Supplementary Material (ESI) for Journal of Materials Chemistry C
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Twisted donor-acceptor molecules for efficient deep-blue electroluminescence with CIE_y ~ 0.06

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I. Supplementary Figures and Tables.

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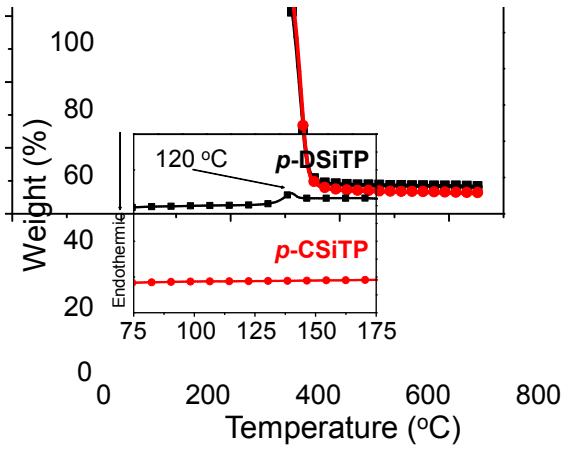


Fig. **S1** TGA traces of ***p*-DSiTP** and ***p*-CSiTP** recorded at heating rate of 20 ℃ min^{-1} under N_2. Inset: DSC traces of ***p*-DSiTP** and ***p*-CSiTP** recorded at heating rate of 10 ℃ min^{-1} under N_2.

Fig. **S2** Picture of solution of ***p*-DSiTP** (Top) and ***p*-CSiTP** (Bottom) in different solvents under UV illumination (λ_{ex} = 365 nm).

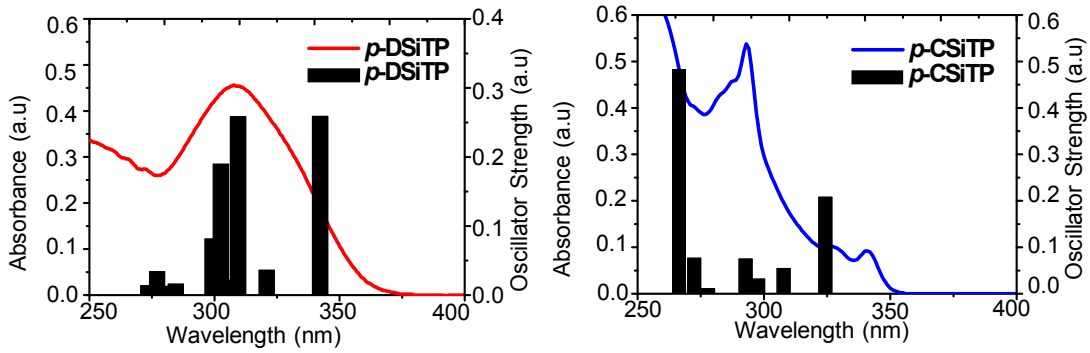


Fig. **S3** Experimental UV-Vis spectra and oscillator strength calculated by B3LYP functional with 6-31G (d, p) basis sets for the dyes.

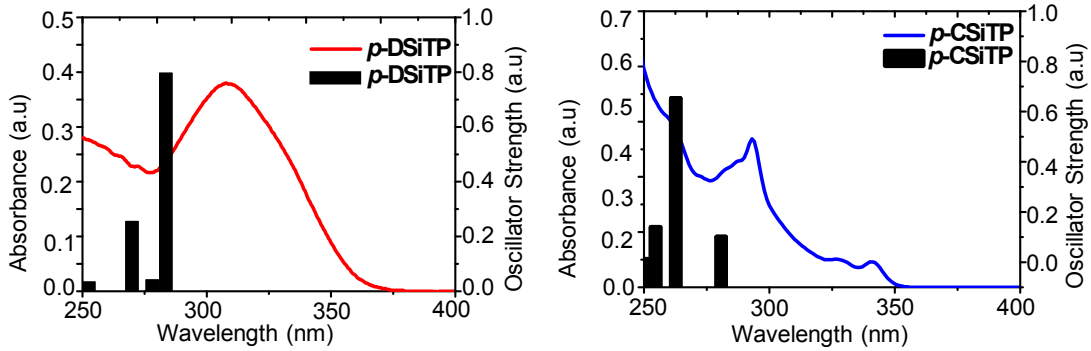


Figure S4. Experimental UV-Vis spectra and oscillator strength calculated by CAM-B3LYP functional (down) with 6-31G (d, p) basis sets for the dyes.

Table S1. Calculated electronic excitation energies, oscillator strengths and related wave functions for ***p*-DSiTP** and ***p*-CSiTP** using the B3LYP function with 6-31G (d) basis sets

	State[a]	E (eV)	λ(nm)	*f*[b]	Wavefunction [c]
***p*-DSiTP**	S_1	3.63	342	0.2589	H→L (89%)
	S_3	4.01	309	0.2585	H→L+2 (53%), H→L+3 (18%), H→L+4 (11%)
	S_5	4.10	303	0.1895	H→L+6 (89%)
***p*-CSiTP**	S_1	3.83	324	0.2077	H→L (86%)
	S_4	4.24	293	0.0748	H→L (14%), H→L+2 (51%), H→L+4 (17%)

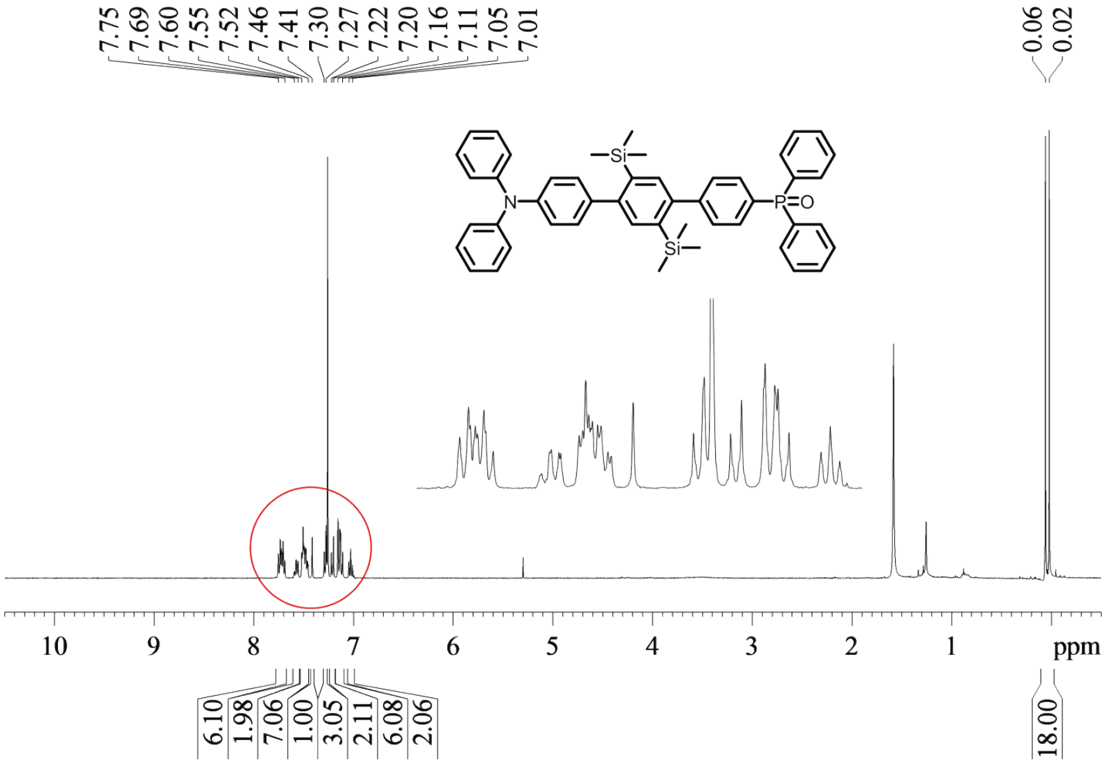
[a] Excited state. [b] Oscillator strength (values < 0.05 are not included). [c] MOs involved the transitions, , H = HOMO, L = LUMO.

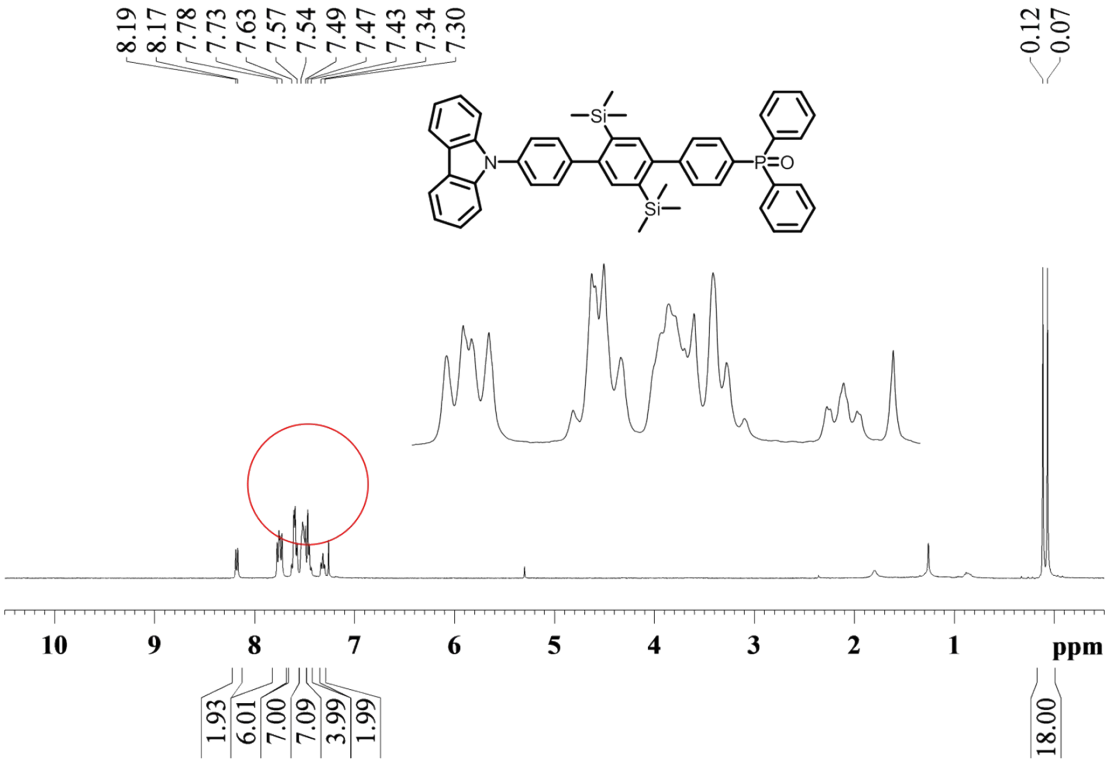
Table S2. Calculated electronic excitation energies, oscillator strengths and related wave functions for ***p*-DSiTP** and ***p*-CSiTP** using the CAM-B3LYP function with 6-31G (d) basis sets

	State[a]	E (eV)	λ(nm)	*f*[b]	Wavefunction [c]
***p*-DSiTP**	S_1	4.37	283	0.7966	H→L (28%), H→L+2 (22%), H→L+3 (14%)
	S_3	4.59	270	0.2551	H→L+6 (93%)
	S_5	5.02	247	0.0766	H-1→L (12%), H→L+10 (25%), H→L+11 (12%)
***p*-CSiTP**	S_1	4.41	280	0.1001	H-1→L+11 (10%), H→L+3 (78%)
	S_2	4.72	262	0.6527	H→L (31%), H→L+1 (13%), H→L+4 (22%)
	S_3	4.87	254	0.139	H-1→L+3 (70%), H→L+11 (14%)

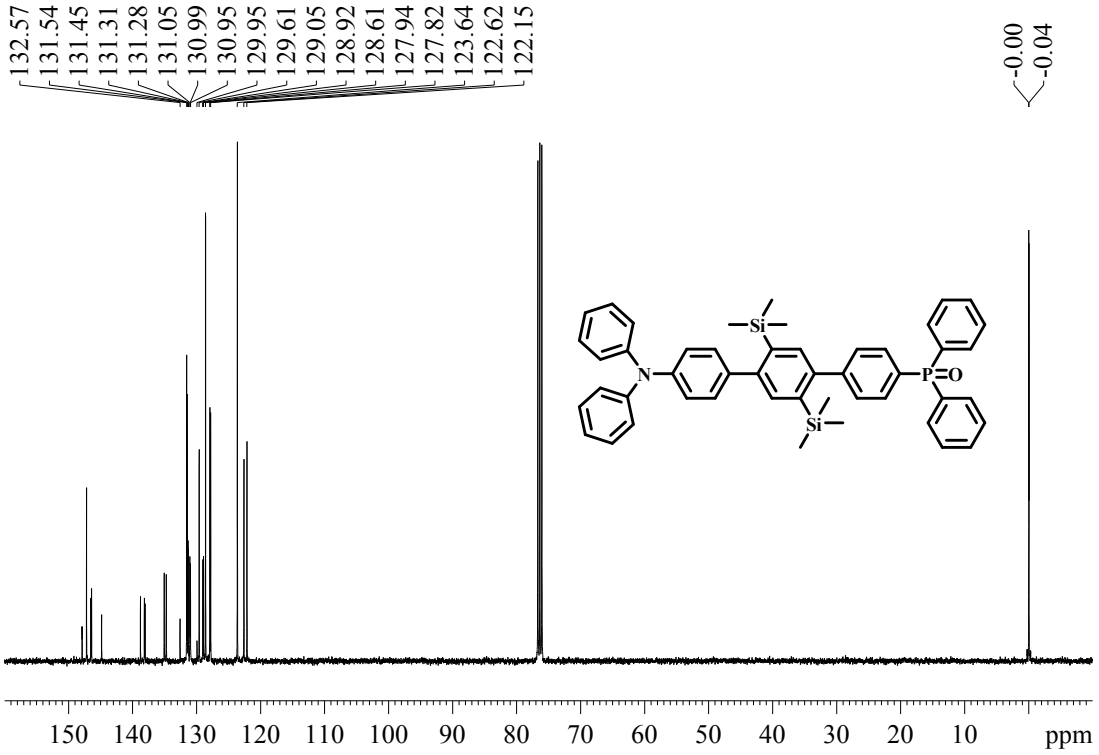
[a] Excited state. [b] Oscillator strength (values < 0.05 are not included). [c] MOs involved the transitions, , H = HOMO, L = LUMO.

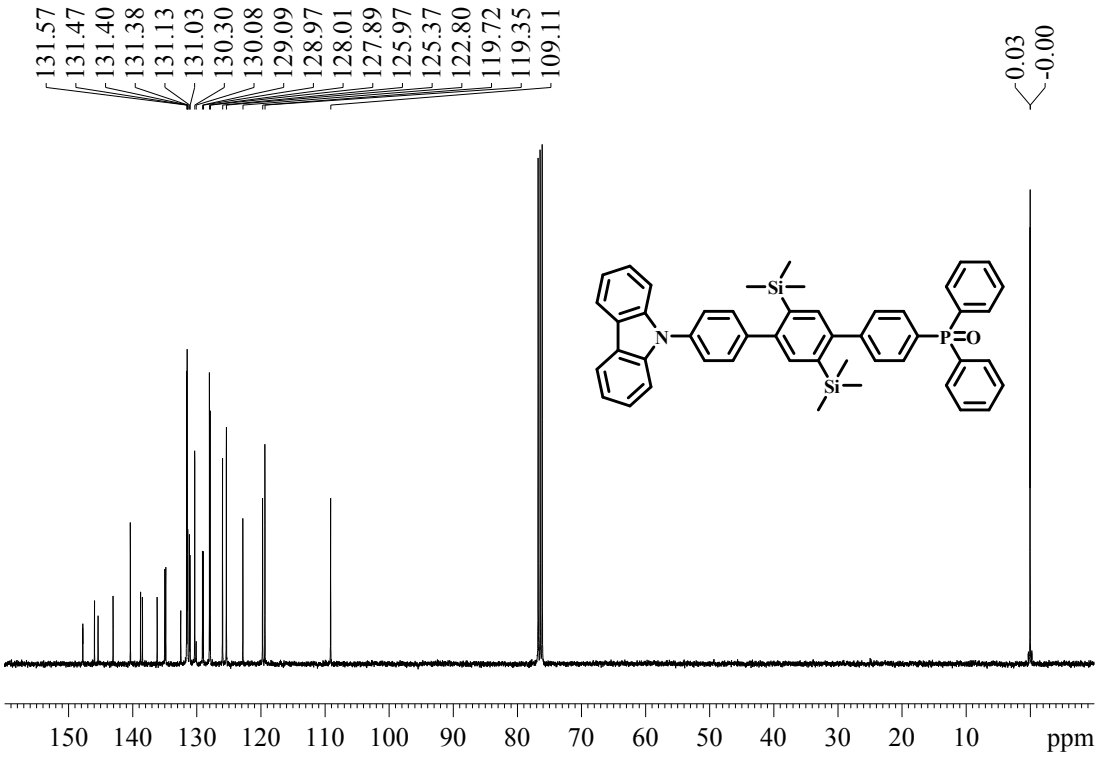
II. **^{1}H NMR** of ***p*-DSiTP** and ***p*-CSiTP** in $CDCl_3$.





III. ^{13}C NMR of *p*-DSiTP and *p*-CSiTP in $CDCl_3$.





IV. **HR-MS** of ***p*-DSiTP** and ***p*-CSiTP**.

Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name	HS11-1-20181123	Instrument / Ser#	microTOF-Q II 228888.10
Comment			324

Acquisition Parameter

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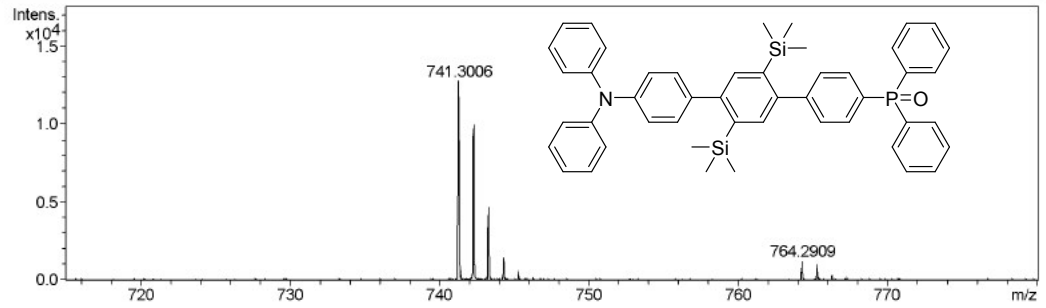
Scan End	1300 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
741.3006	1	C48H48NOPSi2	741.3007	-0.0	84.3	1	100.00	28.0	odd	ok
764.2909	1	C48H48NNaOPSi2	764.2904	-0.6	93.5	1	100.00	27.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\QTOF-LUH-190114-SZQ-9_01.d	Acquisition Date	1/14/2019 4:56:46 PM
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Sample Name	HS11-1-20181123	Instrument / Ser#	microTOF-Q II 228888.10
Comment			324

Acquisition Parameter

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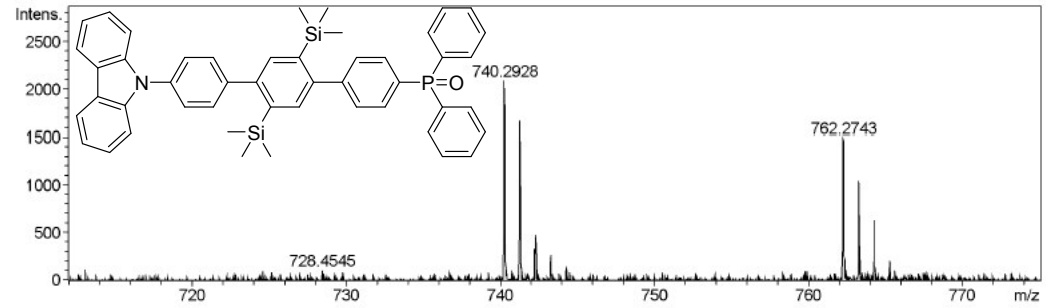
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1300 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
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762.2743	1	C48H46NNaOPSi2	762.2748	0.6	91.3	1	100.00	28.5	even	ok