Supplementary information

Electronic Alteration on End-on Phenyl Groups of *bis*-Triazolyl-silanes: Electron-transport Materials for Blue Phosphorescent OLEDs

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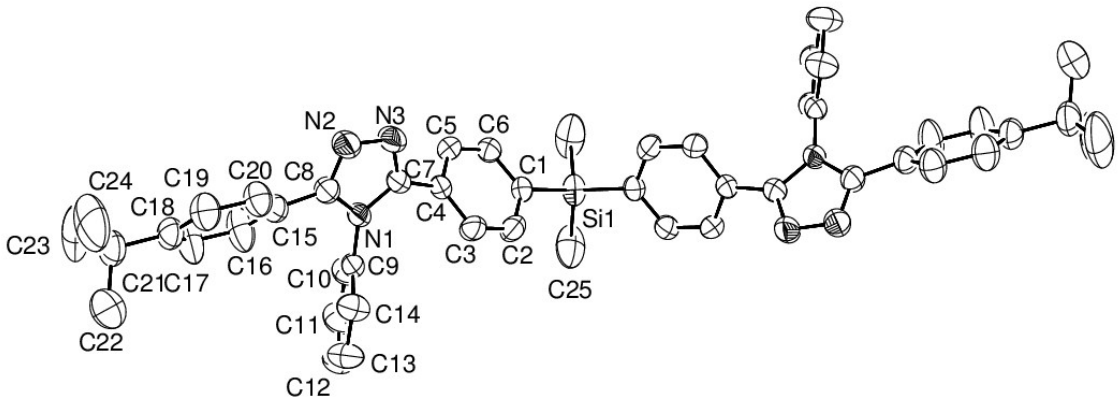

Figure S1. ORTEP structure of **ST-^{t}Bu** showing thermal ellipsoids; the probability level of this structure is 30%. Hydrogen atoms were omitted for clarity.

Table S1. Crystal data and structure refinement for ST-^{t}Bu

Identification code	**ST-^{t}Bu**
Empirical formula	$C_{50}H_{50}N_6Si$
Formula weight	763.05
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $C2/c$
Unit cell dimensions	a = 22.126(5) Å
	b = 11.533(2) Å β = 109.595(4)°
	c = 18.308(4) Å
Volume	4401.4(16) Å^3
Z, Calculated density	4, 1.152 Mg/m^3
Absorption coefficient, μ	0.094 mm^{-1}
F(000)	1624
Crystal size	0.150 × 0.110 × 0.080 mm
ϑ range for data collection	1.954 to 28.376°
Limiting indices	$-29 \le h \le 29$, $-15 \le k \le 15$, $-24 \le l \le 24$
Reflections collected / unique	29637 / 5498 [R_{int} = 0.0579]
Completeness to ϑ = 28.40	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5498 / 0 / 258
Goodness-of-fit on F^2	1.016
Final R indices [$I>2\sigma(I)$]	$R_1{}^a$ = 0.0559, $wR_2{}^b$ = 0.1352
R indices (all data)	$R_1{}^a$ = 0.1202, $wR_2{}^b$ = 0.1807
Largest diff. peak and hole	0.326 and -0.315 e. Å^{-3}

$^a R_1 = \sum||F_o|-|F_c||$ (based on reflections with $F_o^2>2\sigma F^2$), $^b wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; , $P = [\max(F_o^2, 0) + 2F_c^2]/3$(also with $F_o^2>2\sigma F^2$)

Table S2. Bond lengths [Å] for ST-^{t}Bu

Si(1)-C(25)#1	1.860(3)	C(8)-C(15)	1.469(3)
Si(1)-C(25)	1.860(3)	C(9)-C(10)	1.371(3)
Si(1)-C(1)#1	1.876(2)	C(9)-C(14)	1.375(3)
Si(1)-C(1)	1.876(2)	C(10)-C(11)	1.379(3)
N(1)-C(8)	1.370(3)	C(11)-C(12)	1.364(4)
N(1)-C(7)	1.374(3)	C(12)-C(13)	1.366(5)
N(1)-C(9)	1.439(3)	C(13)-C(14)	1.382(4)
N(2)-C(8)	1.308(3)	C(15)-C(16)	1.366(4)
N(2)-N(3)	1.384(3)	C(15)-C(20)	1.376(3)
N(3)-C(7)	1.310(3)	C(16)-C(17)	1.378(4)
C(1)-C(6)	1.386(3)	C(17)-C(18)	1.376(4)
C(1)-C(2)	1.390(3)	C(18)-C(19)	1.370(4)
C(2)-C(3)	1.378(3)	C(18)-C(21)	1.529(3)
C(3)-C(4)	1.384(3)	C(19)-C(20)	1.388(3)
C(4)-C(5)	1.379(3)	C(21)-C(23)	1.510(5)
C(4)-C(7)	1.468(3)	C(21)-C(22)	1.518(5)
C(5)-C(6)	1.378(3)	C(21)-C(24)	1.520(5)

Table S3. Angles [°] for ST-^{t}Bu

C(25)#1-Si(1)-C(25)	110.9(3)	N(1)-C(8)-C(15)	126.19(19)
C(25)#1-Si(1)-C(1)#1	108.74(13)	C(10)-C(9)-C(14)	120.6(2)
C(25)-Si(1)-C(1)#1	109.59(12)	C(10)-C(9)-N(1)	120.2(2)
C(25)#1-Si(1)-C(1)	109.59(12)	C(14)-C(9)-N(1)	119.2(2)
C(25)-Si(1)-C(1)	108.74(13)	C(9)-C(10)-C(11)	119.5(2)
C(1)#1-Si(1)-C(1)	109.31(13)	C(12)-C(11)-C(10)	120.3(3)
C(8)-N(1)-C(7)	105.16(17)	C(11)-C(12)-C(13)	120.3(3)
C(8)-N(1)-C(9)	127.04(17)	C(12)-C(13)-C(14)	120.2(3)
C(7)-N(1)-C(9)	127.75(17)	C(9)-C(14)-C(13)	119.2(3)
C(8)-N(2)-N(3)	107.47(18)	C(16)-C(15)-C(20)	118.1(2)
C(7)-N(3)-N(2)	107.92(18)	C(16)-C(15)-C(8)	122.0(2)
C(6)-C(1)-C(2)	116.8(2)	C(20)-C(15)-C(8)	119.6(2)
C(6)-C(1)-Si(1)	120.88(17)	C(15)-C(16)-C(17)	120.9(3)
C(2)-C(1)-Si(1)	122.34(16)	C(18)-C(17)-C(16)	122.3(3)
C(3)-C(2)-C(1)	122.3(2)	C(19)-C(18)-C(17)	116.2(2)
C(2)-C(3)-C(4)	119.8(2)	C(19)-C(18)-C(21)	123.2(2)
C(5)-C(4)-C(3)	118.8(2)	C(17)-C(18)-C(21)	120.6(2)
C(5)-C(4)-C(7)	117.50(19)	C(18)-C(19)-C(20)	122.3(2)
C(3)-C(4)-C(7)	123.6(2)	C(15)-C(20)-C(19)	120.2(2)
C(6)-C(5)-C(4)	120.7(2)	C(23)-C(21)-C(22)	107.4(3)
C(5)-C(6)-C(1)	121.6(2)	C(23)-C(21)-C(24)	109.4(3)
N(3)-C(7)-N(1)	109.46(19)	C(22)-C(21)-C(24)	107.4(3)

N(3)-C(7)-C(4)	122.75(19)	C(23)-C(21)-C(18)	110.8(2)
N(1)-C(7)-C(4)	127.74(19)	C(22)-C(21)-C(18)	109.1(2)
N(2)-C(8)-N(1)	109.98(19)	C(24)-C(21)-C(18)	112.4(3)
N(2)-C(8)-C(15)	123.6(2)		

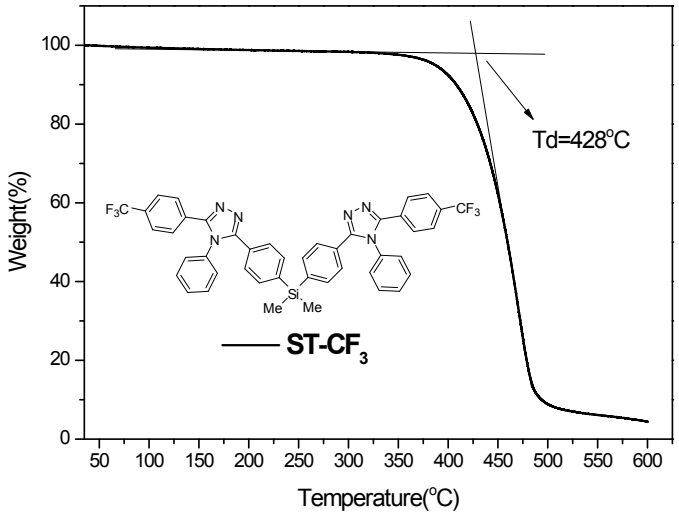

Figure S2. TGA data for **ST-CF_3**.

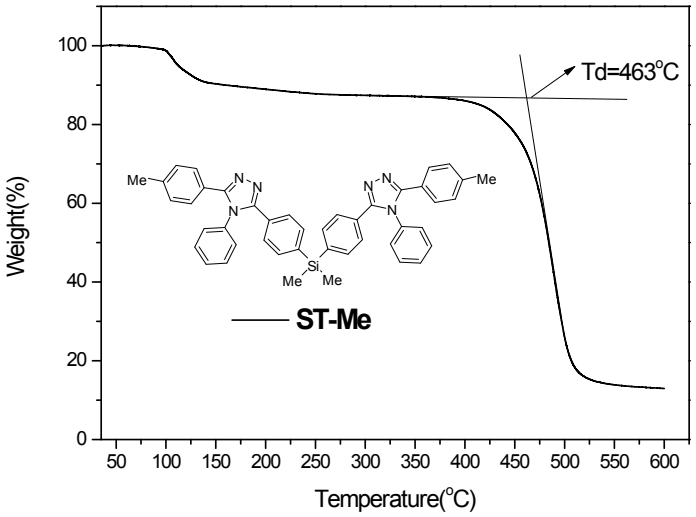

Figure S3. TGA data for **ST-Me**.

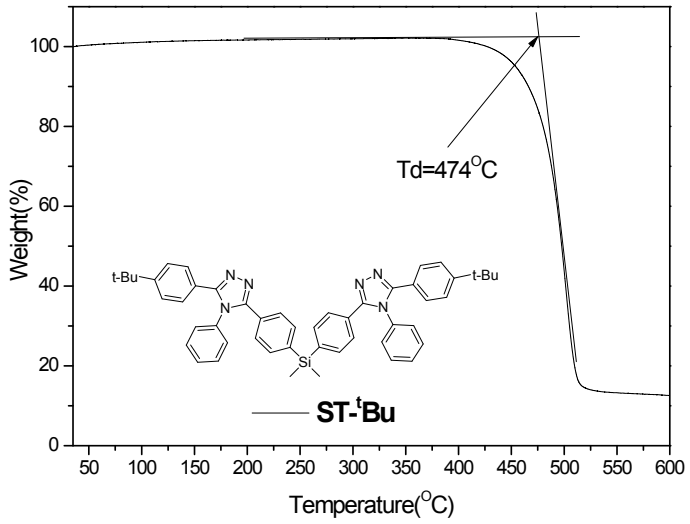

Figure S4. TGA data for **ST-^{t}Bu**.

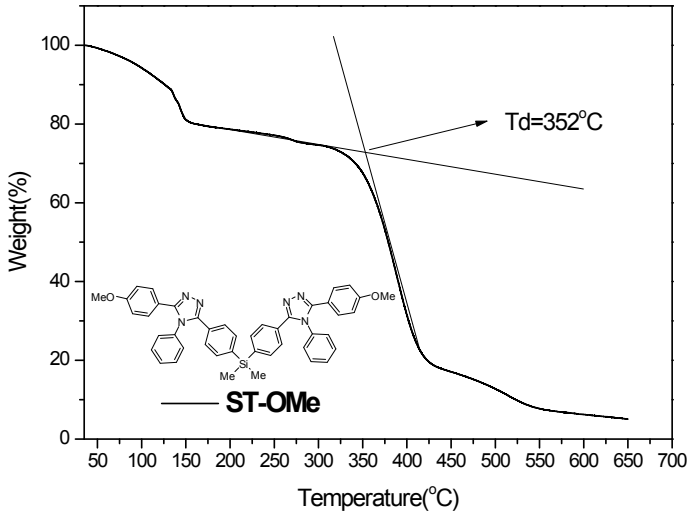

Figure S5. TGA data for **ST-OMe**.

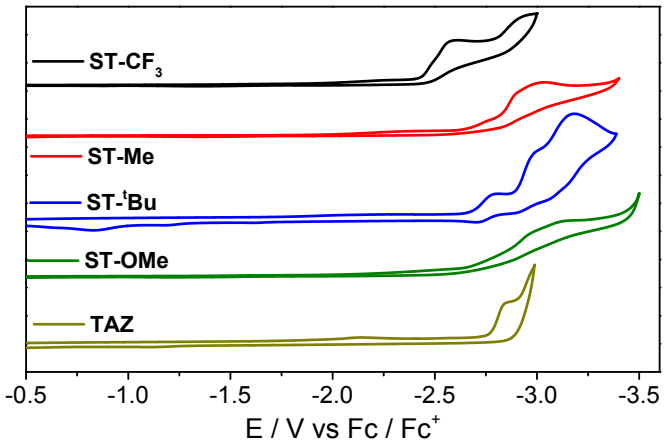

Figure S6. Cyclic voltammograms of **ST-CF_3**, **ST-Me**, **ST-^{t}Bu**, and **ST-OMe** in dichloromethane solution containing 0.1 M TBAP as electrolyte. CVs were obtained at a scan rate of 0.1 V s^{-1}.

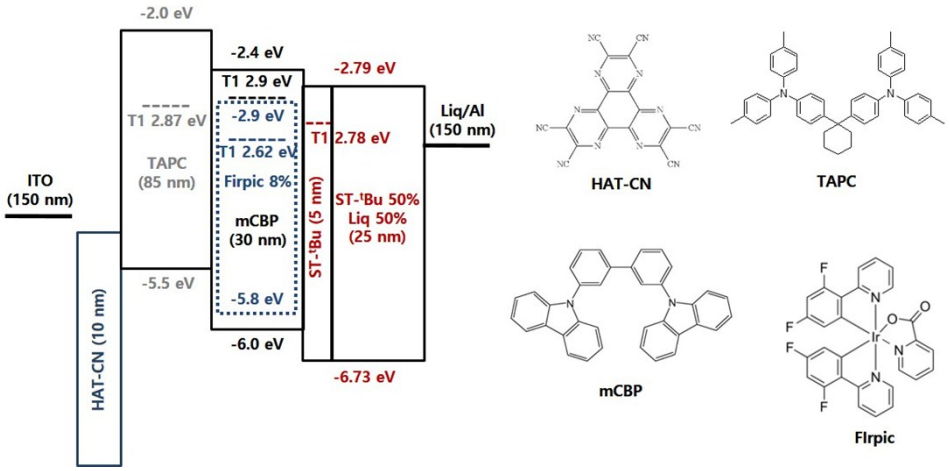

Figure S7. Energy level diagram and chemical structures of the used materials. Device structure: ITO (150 nm)/HATCN (10 nm)/TAPC (85 nm)/mCBP:FIrpic 8% (30 nm)/ST-tBu (5 nm)/ST-tBu:Liq 50% (25 nm)Liq (1 nm)/Al (150 nm).

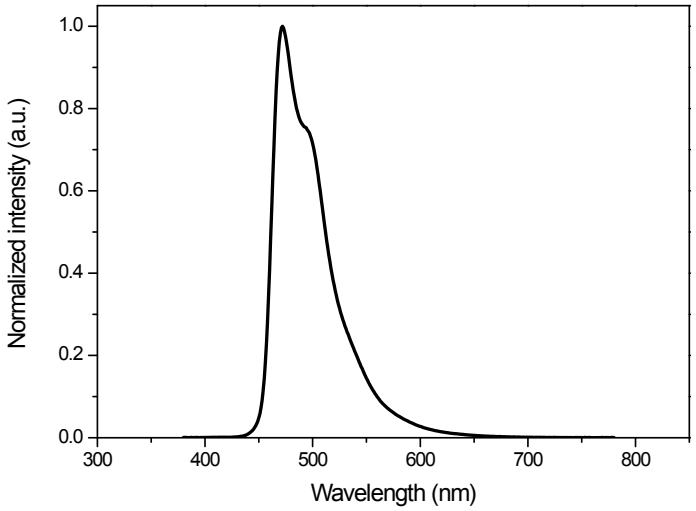

Figure S8. EL spectra of device.

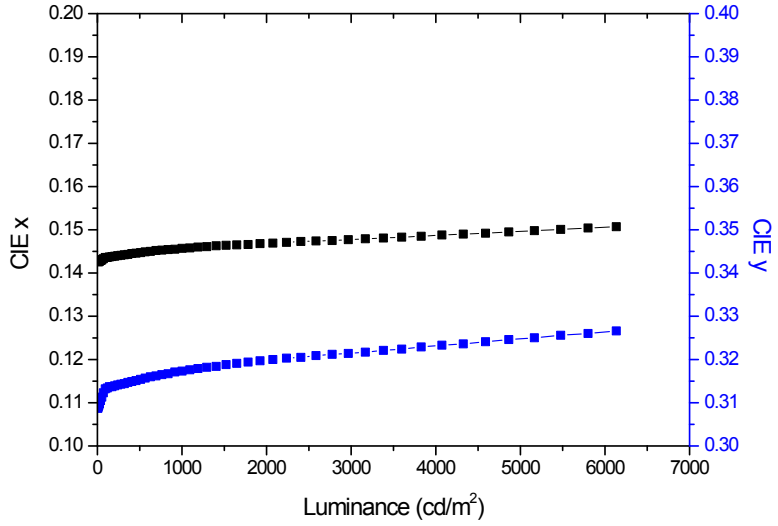

Figure S9. CIE colour coordinate of device.