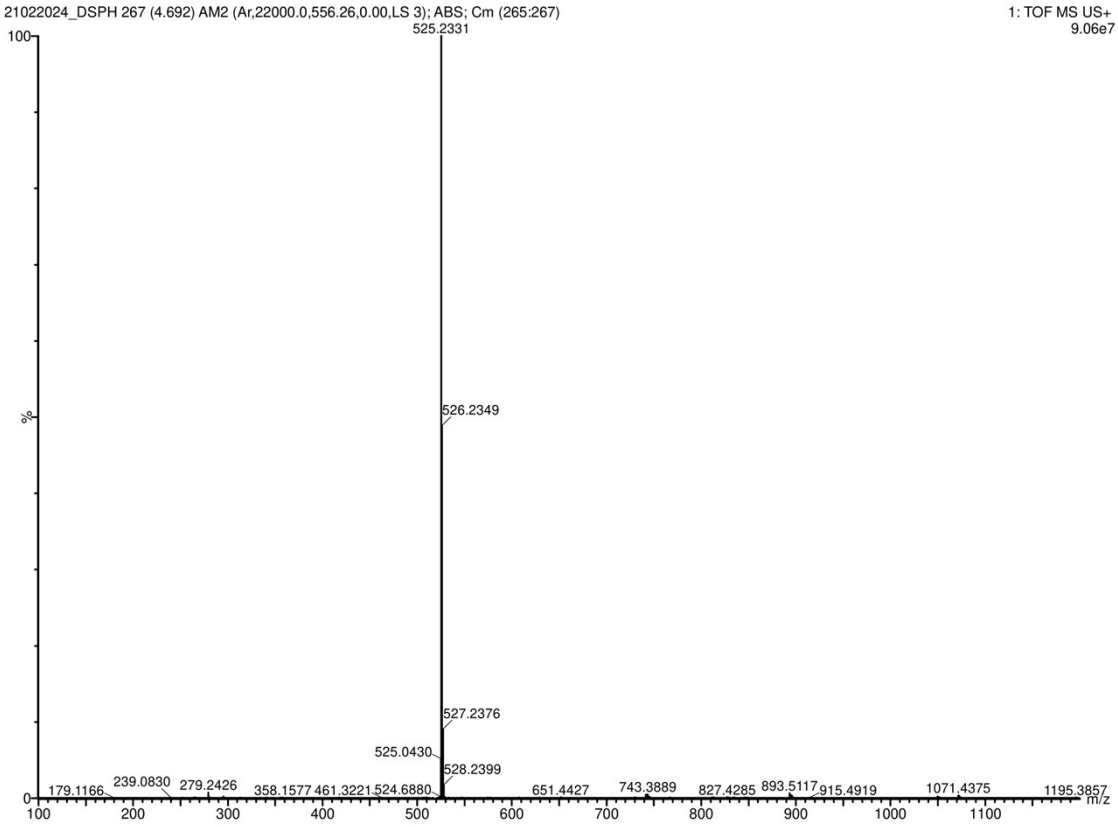


SI Figure S4 ^{13}C NMR spectra of DSPH

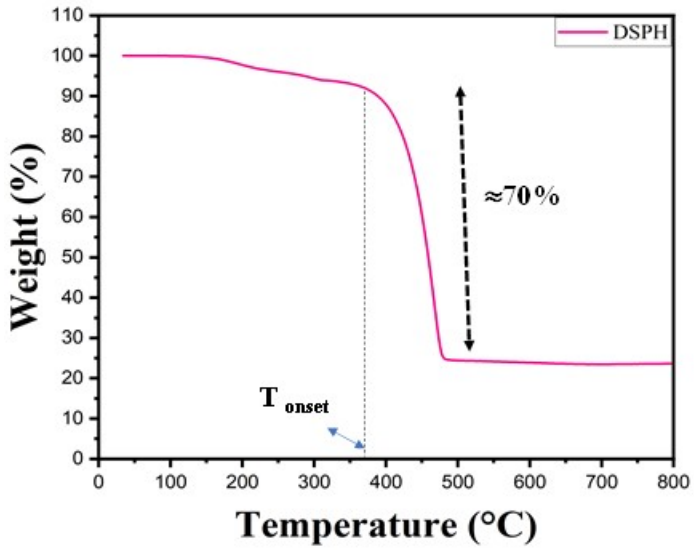


Sr. No	Types of Vibrations	Vø(cm)-1
1	C-H stretch	2943
2	C=C (aromatic)	1600
3	C-H bending	1450.06
4	C-H stretch aliphatic	1105.0
5	C=N stretch	1511.40
6	C-N stretch	1223.70
7	C-H bending	740.44

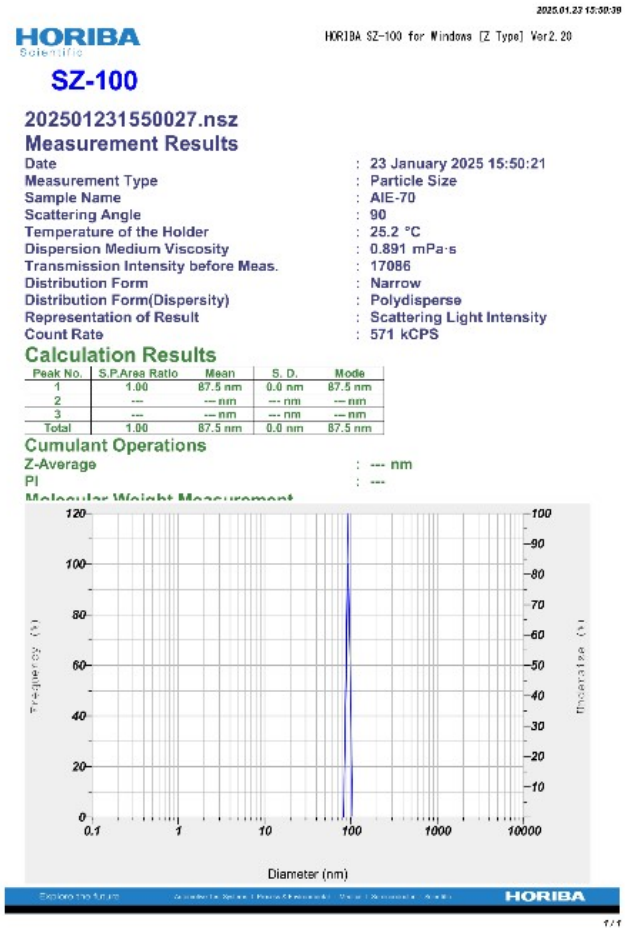
SI Figure S5 FT-IR spectra of DSPH with corresponding band values

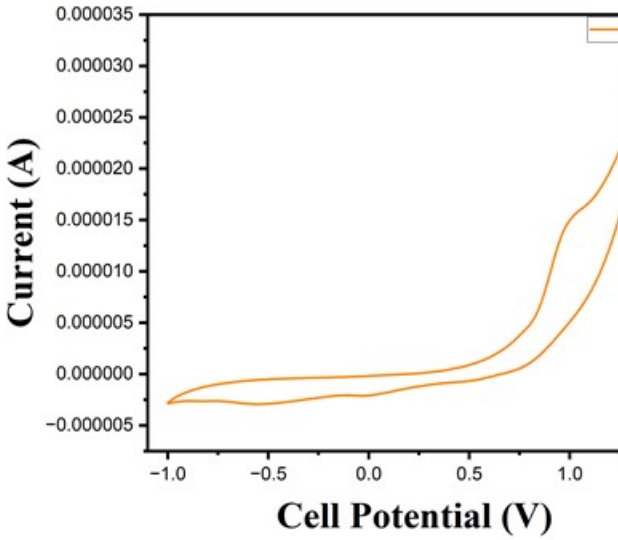


SI Figure S6 HRMS spectra of DSPH: Exact mass= 524.2252 Obtained mass (M+ H^+) = 525.2331



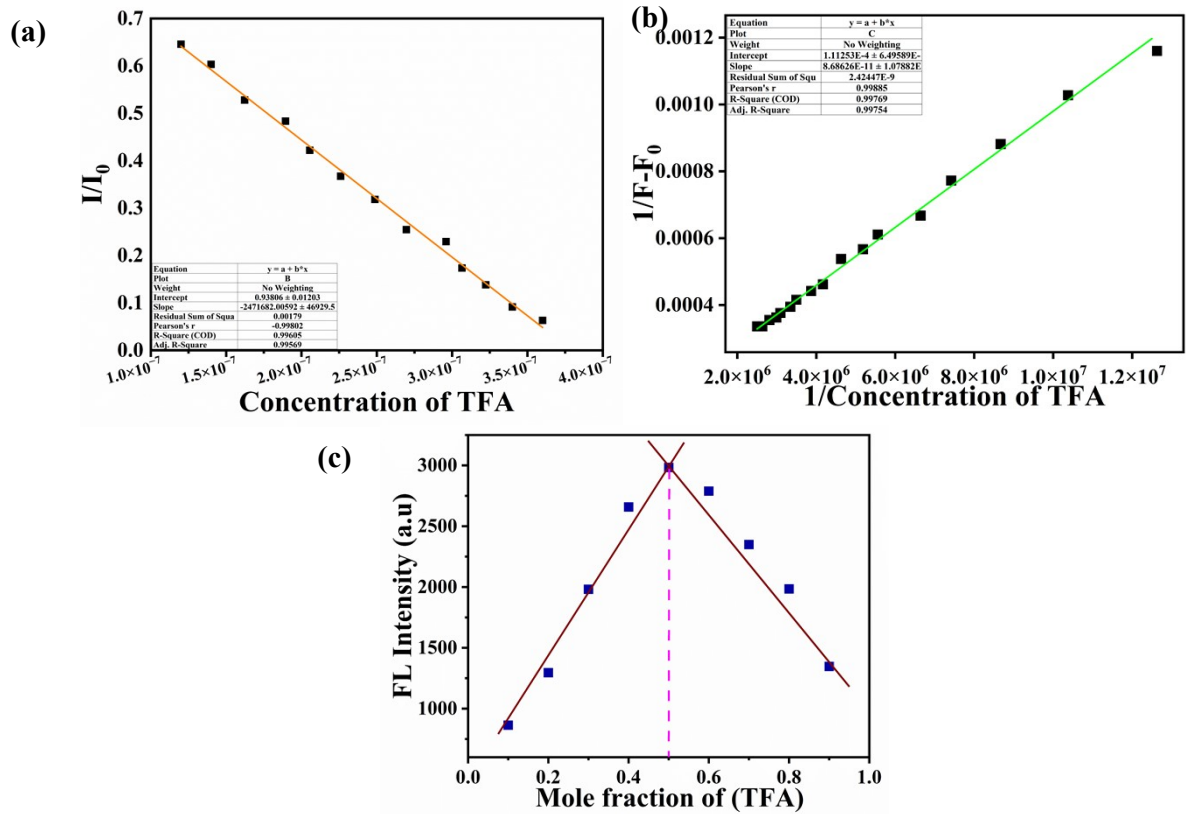
SI Figure S7 TGA plot for probe **DSPH**



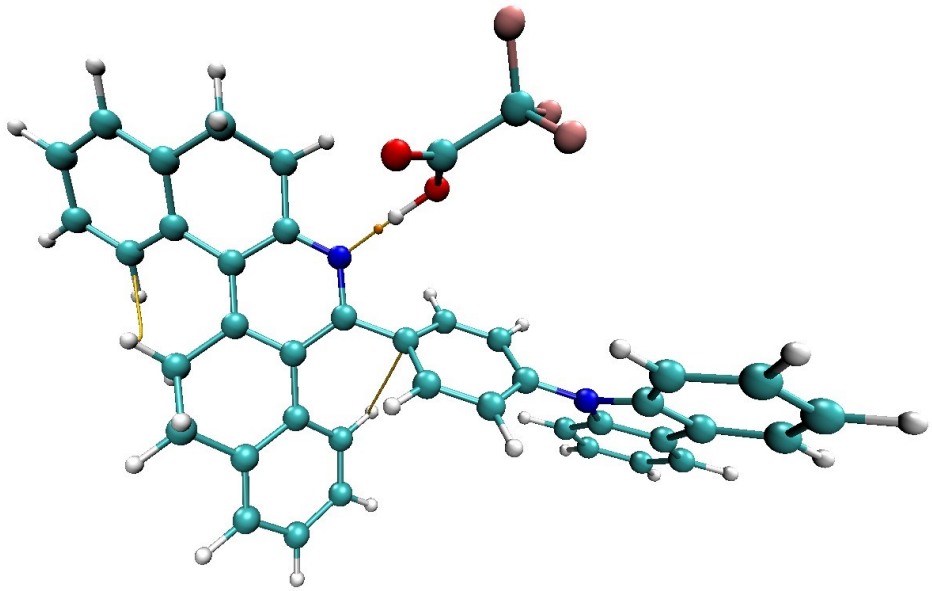


SI Figure S8 Cyclic Voltammogram of probe **DSPH**

SI Figure S9 DLS plot for aggregate size determination



SI Figure S10 (a) Calibration Curve, (b) Benesi – Hildebrand plot of DSPH with TFA, and (c) Job's Plot.



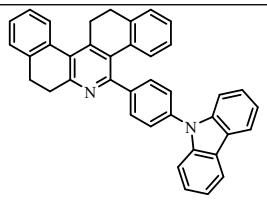
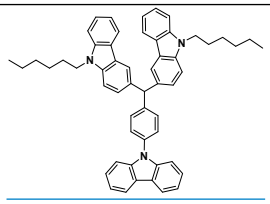
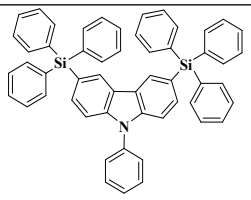
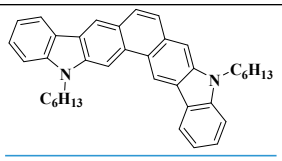
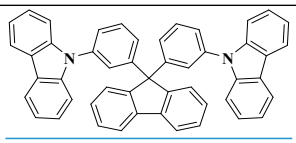
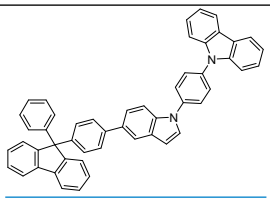
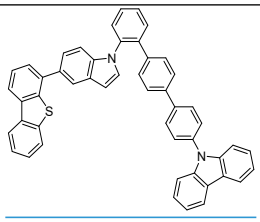
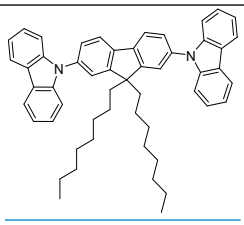
SI Figure S11 Interaction energy plot from DFT-QTAIM model

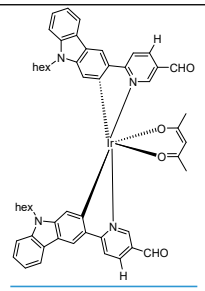
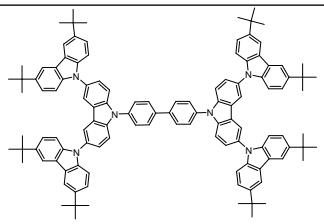
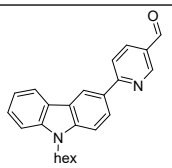
SI Table S1 Photophysical parameters for DSPH in tetrahydrofuran solution at concentration ($2 * 10^{-5}$)

Compound	**Solvent**	**λ_{max}**	**ξ**	**FWHM**	**λ_{em}**	**λ s**
DSPH	THF	327	2.05×10^4	129	413	6368
	EA	327	3.10×10^4	131	412	6309
	DCM	327	1.85×10^4	138	417	6600
	DMSO	327	2.65×10^4	165.8	431	7379
	1,4-dioxane	327	3.45×10^4	121	412	6309
	$CHCl_3$	327	2.35×10^4	123	414	6426

SI Table S2 Comparative study of T_d of different carbazole-based thermally stable probes

Carbazole based probes	T_d (5% weight loss)	Reference

	370 °C	Current work
	417 °C	1
	428 °C	2
	372 °C	3
	480 °C	4
	400 °C	5
	350 °C	6
	488 °C	7

	355 °C	8
	475 °C	9
	309 °C	10

SI Table S3 Energy gap and HOMO – LUMO energy levels of DSPH

Molecule	HOMO (eV)	LUMO (eV)	Energy Gap (ΔE)
DSPH	-5.51	-1.72	-3.79 eV
DSPH+ TFA	-5.62	-2.05	-3.57 eV

SI Table S4 Physical, thermal, and electrochemical parameters for DSPH

Compound	λ_{abs} [a] (nm)	λ_{em} [a] (nm)	T_d [b] (°C)	HOMO/ LUMO[c] (eV)	E_g [d] (eV)	HOMO/ LUMO[e] (eV)	E_g [e] (eV)
DSPH	330	413	370	-5.32/ -1.56	3.75	-5.51/ -1.72	3.79

[a] analysed in THF, [b] determined from TGA, [c] interpreted from CV in THF/TBAP, [d] derived from absorption edge: 1240/ λ_{onset}, [e] evaluated from DFT calculations.

SI Table S5 Oscillator Strengths of Important Transitions for DSPH

Entry	Max(nm)	Oscillator Strength	Energy Gap (ΔE)	Selected Major Transitions
DSPH	370	0.2622	-3.34	H-L (69%)
	324	0.1465	-3.81	H-L_{+1} (52%)
	323	0.0000	-3.83	H_{-1}-L (70%)
	320	0.1406	-3.87	H-L_{+2} (43%)
	317	0.0141	-3.89	H-L_{+2} (52%)

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