Electronic Supplementary Material (ESI) for Materials Advances.

Acenaphthene-Triphenylamine (Acceptor-Donor) based luminophores for organic light emitting diodes: combined experimental and theoretical study

Jairam Tagare, Aravind Babu Kajjam, Kasturi Singh, Sabita Patel and Sivakumar Vaidyanathan*

Department of Chemistry, National Institute of Technology Rourkela, India.

Contents:

SI5 DFT data of Acenaphthene derivatives

SI1 NMR spectra (^{1}H, ^{13}C and ^{19}F) of the compounds

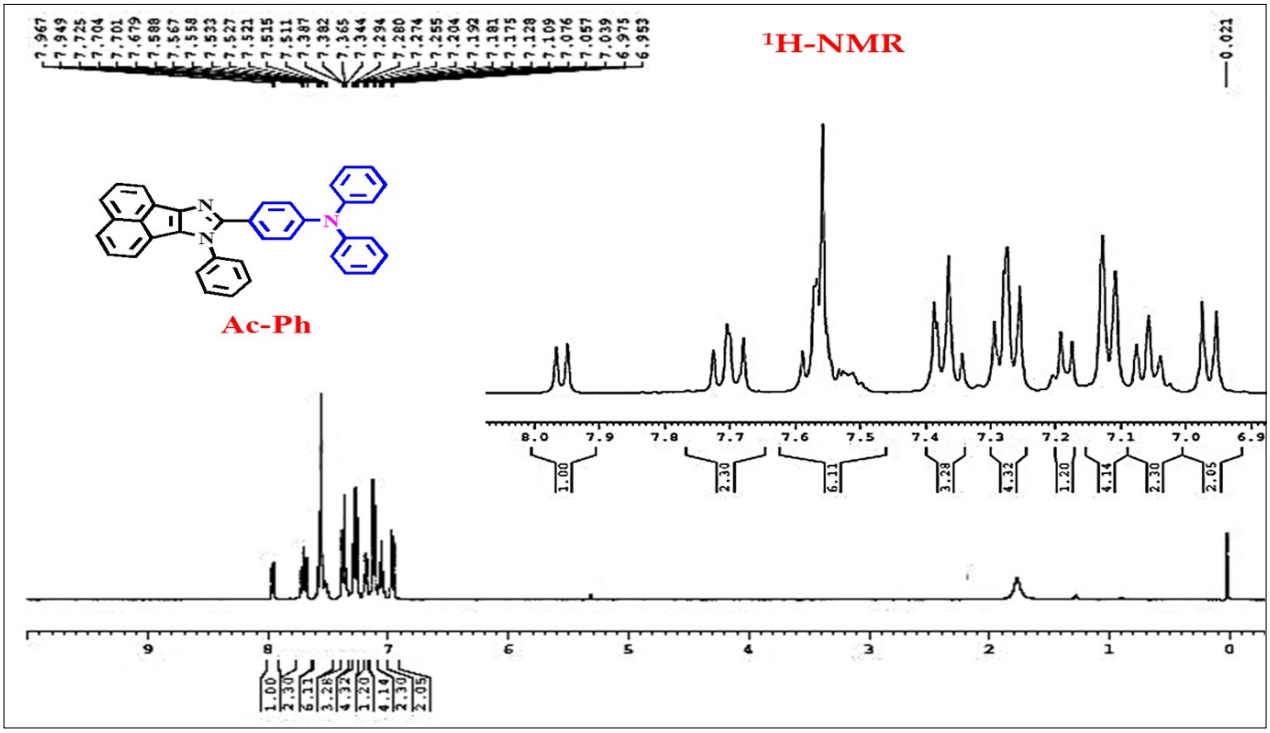

Fig. S1. The ^{1}H NMR spectra of the AC-Ph

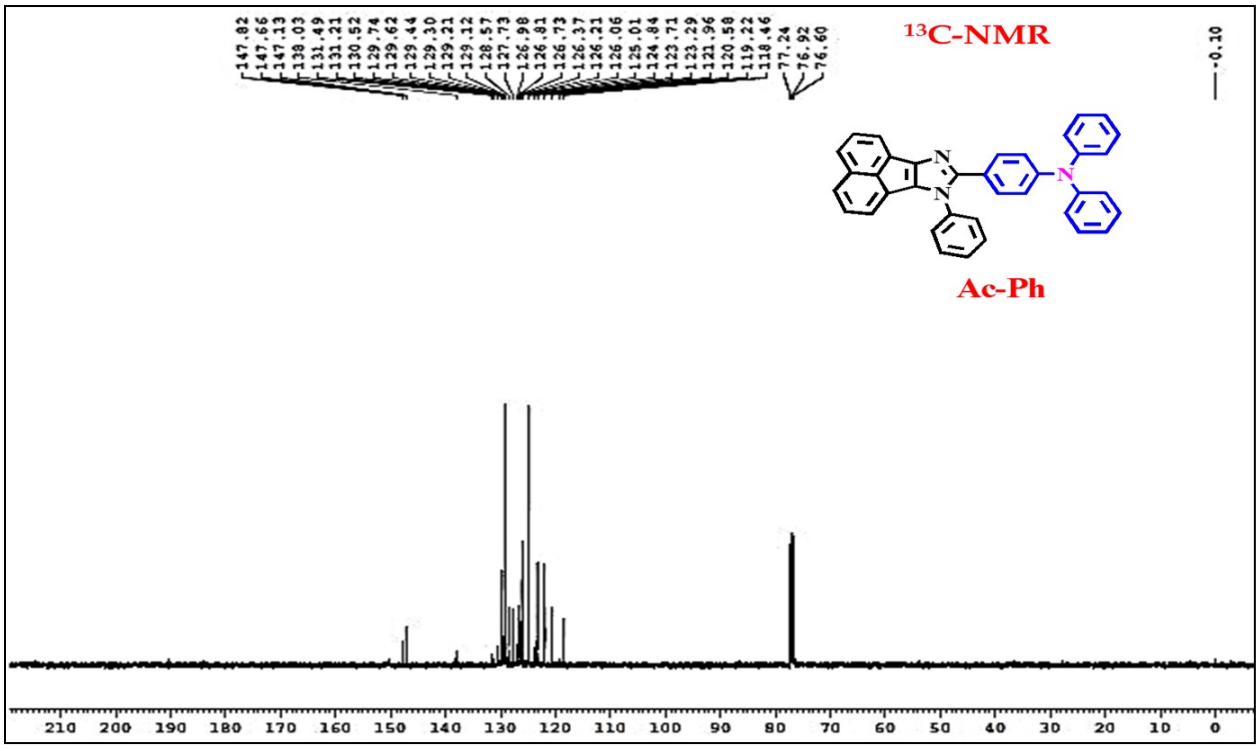

Fig. S2. The ^{13}C NMR spectra of the AC-Ph

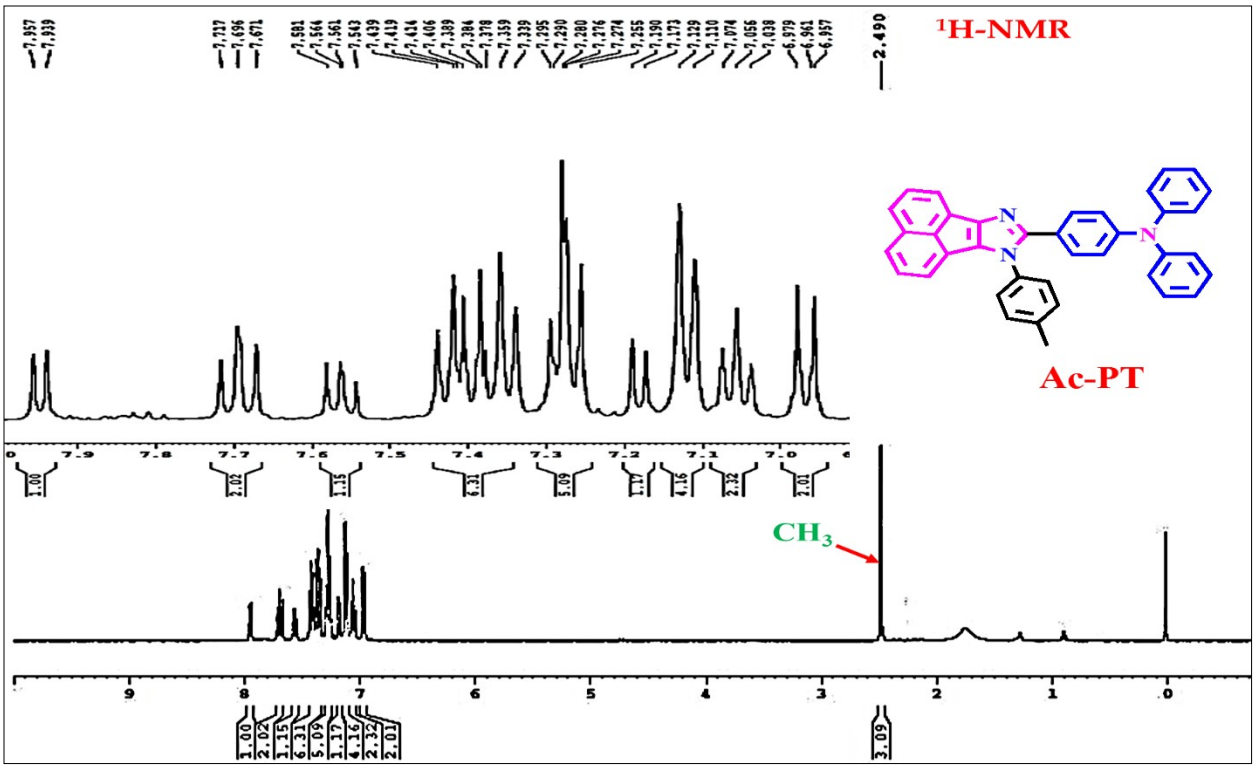

Fig. S3. The ^{1}H NMR spectra of the AC-PT

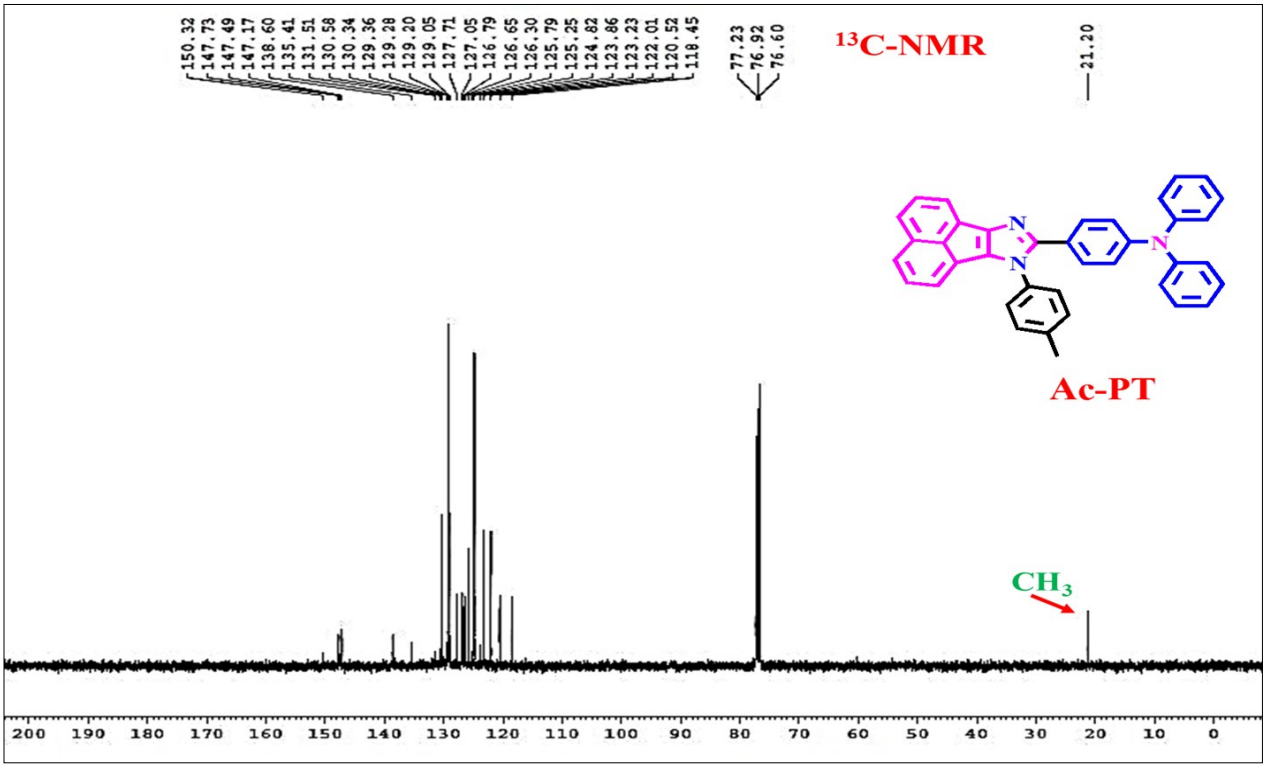

Fig. S4. The ^{13}C NMR spectra of the AC-PT

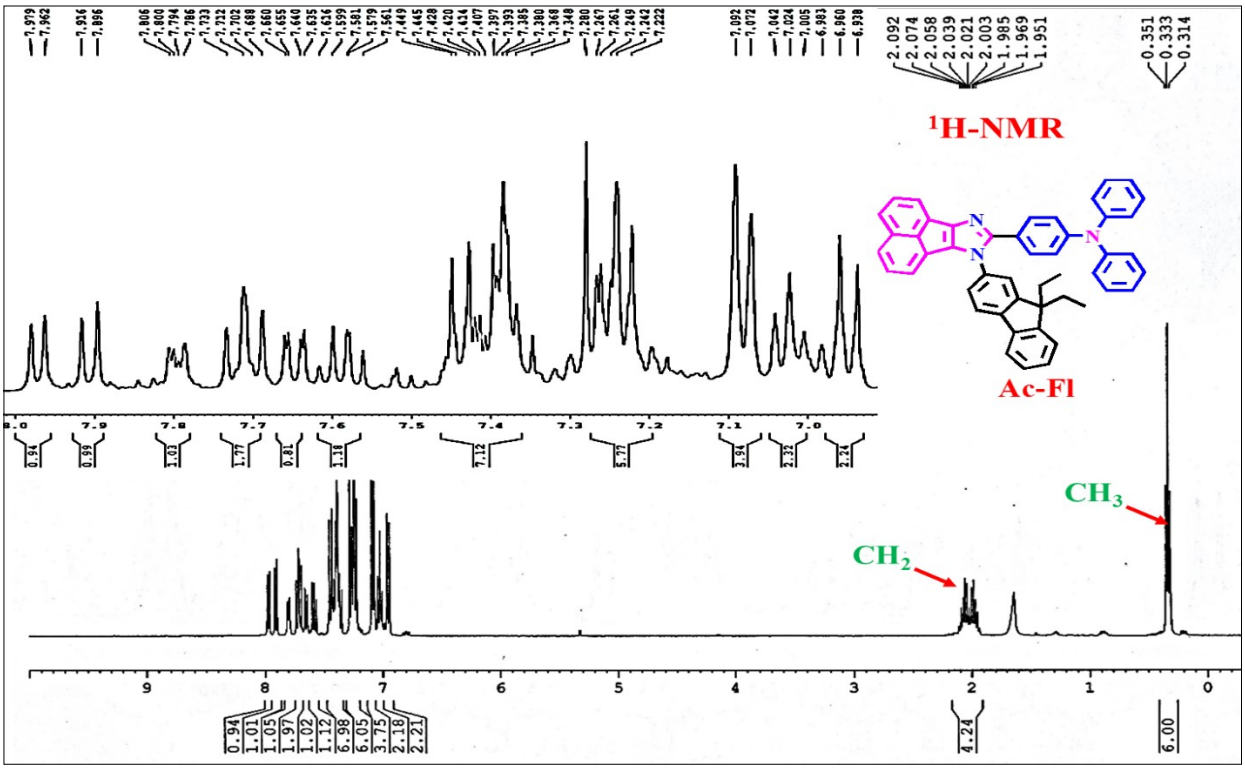

Fig. S5. The ^{1}H NMR spectra of the AC-Fl

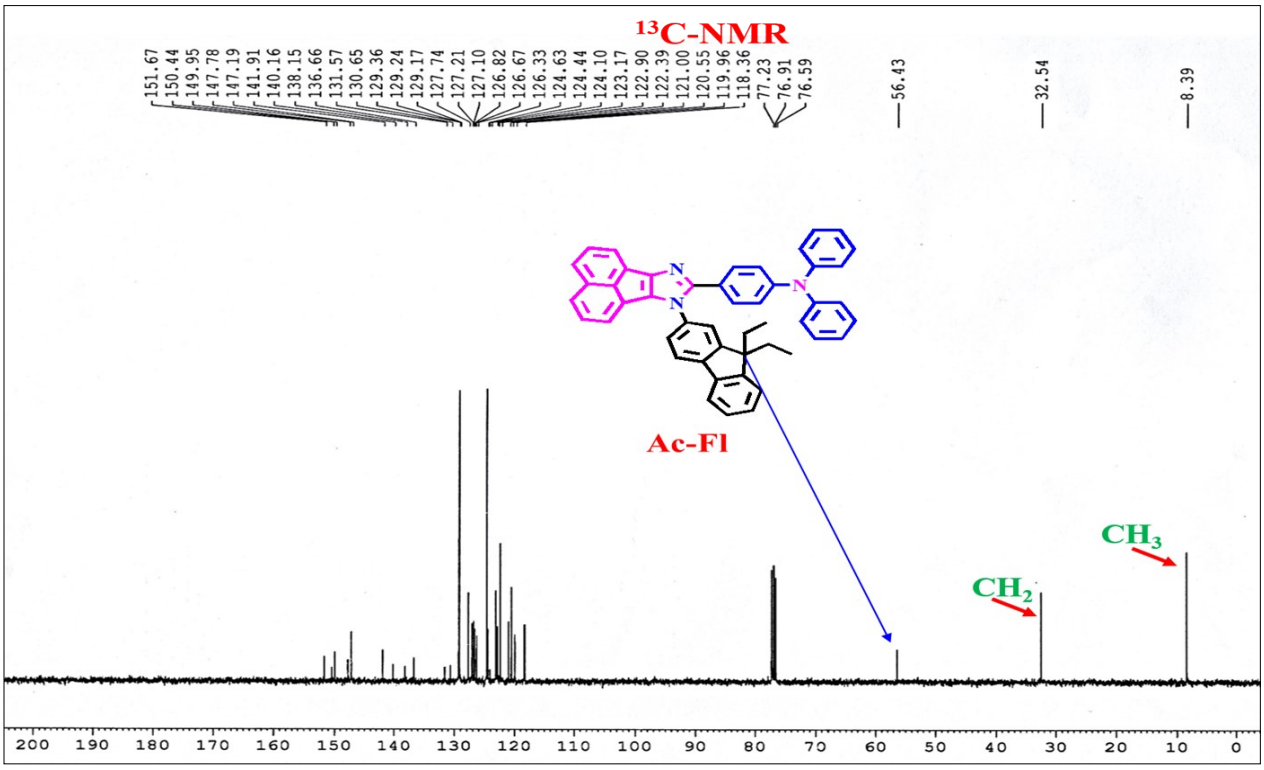

Fig. S6. The ^{13}C NMR spectra of the AC-Fl

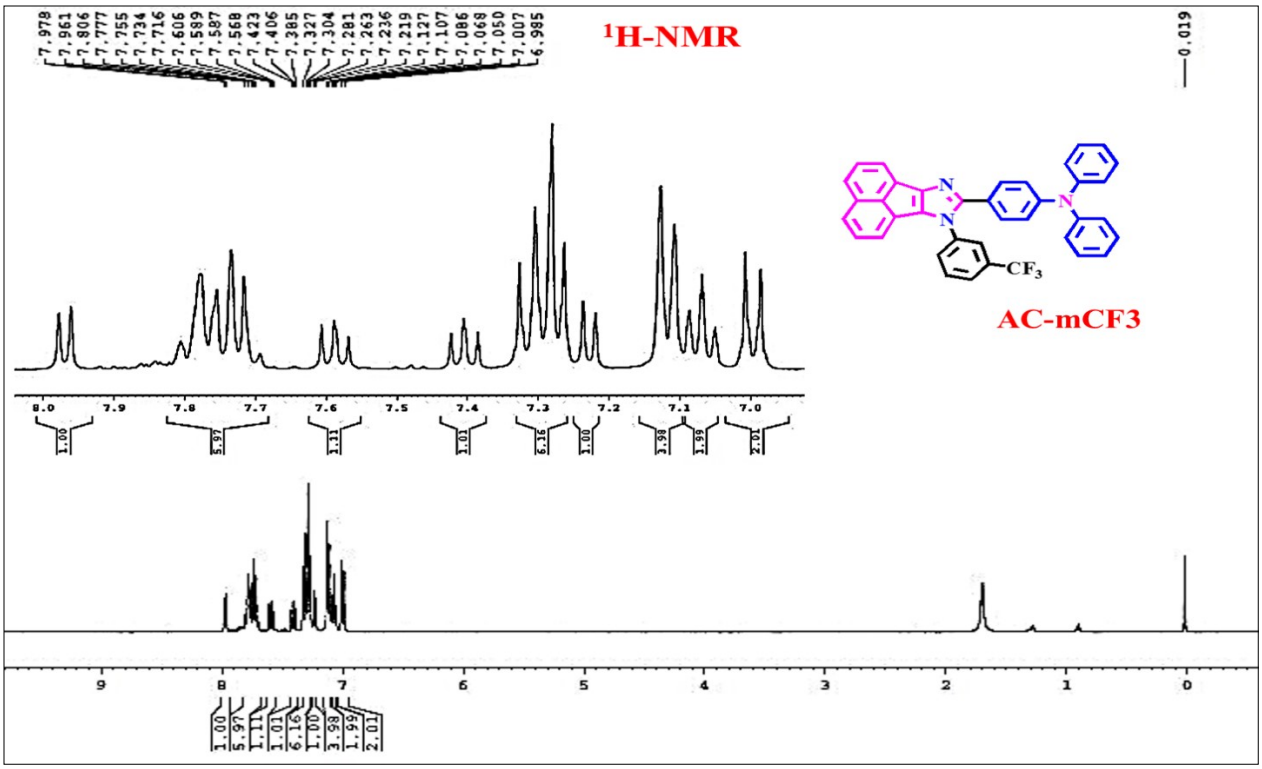

Fig. S7. The [1]H NMR spectra of the AC-mCF3

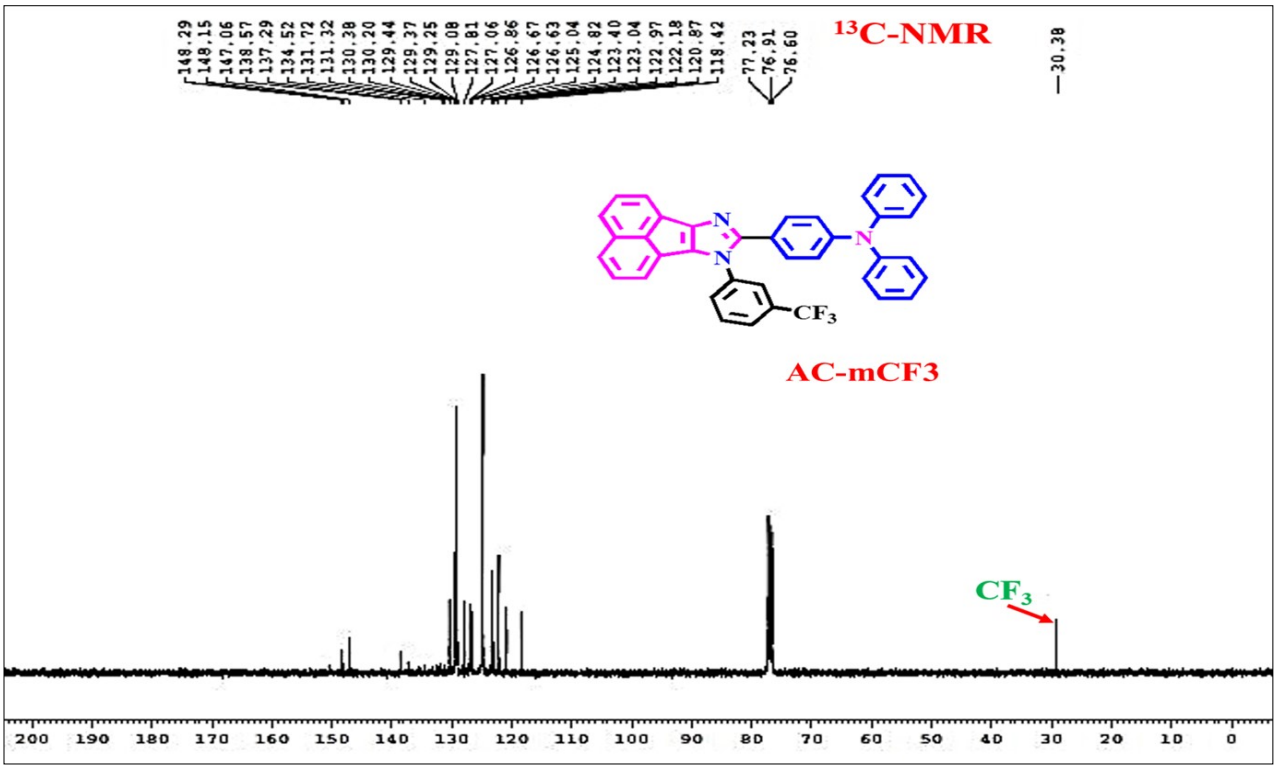

Fig. S8. The [13]C NMR spectra of the AC-mCF3

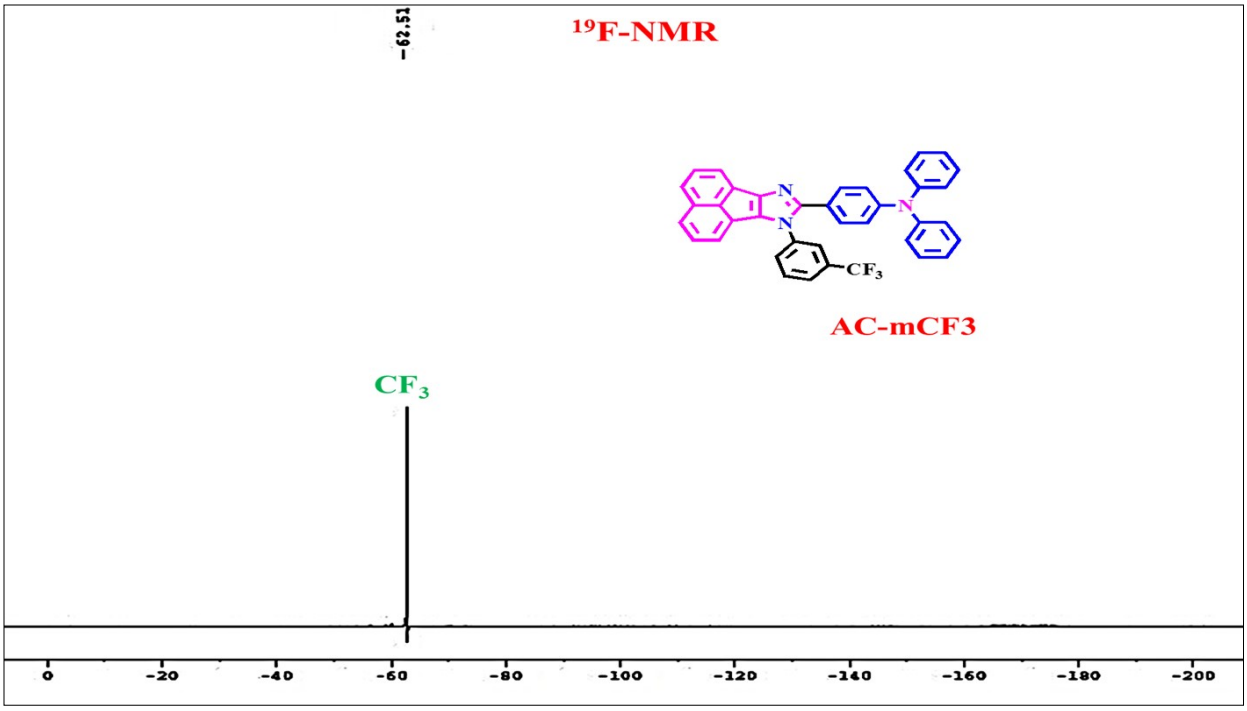

Fig. S9. The ^{19}F NMR spectra of the AC-mCF3

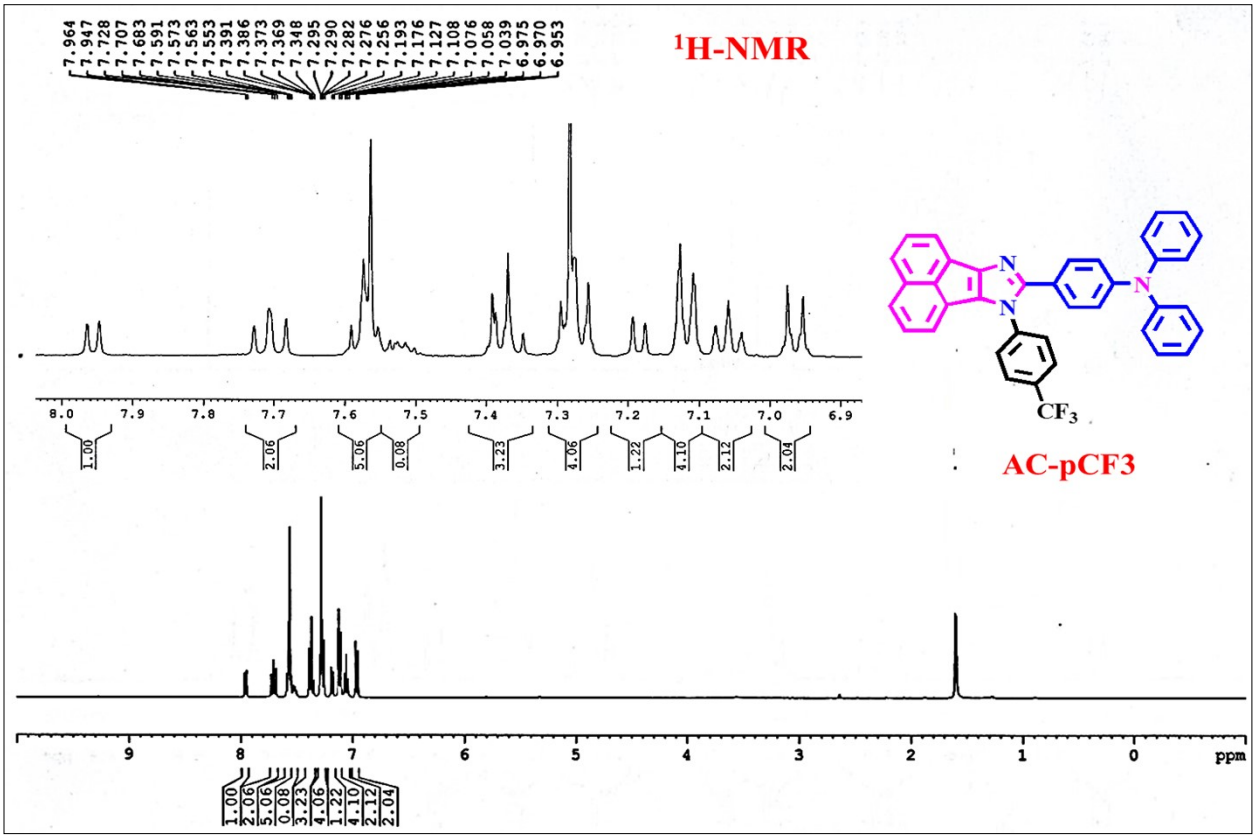

Fig. S10. The ^{1}H NMR spectra of the AC-pCF3

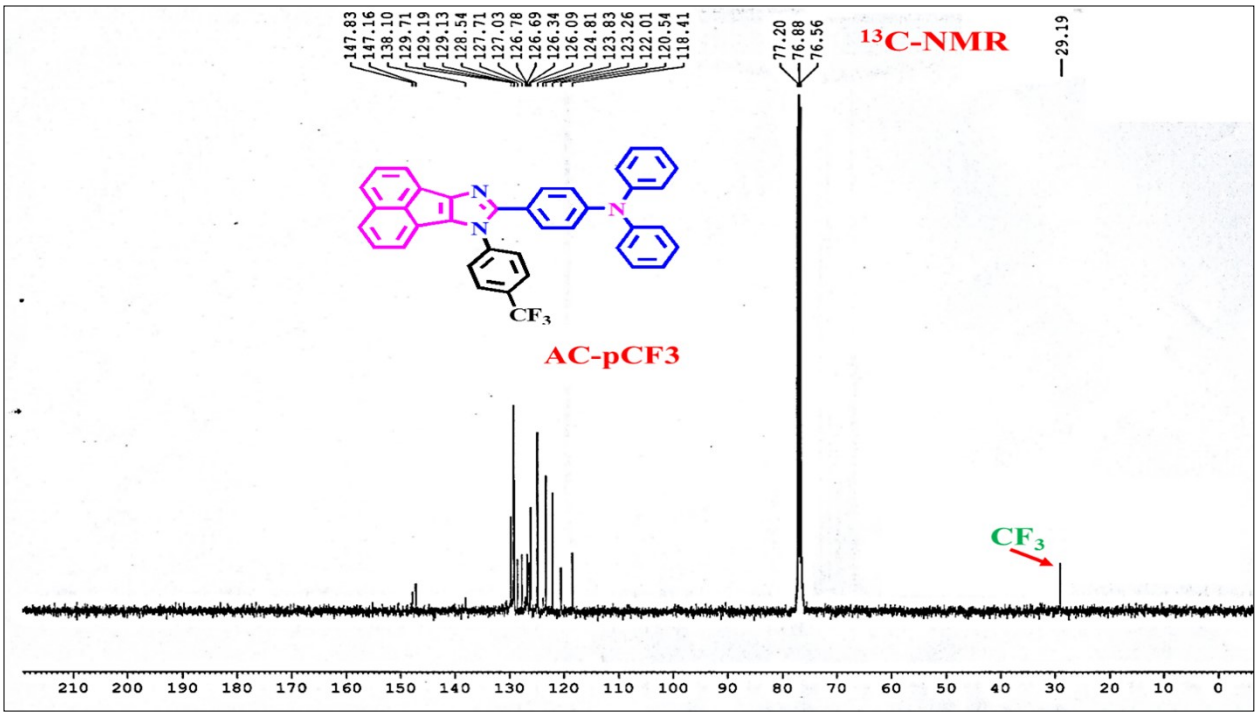

Fig. S11. The ^{13}C NMR spectra of the AC-pCF3

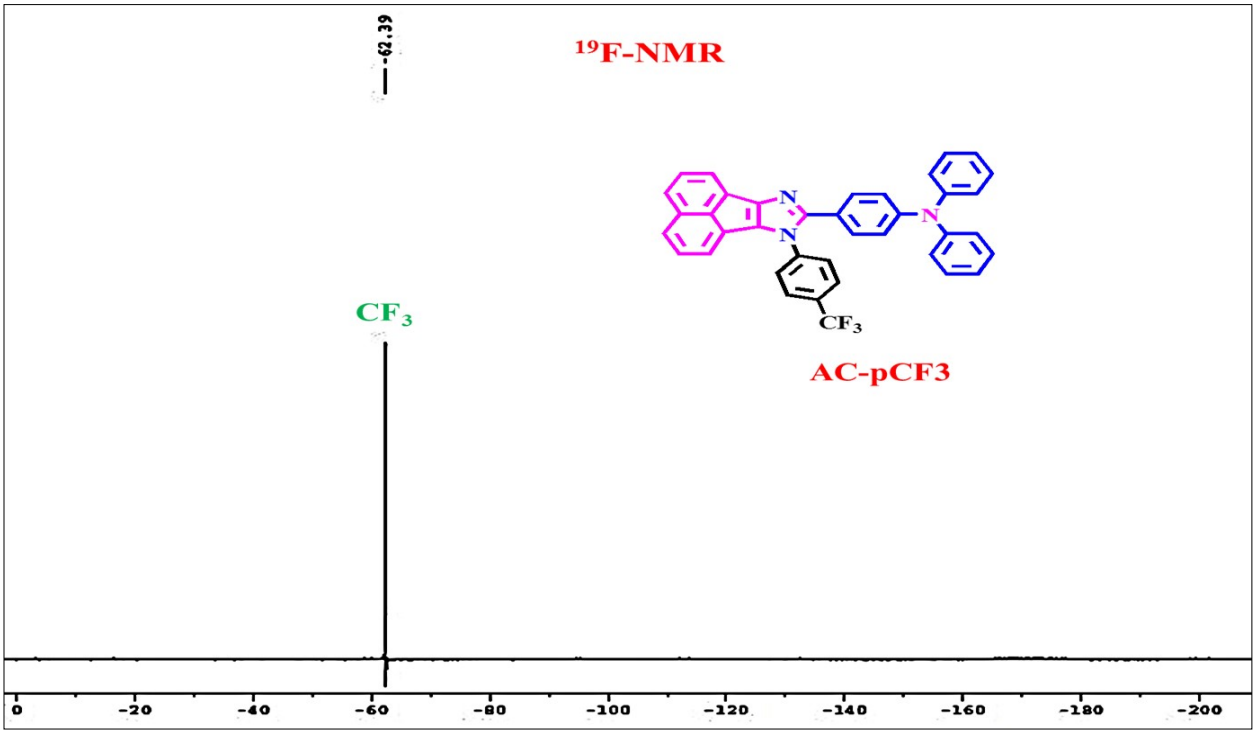

Fig. S12. The ^{19}F NMR spectra of the AC-pCF3

SI2 Mass spectra of the compounds

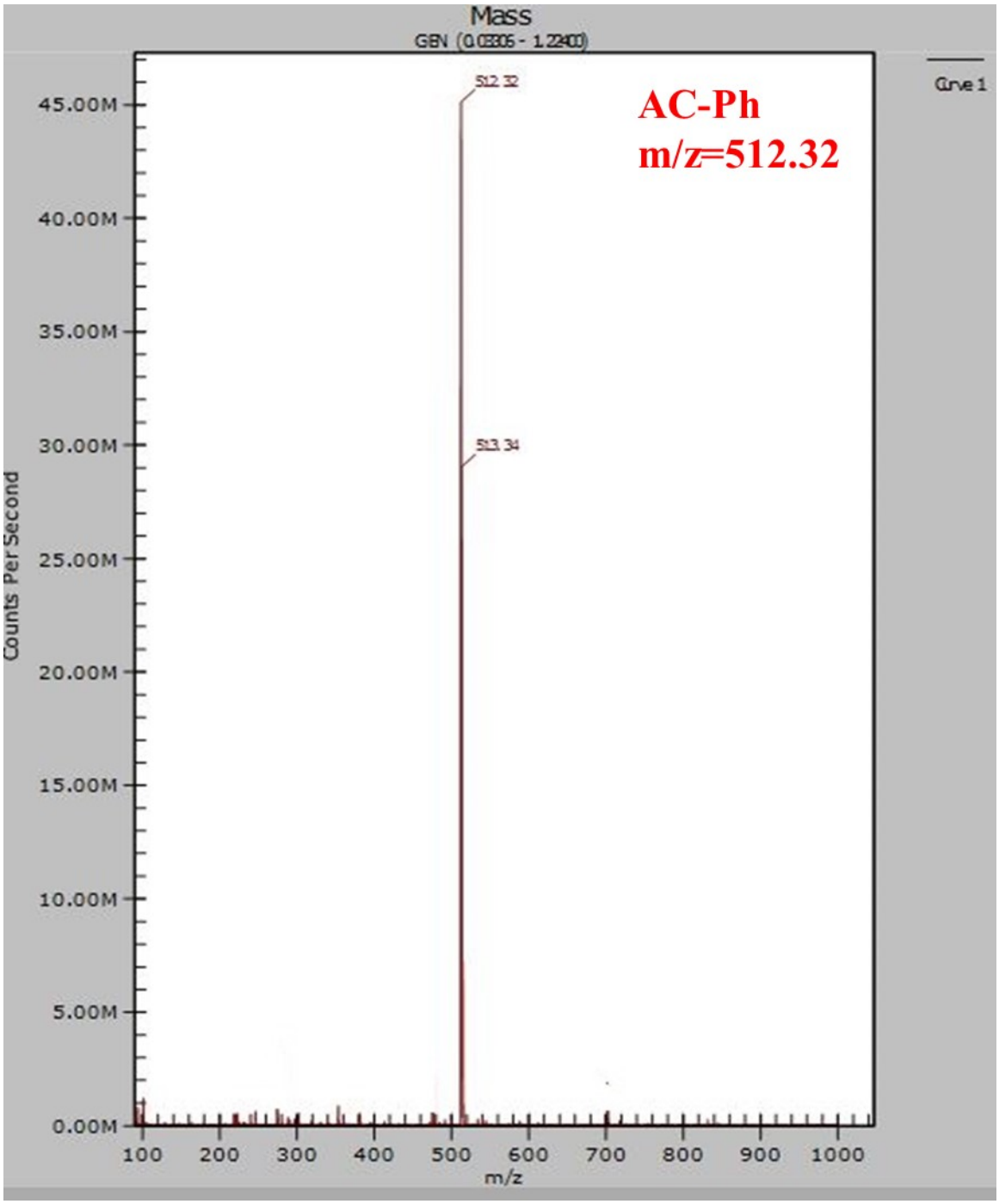

Fig. S13. The mass spectra of the AC-Ph

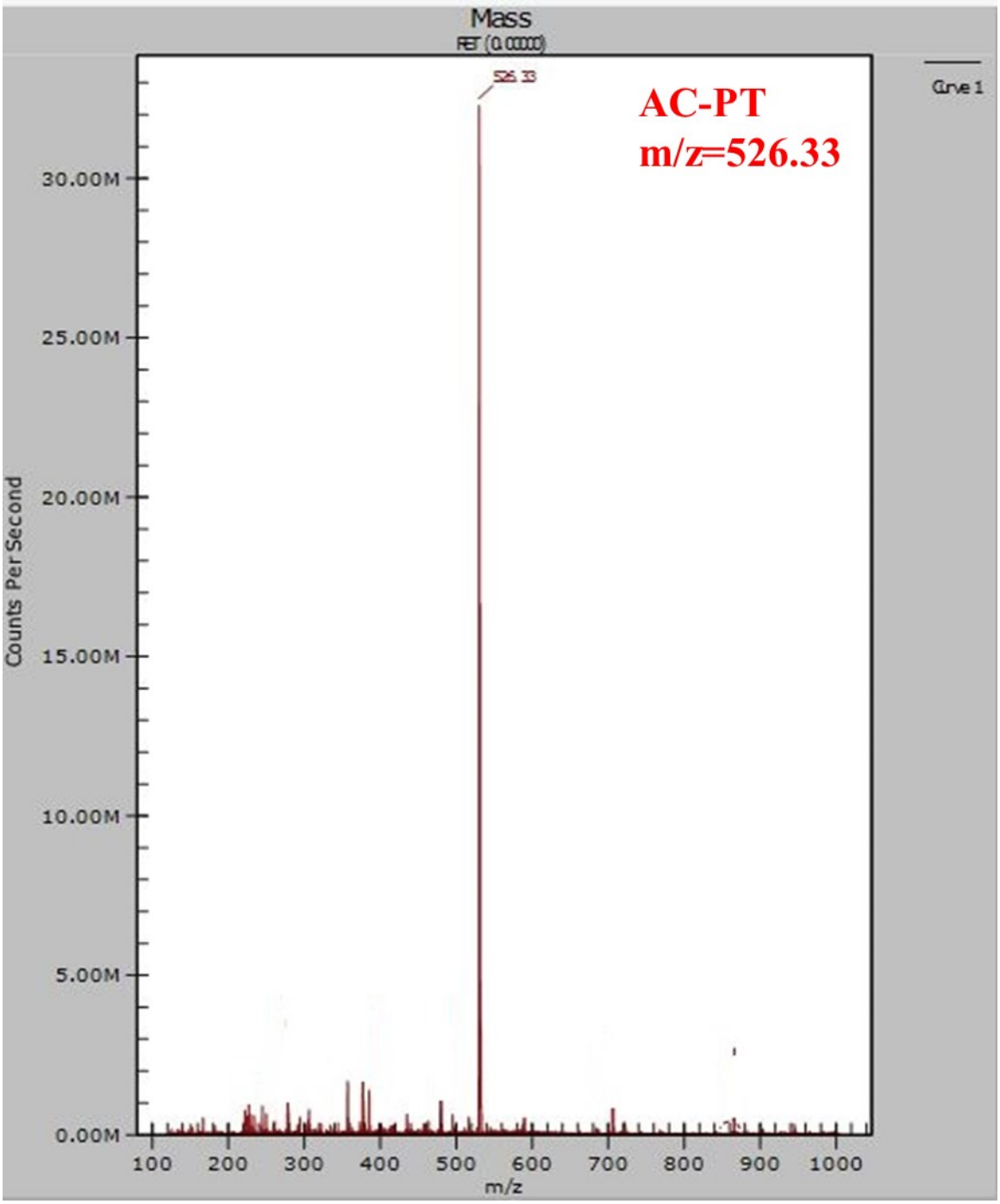

Fig. S14. The mass spectra of the AC-PT

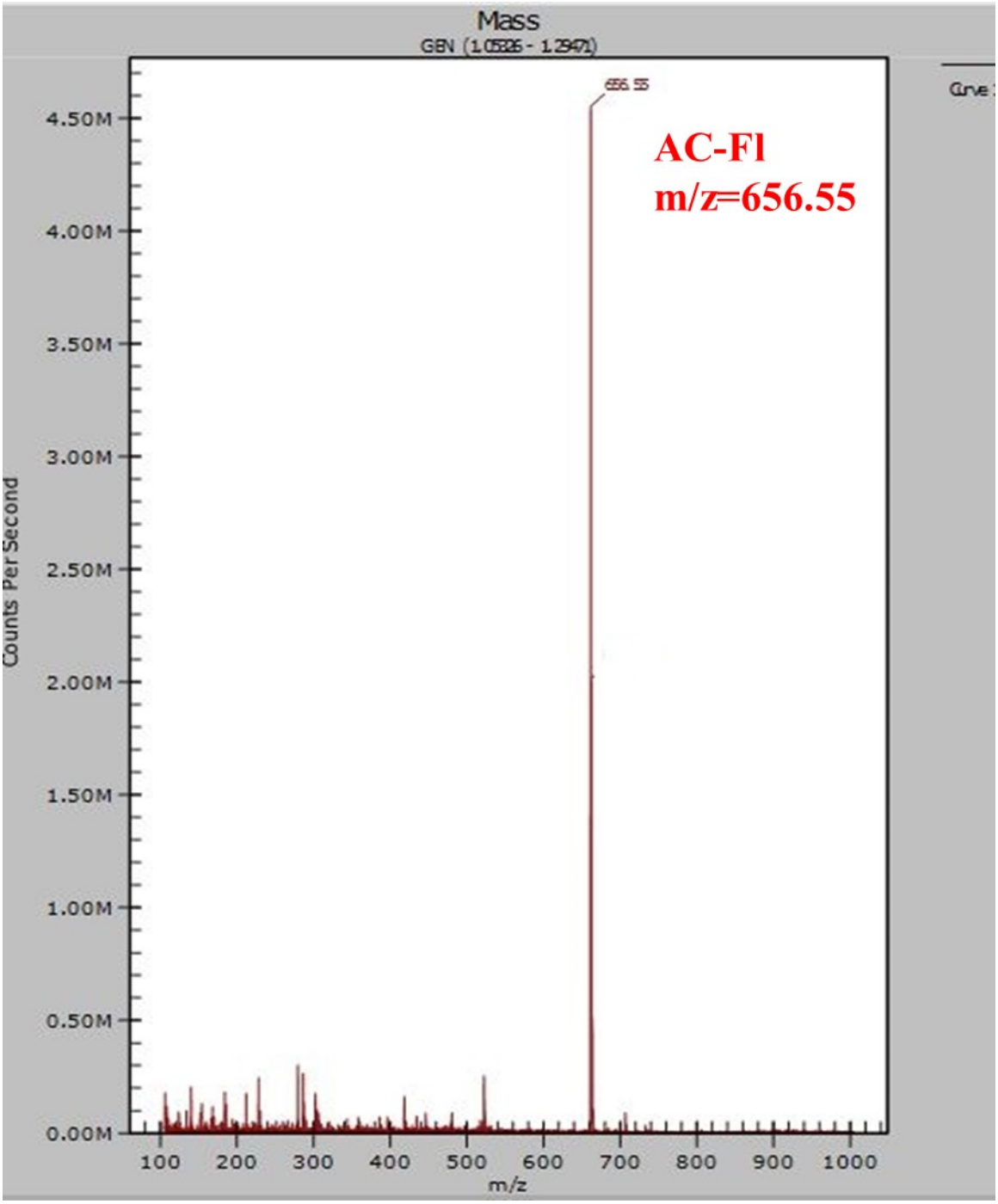

Fig. S15. The mass spectra of the AC-Fl

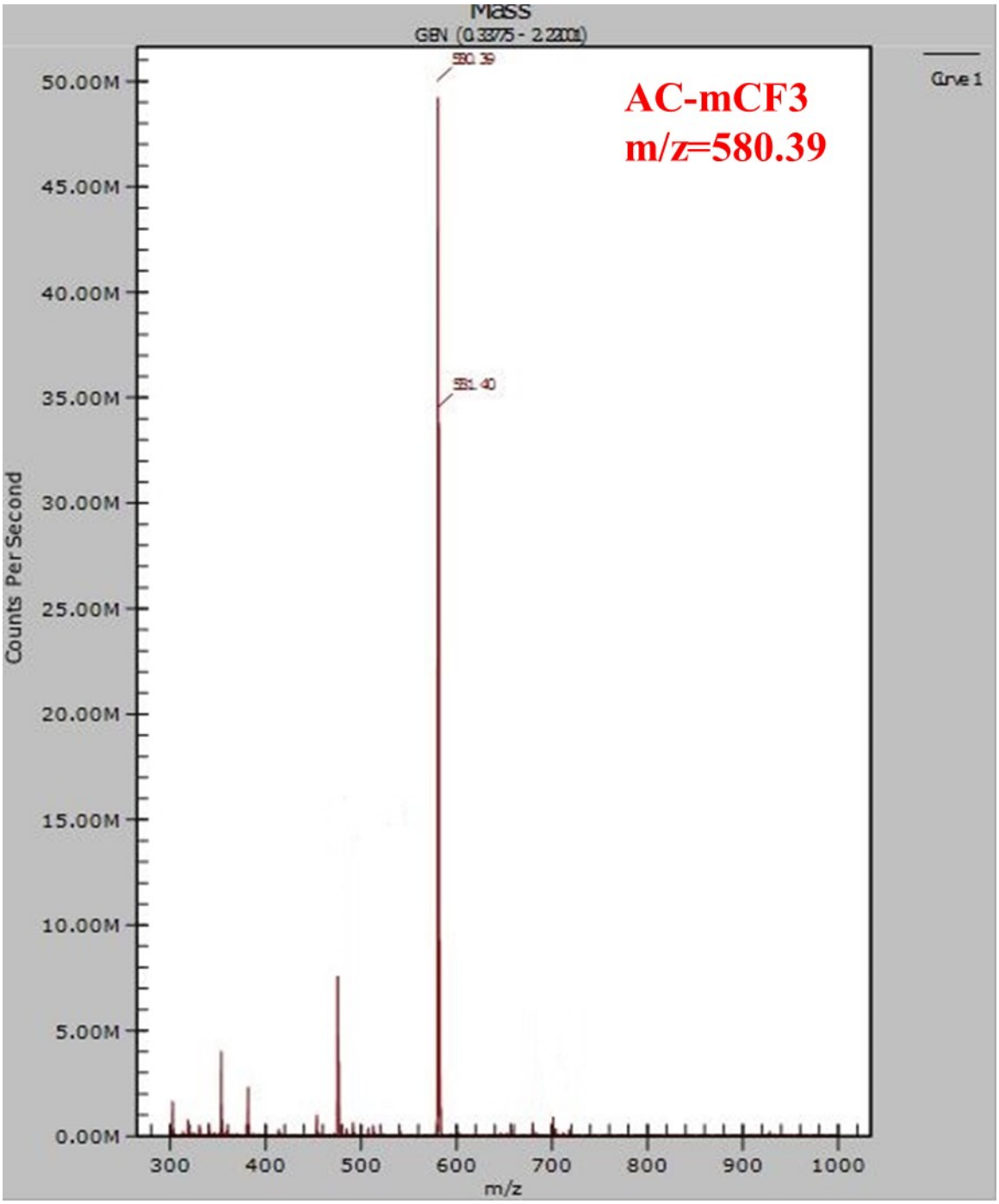

Fig. S16. The mass spectra of the AC-mCF3

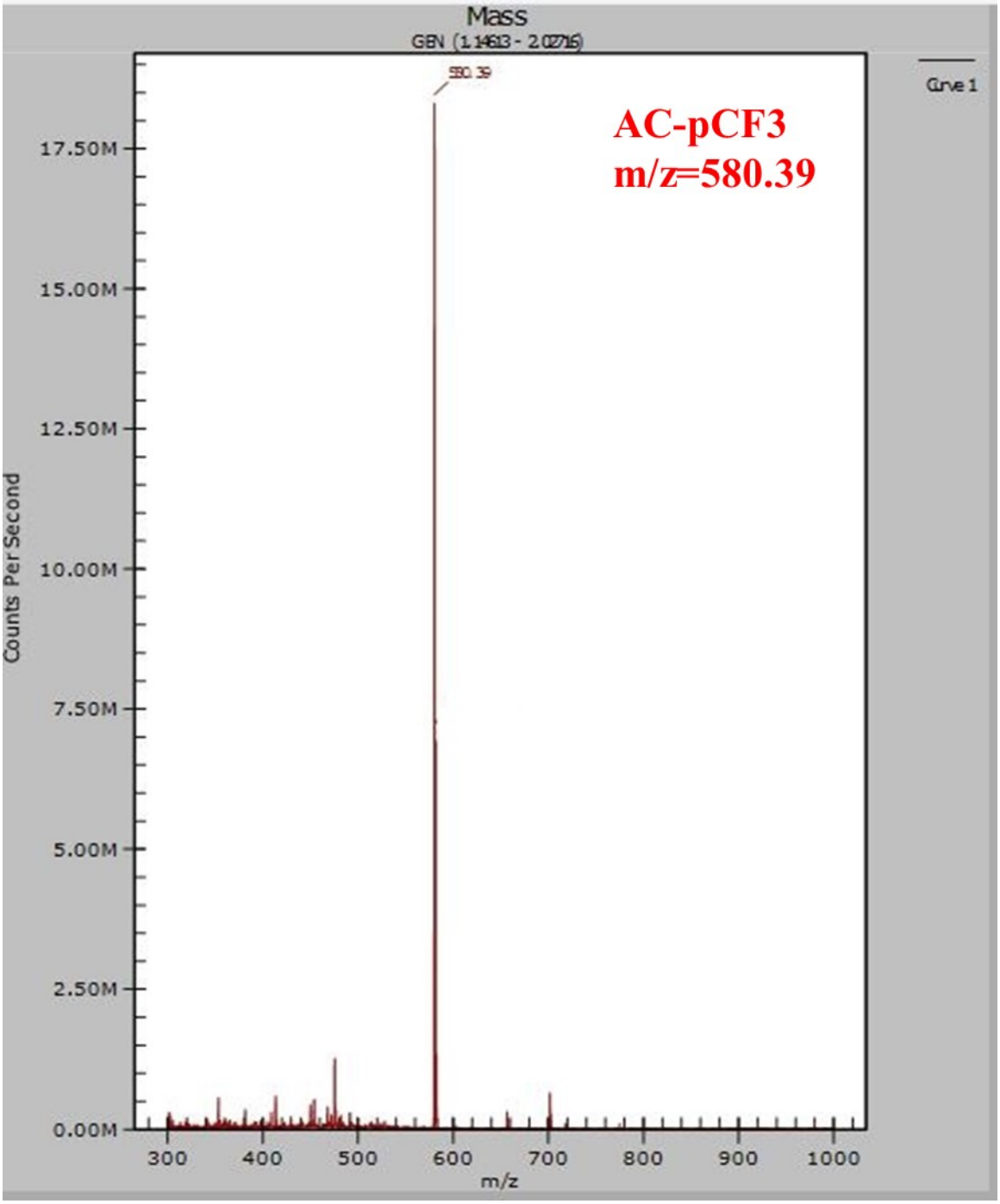

Fig. S17. The mass spectra of the AC-pCF3

SI3 Fourier transform infrared (FTIR) Spectroscopy

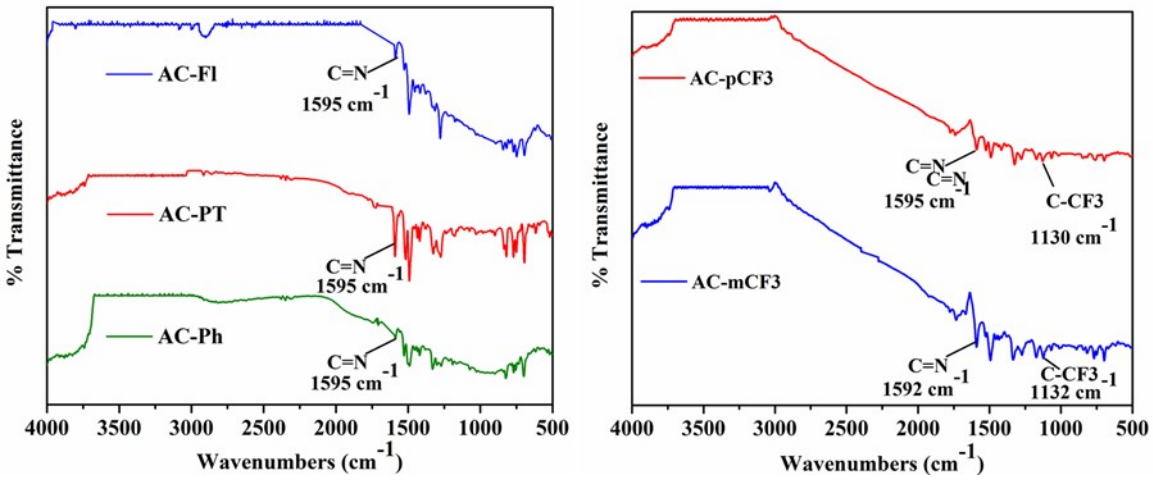

Fig. S18. Fourier transform infrared spectra of all the dyes

Table S1 The major FT-IR bands [cm^{-1}] of all the dyes

Bonding	AC-Ph	AC-PT	AC-Fl	AC-mCF3	AC-pCF3
C=N	1595	1595	1595	1592	1595
C-CF3	-	-	-	1130	1132
Aromatic -CH2-CH3, C–C, C=C stretching frequency.	1496, 1416, 1336, 1266	1488, 1420, 1324, 1274, 1180	2894, 1488, 1418, 1318, 1278	1492, 1333, 1273, 1163, 1073	1486, 1416, 1326, 1276, 1166, 1066
C–H bending	816, 766, 696	825, 755, 695	838, 749, 699	813, 773, 703	836, 766, 696

Table S2. Crystal data and structure-refinement parameters of AC-Ph, AC-PT and AC-mCF3.

Identification code	AC-Ph	AC-PT	AC-mCF3
Empirical formula	$C_{37}H_{25}N_3$	$C_{38}H_{27}N_3$	$C_{76}H_{48}F_6N_6$
Formula weight	511.60	525.63	1160.21
Temperature/K	293(2)	293(2)	293(2)
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	P1	P1
a/Å	9.4757(3)	11.9844(5)	10.5459(7)
b/Å	33.1303(8)	13.3254(5)	10.6770(8)
c/Å	9.4560(5)	17.9582(8)	14.3890(10)
α/°	90.00	101.962(4)	103.037(6)
β/°	115.253(5)	95.302(4)	97.282(6)
γ/°	90.00	92.222(3)	107.693(6)

Volume/Å^3	2684.84(17)	2788.6(2)	1470.08(18)
Z	4	4	1
ρ_{calc}g/cm^3	1.266	1.252	1.311
μ/mm^{-1}	0.575	0.567	0.741
F(000)	1072.0	1104.0	601.0
Crystal size/mm^3	0.396 × 0.283 × 0.149	0.313 × 0.156 × 0.114	0.252 × 0.187 × 0.122
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.32 to 133.76	7.56 to 133.86	9.06 to 133.96
Index ranges	-11 ≤ h ≤ 7, -39 ≤ k ≤ 39, -10 ≤ l ≤ 9	-14 ≤ h ≤ 11, -15 ≤ k ≤ 15, -21 ≤ l ≤ 20	-12 ≤ h ≤ 11, -10 ≤ k ≤ 12, -17 ≤ l ≤ 16
Reflections collected	5501	17383	8334
Independent reflections	3529 [R_{int} = 0.0155, R_{sigma} = 0.0234]	9799 [R_{int} = 0.0342, R_{sigma} = 0.0458]	5787 [R_{int} = 0.0495, R_{sigma} = 0.0430]
Data/restraints/parameters	3529/0/361	9799/0/741	5787/3/793
Goodness-of-fit on F^2	1.075	1.030	1.096
Final R indexes [I>=2σ (I)]	R_1 = 0.0409, wR_2 = 0.1072	R_1 = 0.0553, wR_2 = 0.1543	R_1 = 0.0667, wR_2 = 0.1955
Final R indexes [all data]	R_1 = 0.0471, wR_2 = 0.1124	R_1 = 0.0664, wR_2 = 0.1688	R_1 = 0.0905, wR_2 = 0.2513
Largest diff. peak/hole / e Å^{-3}	0.13/-0.15	0.43/-0.34	0.38/-0.34

Table S3, S4, S5, S6, S7 and S8. The Bond Lengths and Bond Angles from single crystal XRD data of AC-Ph, AC-PT and AC-mCF3 dyes.

Table S3 Bond Lengths for AC-Ph						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
N28	C29	1.434(2)		C10	C5	1.397(2)
N28	C25	1.396(2)		C8	C9	1.367(2)
N28	C35	1.431(2)		C8	C7	1.418(3)
N21	C13	1.3267(19)		C11	C12	1.362(2)
N21	C12	1.368(2)		C11	C1	1.456(2)
C26	C27	1.381(2)		C30	C31	1.384(3)
C26	C25	1.395(2)		C18	C19	1.375(3)
C27	C22	1.390(2)		C18	C17	1.364(4)
N14	C13	1.3863(19)		C9	C12	1.473(2)
N14	C15	1.4375(18)		C1	C2	1.364(2)
N14	C11	1.371(2)		C34	C33	1.384(3)

C24	C25	1.397(2)		C33	C32	1.364(3)
C24	C23	1.378(2)		C3	C4	1.363(3)
C13	C22	1.470(2)		C3	C2	1.419(3)
C29	C30	1.383(3)		C7	C6	1.362(3)
C29	C34	1.374(3)		C4	C5	1.413(3)
C15	C16	1.378(3)		C5	C6	1.416(3)
C15	C20	1.369(3)		C36	C37	1.387(3)
C40	C35	1.386(2)		C39	C38	1.363(4)
C40	C39	1.380(3)		C16	C17	1.385(3)
C35	C36	1.375(3)		C37	C38	1.370(3)
C23	C22	1.386(2)		C19	C20	1.382(2)
C10	C9	1.421(2)		C32	C31	1.371(4)
C10	C1	1.424(2)				

Table S4 Bond Angles for AC-Ph

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C25	N28	C29	121.88(13)		N14	C11	C1	141.67(15)
C25	N28	C35	121.08(14)		C12	C11	N14	106.53(13)
C35	N28	C29	116.43(13)		C12	C11	C1	111.79(14)
C13	N21	C12	104.27(12)		C29	C30	C31	119.3(2)
C27	C26	C25	121.04(15)		C17	C18	C19	119.64(17)
C26	C27	C22	121.29(15)		C10	C9	C12	103.86(14)
C13	N14	C15	129.66(13)		C8	C9	C10	118.57(16)
C11	N14	C13	105.43(12)		C8	C9	C12	137.57(16)
C11	N14	C15	124.58(12)		N21	C12	C9	139.93(14)
C23	C24	C25	120.90(16)		C11	C12	N21	111.46(13)
N21	C13	N14	112.31(14)		C11	C12	C9	108.60(14)
N21	C13	C22	122.99(13)		C10	C1	C11	102.71(14)
N14	C13	C22	124.52(13)		C2	C1	C10	118.94(18)
C30	C29	N28	121.55(19)		C2	C1	C11	138.34(18)
C34	C29	N28	119.18(16)		C29	C34	C33	120.82(19)
C34	C29	C30	119.26(16)		C32	C33	C34	120.0(2)

N28	C25	C24	120.71(15)		C4	C3	C2	122.42(19)
C26	C25	N28	121.77(15)		C6	C7	C8	122.74(17)
C26	C25	C24	117.52(14)		C3	C4	C5	120.95(19)
C16	C15	N14	120.64(16)		C10	C5	C4	116.02(18)
C20	C15	N14	118.46(16)		C10	C5	C6	115.95(17)
C20	C15	C16	120.82(15)		C4	C5	C6	128.02(19)
C39	C40	C35	119.3(2)		C35	C36	C37	120.13(19)
C40	C35	N28	120.38(19)		C38	C39	C40	121.2(2)
C36	C35	N28	120.11(16)		C1	C2	C3	118.4(2)
C36	C35	C40	119.51(17)		C15	C16	C17	119.01(19)
C24	C23	C22	121.65(15)		C7	C6	C5	120.60(17)
C27	C22	C13	122.70(15)		C38	C37	C36	120.2(2)
C23	C22	C27	117.59(14)		C18	C19	C20	120.5(2)
C23	C22	C13	119.50(14)		C18	C17	C16	120.7(2)
C9	C10	C1	113.03(15)		C33	C32	C31	119.59(19)
C5	C10	C9	123.69(16)		C15	C20	C19	119.30(19)
C5	C10	C1	123.27(16)		C39	C38	C37	119.56(19)
C9	C8	C7	118.43(17)		C32	C31	C30	121.0(2)

Table S5 Bond Lengths for AC-PT.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
N0AA	C6	1.363(2)		C28	C62	1.505(3)
N0AA	C10	1.329(2)		C31	C50	1.383(3)
N2	C9	1.435(2)		C32	C47	1.383(3)
N2	C10	1.389(2)		C33	C42	1.423(3)
N2	C16	1.374(2)		C33	C48	1.393(3)
N1AA	C2AA	1.397(2)		C34	N35	1.412(3)
N1AA	C7	1.369(2)		C34	C54	1.374(3)
N1AA	C19	1.438(2)		C34	C67	1.383(4)
C2AA	N3AA	1.325(2)		N35	C55	1.418(3)
C2AA	C20	1.469(2)		C37	C39	1.383(3)

N3AA	C21	1.369(2)		C38	C52	1.385(3)
C6	C13	1.472(2)		C40	C1	1.375(3)
C6	C16	1.362(3)		C40	C2	1.388(3)
C7	C21	1.368(3)		C41	C45	1.423(3)
C7	C24	1.455(2)		C41	C59	1.405(3)
C8	C13	1.418(3)		C42	C57	1.364(3)
C8	C17	1.426(3)		C43	C1AA	1.394(4)
C8	C41	1.396(3)		C43	C4AA	1.345(4)
C9	C37	1.381(3)		C44	C58	1.417(3)
C9	C38	1.368(3)		C45	C49	1.355(4)
C10	C15	1.469(2)		C46	C60	1.416(3)
C11	C20	1.396(2)		C47	C51	1.371(4)
C11	C36	1.377(3)		C48	C63	1.411(4)
C12	C15	1.393(3)		C48	C65	1.422(3)
C12	C23	1.375(3)		C50	C51	1.381(4)
C13	C27	1.367(3)		C51	C74	1.507(3)
C14	C15	1.392(2)		C54	C71	1.392(4)
C14	C22	1.384(3)		C55	C56	1.389(4)
C16	C17	1.452(2)		C55	C61	1.375(4)
C17	C44	1.365(3)		C56	C72	1.381(4)
C18	C30	1.388(3)		C57	C70	1.421(3)
C18	N35	1.421(2)		C58	C59	1.362(4)
C18	C36	1.387(3)		C60	C65	1.358(4)
C19	C31	1.364(3)		C61	C69	1.409(5)
C19	C32	1.374(3)		C63	C70	1.363(4)
C20	C25	1.385(3)		C67	C77	1.382(4)
C21	C42	1.469(3)		C69	C76	1.372(7)
C22	C29	1.387(3)		C71	C75	1.358(5)
C23	C29	1.395(3)		C72	C76	1.367(6)
C24	C33	1.420(3)		C75	C77	1.357(5)
C24	C46	1.368(3)		C1AA	C3AA	1.347(4)
C25	C30	1.389(3)		C0AA	C3AA	1.311(7)
N26	C29	1.412(2)		C0AA	C5AA	1.390(8)
N26	C40	1.408(3)		C5AA	C4AA	1.446(6)
N26	C43	1.422(3)		C1	C5	1.380(3)
C27	C49	1.424(3)		C2	C4	1.375(4)

C28	C39	1.377(3)		C3	C4	1.361(5)	
C28	C52	1.378(3)		C3	C5	1.370(5)	

Table S6 Bond Angles for AC-PT.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C10	N0AA	C6	104.36(14)		C19	C31	C50	119.2(2)
C10	N2	C9	130.31(14)		C19	C32	C47	119.3(2)
C16	N2	C9	123.61(14)		C24	C33	C42	113.02(17)
C16	N2	C10	105.47(14)		C48	C33	C24	123.2(2)
C2AA	N1AA	C19	130.31(14)		C48	C33	C42	123.8(2)
C7	N1AA	C2AA	105.38(14)		C54	C34	N35	121.7(2)
C7	N1AA	C19	123.52(14)		C54	C34	C67	118.8(2)
N1AA	C2AA	C20	125.15(15)		C67	C34	N35	119.5(2)
N3AA	C2AA	N1AA	112.10(14)		C34	N35	C18	120.09(16)
N3AA	C2AA	C20	122.71(15)		C34	N35	C55	120.65(16)
C2AA	N3AA	C21	104.57(15)		C55	N35	C18	118.39(17)
N0AA	C6	C13	139.42(17)		C11	C36	C18	120.42(17)
C16	C6	N0AA	111.80(15)		C9	C37	C39	118.8(2)
C16	C6	C13	108.72(16)		C9	C38	C52	119.98(19)
N1AA	C7	C24	141.73(17)		C28	C39	C37	122.1(2)
C21	C7	N1AA	106.62(15)		C1	C40	N26	122.35(19)
C21	C7	C24	111.57(16)		C1	C40	C2	118.2(2)
C13	C8	C17	112.75(16)		C2	C40	N26	119.4(2)
C41	C8	C13	123.50(19)		C8	C41	C45	116.0(2)
C41	C8	C17	123.74(19)		C8	C41	C59	116.0(2)
C37	C9	N2	120.26(17)		C59	C41	C45	128.0(2)
C38	C9	N2	119.54(16)		C33	C42	C21	103.91(16)
C38	C9	C37	120.14(17)		C57	C42	C21	137.68(19)
N0AA	C10	N2	112.04(15)		C57	C42	C33	118.40(19)
N0AA	C10	C15	122.60(15)		C1AA	C43	N26	118.8(2)
N2	C10	C15	125.36(15)		C4AA	C43	N26	120.8(3)
C36	C11	C20	121.32(17)		C4AA	C43	C1AA	120.4(3)
C23	C12	C15	121.65(17)		C17	C44	C58	118.2(2)
C8	C13	C6	103.96(15)		C49	C45	C41	120.73(19)
C27	C13	C6	137.29(18)		C24	C46	C60	118.3(2)
C27	C13	C8	118.75(17)		C51	C47	C32	121.4(2)
C22	C14	C15	120.83(17)		C33	C48	C63	116.1(2)

C12	C15	C10	118.00(15)		C33	C48	C65	116.2(2)
C14	C15	C10	124.12(16)		C63	C48	C65	127.7(2)
C14	C15	C12	117.86(16)		C45	C49	C27	122.5(2)
N2	C16	C17	142.03(17)		C51	C50	C31	121.6(2)
C6	C16	N2	106.32(15)		C47	C51	C50	117.9(2)
C6	C16	C17	111.53(16)		C47	C51	C74	121.2(3)
C8	C17	C16	103.01(16)		C50	C51	C74	120.9(3)
C44	C17	C8	118.35(18)		C28	C52	C38	121.2(2)
C44	C17	C16	138.61(19)		C34	C54	C71	119.7(3)
C30	C18	N35	120.99(18)		C56	C55	N35	120.2(2)
C36	C18	C30	118.88(16)		C61	C55	N35	120.3(3)
C36	C18	N35	120.11(18)		C61	C55	C56	119.5(3)
C31	C19	N1AA	119.63(17)		C72	C56	C55	121.0(3)
C31	C19	C32	120.65(18)		C42	C57	C70	118.4(2)
C32	C19	N1AA	119.63(18)		C59	C58	C44	123.1(2)
C11	C20	C2AA	117.96(15)		C58	C59	C41	120.5(2)
C25	C20	C2AA	123.97(16)		C65	C60	C46	122.7(2)
C25	C20	C11	118.00(16)		C55	C61	C69	118.9(4)
N3AA	C21	C42	140.02(17)		C70	C63	C48	120.5(2)
C7	C21	N3AA	111.33(16)		C60	C65	C48	120.6(2)
C7	C21	C42	108.58(16)		C77	C67	C34	120.3(3)
C14	C22	C29	120.79(17)		C76	C69	C61	120.8(3)
C12	C23	C29	120.15(18)		C63	C70	C57	122.7(2)
C33	C24	C7	102.92(16)		C75	C71	C54	121.1(3)
C46	C24	C7	138.06(19)		C76	C72	C56	119.9(4)
C46	C24	C33	119.01(18)		C77	C75	C71	119.3(3)
C20	C25	C30	120.91(17)		C72	C76	C69	119.9(3)
C29	N26	C43	119.90(17)		C75	C77	C67	120.8(3)
C40	N26	C29	122.05(16)		C3AA	C1AA	C43	122.5(4)
C40	N26	C43	116.91(16)		C3AA	C0AA	C5AA	122.7(4)
C13	C27	C49	118.5(2)		C0AA	C3AA	C1AA	118.6(5)
C39	C28	C52	117.69(18)		C0AA	C5AA	C4AA	118.7(4)
C39	C28	C62	121.4(2)		C43	C4AA	C5AA	117.0(4)
C52	C28	C62	120.9(2)		C40	C1	C5	120.5(2)
C22	C29	C23	118.72(17)		C4	C2	C40	120.6(3)
C22	C29	N26	121.14(17)		C4	C3	C5	119.0(3)

C23	C29	N26	120.14(18)		C3	C4	C2	120.9(3)
C18	C30	C25	120.46(17)		C3	C5	C1	120.8(3)

Table S7 Bond Lengths for AC-mCF3.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
N9	C10	1.409(11)		C72	C71	1.301(19)
N9	C36	1.427(11)		C6	C5	1.418(14)
N9	C8	1.393(11)		N62	C69	1.432(13)
N45	C44	1.339(11)		N62	C56	1.447(12)
N45	C46	1.368(11)		C58	C57	1.375(14)
N55	C75	1.443(10)		C1	C13	1.349(14)
N55	C44	1.381(11)		C61	C56	1.378(15)
N55	C54	1.349(11)		C21	C16	1.393(14)
N11	C10	1.296(12)		C18	C17	1.395(12)
N11	C12	1.370(12)		C51	C88	1.453(16)
C52	C53	1.430(13)		C51	C50	1.393(16)
C52	C47	1.427(13)		C69	C70	1.361(13)
C52	C51	1.400(12)		C69	C74	1.381(14)
C10	C19	1.481(12)		C88	C87	1.303(16)
C75	C80	1.367(13)		C65	C64	1.393(16)
C75	C76	1.381(13)		C65	C66	1.38(2)
C36	C37	1.378(13)		C29	C34	1.379(14)
C36	C35	1.402(13)		C29	C30	1.398(14)
C44	C59	1.462(12)		C38	C39	1.373(15)
C2	C3	1.392(13)		C38	C41	1.510(14)
C2	C7	1.408(13)		C50	C49	1.360(18)
C2	C1	1.407(13)		C4	C5	1.409(16)
C54	C46	1.400(12)		C79	C78	1.377(17)
C54	C53	1.458(12)		C79	C0AA	1.489(17)
C80	C79	1.395(13)		C16	C17	1.370(14)
C8	C12	1.338(12)		C70	C71	1.437(16)
C8	C7	1.453(11)		C56	C57	1.393(14)
C59	C60	1.387(13)		C13	C14	1.437(16)
C59	C58	1.386(13)		C15	C14	1.357(18)
C23	N22	1.442(12)		C35	C40	1.417(15)
C23	C24	1.370(14)		C34	C33	1.379(17)

C23	C28	1.407(14)		C48	C49	1.410(17)
C19	C20	1.399(12)		C30	C31	1.337(16)
C19	C18	1.386(13)		C24	C25	1.380(18)
N22	C29	1.389(13)		C77	C76	1.350(15)
N22	C16	1.413(11)		C77	C78	1.370(18)
C46	C47	1.446(12)		C28	C27	1.46(2)
C12	C1	1.486(12)		C33	C32	1.355(18)
C63	N62	1.389(12)		C26	C27	1.30(3)
C63	C64	1.368(15)		C26	C25	1.37(3)
C63	C68	1.367(14)		C68	C67	1.309(17)
C3	C4	1.396(16)		C74	C73	1.390(17)
C3	C15	1.432(16)		C40	C39	1.377(17)
C37	C38	1.386(13)		C31	C32	1.418(17)
C20	C21	1.365(12)		C66	C67	1.36(2)
C53	C86	1.328(12)		C41	F0AA	1.227(14)
C60	C61	1.404(13)		C41	F7	1.237(14)
C7	C6	1.407(12)		C41	F9	1.239(15)
C86	C87	1.435(12)		F2	C0AA	1.180(14)
C47	C48	1.383(14)		C0AA	F4	1.295(17)
C72	C73	1.38(2)		C0AA	F5	1.200(16)

Table S8 Bond Angles for AC-mCF3

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C10	N9	C36	128.7(7)		C2	C1	C12	103.5(7)
C8	N9	C10	104.0(7)		C13	C1	C2	119.8(9)
C8	N9	C36	127.2(7)		C13	C1	C12	136.7(9)
C44	N45	C46	104.6(7)		C56	C61	C60	117.8(9)
C44	N55	C75	126.3(6)		C20	C21	C16	121.5(10)
C54	N55	C75	126.0(7)		C19	C18	C17	118.6(9)
C54	N55	C44	107.7(7)		C52	C51	C88	115.2(9)
C10	N11	C12	106.0(7)		C50	C51	C52	117.0(10)
C47	C52	C53	112.7(8)		C50	C51	C88	127.7(10)
C51	C52	C53	123.8(9)		C70	C69	N62	119.6(9)
C51	C52	C47	123.4(8)		C70	C69	C74	121.6(10)
N9	C10	C19	120.6(7)		C74	C69	N62	118.7(8)
N11	C10	N9	111.8(8)		C87	C88	C51	119.1(9)
N11	C10	C19	127.3(8)		C66	C65	C64	117.3(13)

C80	C75	N55	120.6(7)		N22	C29	C30	122.9(9)
C80	C75	C76	119.8(9)		C34	C29	N22	120.8(9)
C76	C75	N55	119.5(8)		C34	C29	C30	116.4(10)
C37	C36	N9	120.0(8)		C37	C38	C41	117.9(10)
C37	C36	C35	121.9(9)		C39	C38	C37	119.9(10)
C35	C36	N9	118.0(8)		C39	C38	C41	122.2(10)
N45	C44	N55	111.4(7)		C63	C64	C65	120.5(11)
N45	C44	C59	125.4(8)		C49	C50	C51	119.8(10)
N55	C44	C59	122.9(7)		C3	C4	C5	121.7(9)
C3	C2	C7	123.3(9)		C80	C79	C0AA	119.3(10)
C3	C2	C1	123.4(8)		C78	C79	C80	121.0(10)
C1	C2	C7	113.3(8)		C78	C79	C0AA	119.7(10)
N55	C54	C46	105.4(8)		C21	C16	N22	121.2(9)
N55	C54	C53	143.4(8)		C17	C16	N22	120.1(9)
C46	C54	C53	110.5(7)		C17	C16	C21	118.7(8)
C75	C80	C79	118.9(9)		C4	C5	C6	120.5(9)
N9	C8	C7	140.9(8)		C69	C70	C71	118.4(11)
C12	C8	N9	107.0(7)		C61	C56	N62	119.7(9)
C12	C8	C7	112.0(8)		C61	C56	C57	122.3(9)
C60	C59	C44	121.0(8)		C57	C56	N62	117.9(10)
C58	C59	C44	121.6(9)		C1	C13	C14	118.4(11)
C58	C59	C60	117.4(9)		C88	C87	C86	124.8(10)
C24	C23	N22	120.3(9)		C14	C15	C3	120.5(10)
C24	C23	C28	121.4(9)		C36	C35	C40	117.6(10)
C28	C23	N22	118.3(9)		C58	C57	C56	117.5(9)
C20	C19	C10	120.0(8)		C33	C34	C29	120.6(12)
C18	C19	C10	119.5(8)		C47	C48	C49	117.7(11)
C18	C19	C20	120.5(8)		C31	C30	C29	122.4(11)
C29	N22	C23	121.5(7)		C23	C24	C25	119.1(13)
C29	N22	C16	121.4(8)		C76	C77	C78	121.6(11)
C16	N22	C23	117.1(8)		C23	C28	C27	114.6(12)
N45	C46	C54	110.9(8)		C32	C33	C34	123.6(12)
N45	C46	C47	140.3(9)		C16	C17	C18	121.5(9)
C54	C46	C47	108.8(8)		C27	C26	C25	119.5(12)
N11	C12	C1	140.5(8)		C67	C68	C63	125.0(14)
C8	C12	N11	111.1(8)		C69	C74	C73	118.1(11)

C8	C12	C1	108.3(8)		C77	C76	C75	120.3(11)
C64	C63	N62	122.8(9)		C77	C78	C79	118.2(10)
C68	C63	N62	120.1(10)		C39	C40	C35	119.4(10)
C68	C63	C64	117.1(10)		C72	C73	C74	119.7(12)
C2	C3	C4	117.0(9)		C38	C39	C40	121.8(10)
C2	C3	C15	116.0(10)		C15	C14	C13	121.9(11)
C4	C3	C15	127.1(10)		C72	C71	C70	119.3(11)
C36	C37	C38	119.3(9)		C50	C49	C48	124.2(10)
C21	C20	C19	119.2(9)		C30	C31	C32	121.6(11)
C52	C53	C54	103.1(7)		C26	C27	C28	123.5(13)
C86	C53	C52	117.9(8)		C67	C66	C65	122.3(12)
C86	C53	C54	139.0(8)		C68	C67	C66	117.5(13)
C59	C60	C61	121.8(9)		C33	C32	C31	115.4(10)
C2	C7	C8	102.9(8)		C26	C25	C24	121.7(15)
C6	C7	C2	119.3(8)		F0AA	C41	C38	116.4(9)
C6	C7	C8	137.8(8)		F0AA	C41	F7	106.5(13)
C53	C86	C87	118.8(9)		F0AA	C41	F9	106.8(16)
C52	C47	C46	104.7(7)		F7	C41	C38	113.3(12)
C48	C47	C52	117.8(9)		F7	C41	F9	102.2(15)
C48	C47	C46	137.5(10)		F9	C41	C38	110.7(10)
C71	C72	C73	122.6(12)		F2	C0AA	C79	118.1(13)
C7	C6	C5	118.2(8)		F2	C0AA	F4	94.9(16)
C63	N62	C69	121.4(7)		F2	C0AA	F5	111.6(16)
C63	N62	C56	119.9(8)		F4	C0AA	C79	110.6(13)
C69	N62	C56	118.6(8)		F5	C0AA	C79	116.9(9)
C57	C58	C59	123.2(9)		F5	C0AA	F4	100.8(17)

Thermal properties:

The thermal properties of the AC-derivatives were examined by thermogravimetric analysis (TGA) under a nitrogen atmosphere at the scanning rate of 10 °C/min. Thermogravimetric grap of the dyes are shown in Fig. 2 and the corresponding data are listed in Table 2. All the dyes shown good thermal stability and the thermal decomposition temperatures (T_d) are in the range of 390-430 °C. Fluorene substituted AC-derivative (AC-Fl) display higher thermal decomposition

temperatures ~ 430 °C and the order of stability is AC-mCF3 < AC-pCF3 < AC-PT < AC-Ph < AC-Fl. This difference probably arises due to N1 functionilization of imidazole group with defferent substitutions. Thermal stability of the material is important for applications in organic electronic devices.

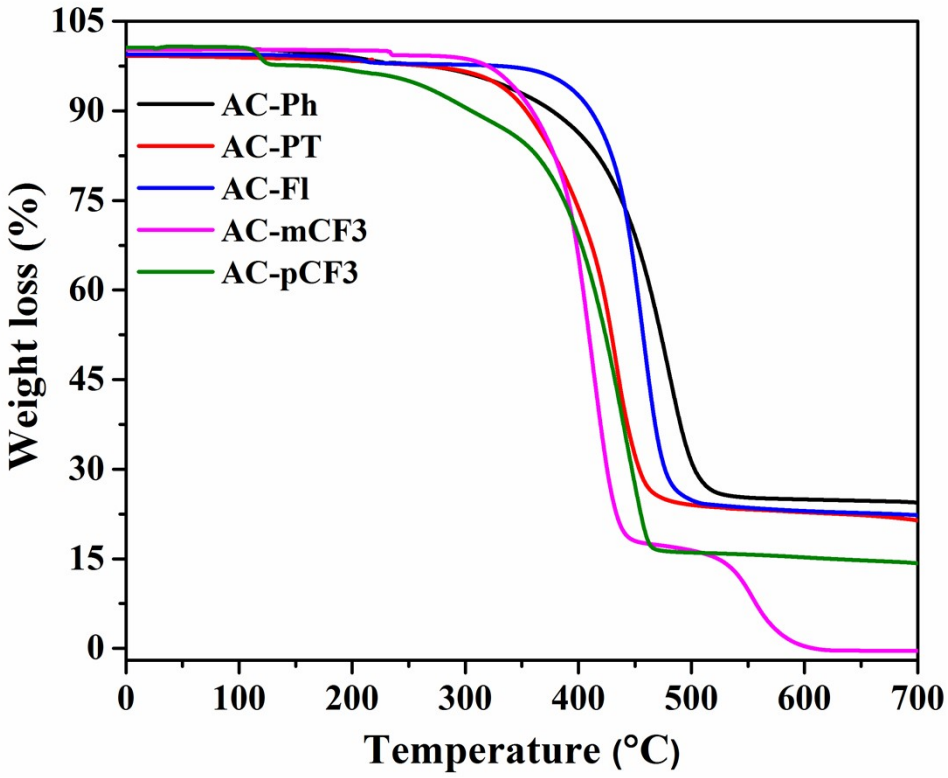

Fig. 2. Thermogravimetric curves AC-derivatives.

Table SI9. Computed vertical transitions and their oscillator strengths and configurations.[1,2]

Compound	State	f	λ_{max} nm	Energy (eV)	Configuration
AC-Ph					
Gas	Triplet	0	553.7	2.239	HOMO-2 → LUMO (20.65%) HOMO-1 → LUMO (48.94%) HOMO-1 →LUMO+1 (13.37%)
	S1	0.073	424.03	2.924	HOMO → LUMO (68.12%)
	S2	0.543	338.64	3.661	HOMO-1 → LUMO (43.48%) HOMO → LUMO+1 (44.20%)
DCM	Triplet	0	548.98	2.258	HOMO-2 → LUMO (16.89%) HOMO-1 → LUMO (54.89%)

					HOMO-1 →LUMO+1 (12.62%)
	S1	0.108	419.68	2.954	HOMO → LUMO (68.12%)
	S2	0.701	343.06	3.614	HOMO-1 → LUMO (43.48%) HOMO → LUMO+1 (44.20%)
AC-PT					
Gas	Triplet	0	624.95	1.983	HOMO-1 → LUMO (33.45%)
					HOMO → LUMO (60.35%)
	S1	0.071	491.40	2.523	HOMO-1 → LUMO (19.44%) HOMO → LUMO (67.21%)
DCM	Triplet	0	614.54	2.017	HOMO-1 → LUMO (36.10%) HOMO → LUMO (58.74%)
	S1	0.086	491.49	2.522	HOMO-1 → LUMO (20.49%)
					HOMO → LUMO (67.10%)
AC-Fl					
Gas	Triplet	0	627.89	1.974	HOMO → LUMO (60.73%)
	S1	0.0795	493.71	2.511	HOMO → LUMO (67.39%)
	S2	0.0718	408.57	3.034	HOMO-1 → LUMO (67.5%)
DCM	Triplet	0	617.99	2.006	HOMO → LUMO (59.25%)
	S1	0.096	494.10	2.509	HOMO → LUMO (67.34%)
	S2	0.297	394.35	3.144	HOMO-1 → LUMO (52.53%)
AC-mCF3					
Gas	Triplet	0	625.29	1.982	HOMO → LUMO (59.62%) HOMO-1 → LUMO (34.60%)
	S1	2.539	488.22	2.539	HOMO → LUMO (67.38%)
DCM	Triplet	0	617.73	2.007	HOMO → LUMO (59.25%)
	S1	0.0795	493.71	2.511	HOMO → LUMO (57.93%) HOMO-1 → LUMO (37.40%)
AC-pCF3					
Gas	Triplet	0	629.58	1.969	HOMO→LUMO (59.36%) HOMO-1→LUMO (34.95%)
	S1	0.091	494.10	2.509	HOMO → LUMO (67.45%)
	S2	0.112	403.12	3.075	HOMO-1 → LUMO (27.83%) HOMO → LUMO (11.42%) HOMO → LUMO+1 (62.48%)
DCM	Triplet	0	618.93	2.003	HOMO→LUMO (58.19%) HOMO-1→LUMO (36.99%)
	S1	0.107	493.54	2.512	HOMO → LUMO (67.38%)
	S2	0.212	395.37	3.135	HOMO-1 → LUMO (52.94%) HOMO → LUMO (17.34%) HOMO → LUMO+1 (41.75%)

SI10 Atomic coordinates of Acenaphthene derivatives

AC-Ph:

6	-5.748327	1.399372	0.405711
6	-4.952490	0.329404	0.050151
6	-5.591155	-0.888886	-0.356415
6	-6.978571	-1.053790	-0.416581
6	-7.771972	0.072245	-0.044295
6	-7.163827	1.248672	0.351567
1	-5.322817	2.345423	0.725249
6	-4.653375	-1.914542	-0.686431
6	-7.448103	-2.333827	-0.839062
1	-8.855971	0.001291	-0.071272
1	-7.782349	2.095797	0.633925
6	-6.547435	-3.331444	-1.160698
6	-5.136754	-3.139744	-1.089238
1	-8.516507	-2.520970	-0.904975
1	-6.921800	-4.299957	-1.479771
1	-4.467198	-3.953421	-1.350773
6	-3.532282	0.014781	-0.052784
6	-3.340881	-1.293545	-0.471027
6	-1.377035	-0.503415	-0.161427
7	-2.271797	0.533242	0.157440
7	-2.019477	-1.608962	-0.536619
6	-2.004423	1.814562	0.731547
6	-2.448784	2.966661	0.075259
6	-1.337202	1.911395	1.956304
6	-2.221892	4.218492	0.648480
1	-2.961138	2.873239	-0.876849
6	-1.103033	3.167214	2.514304
1	-1.009094	1.007950	2.458444
6	-1.545604	4.321771	1.865201
1	-2.567135	5.112418	0.138009
1	-0.582107	3.241989	3.463925
1	-1.365512	5.297133	2.306628
6	0.086068	-0.402552	-0.139743
6	0.795525	0.789967	-0.365432
6	0.830132	-1.581589	0.055365
6	2.185870	0.809627	-0.364340
1	0.263741	1.715988	-0.550101
6	2.217261	-1.569781	0.038244
1	0.294771	-2.513553	0.198432
6	2.921676	-0.369356	-0.162614
1	2.709869	1.744109	-0.532642
1	2.766805	-2.493771	0.181783
7	4.339305	-0.351807	-0.169411

6	5.039642	0.470571	-1.095509
6	4.622655	0.553415	-2.433685
6	6.161105	1.208648	-0.684687
6	5.309245	1.365275	-3.334123
1	3.761480	-0.020126	-2.759601
6	6.852058	2.003133	-1.597230
1	6.485459	1.152988	0.349026
6	6.429512	2.091422	-2.925026
1	7.718147	2.567004	-1.262544
6	5.068743	-1.160618	0.745583
6	6.206958	-1.865179	0.322045
6	4.664217	-1.263969	2.086200
6	6.925237	-2.647129	1.224152
1	6.521859	-1.794542	-0.713588
6	5.378532	-2.063278	2.976182
1	3.789717	-0.716861	2.421884
6	6.514901	-2.756126	2.554264
1	7.803201	-3.185802	0.879160
1	5.050912	-2.132366	4.009598
1	7.072765	-3.372619	3.252256
1	6.966256	2.716960	-3.631521
1	4.973284	1.417250	-4.365829

AC-PT:

6	-5.697144	1.086461	0.430798
6	-4.874323	0.041312	0.063414
6	-5.481924	-1.188014	-0.357382
6	-6.864682	-1.387261	-0.420346
6	-7.686491	-0.286056	-0.035521
6	-7.108398	0.900723	0.374227
1	-5.295188	2.038927	0.761491
6	-4.518214	-2.185417	-0.699236
6	-7.301517	-2.673669	-0.858383
1	-8.768341	-0.384178	-0.063910
1	-7.748332	1.728546	0.666064
6	-6.375688	-3.644100	-1.191501
6	-4.970311	-3.417529	-1.116981
1	-8.364814	-2.887061	-0.927179
1	-6.725225	-4.617914	-1.522436
1	-4.280297	-4.210757	-1.388008
6	-3.446533	-0.235423	-0.042881
6	-3.221990	-1.533628	-0.476344
6	-1.279373	-0.696377	-0.158543
7	-2.199973	0.312971	0.172450
7	-1.893145	-1.814174	-0.546172
6	-1.963571	1.595234	0.759849
6	-2.430590	2.740656	0.107299

6	-1.301037	1.696464	1.984419
6	-2.242800	4.008967	0.668092
1	-2.936036	2.633295	-0.847958
6	-1.097756	2.959132	2.539879
1	-0.951502	0.799891	2.483846
6	-1.563620	4.101943	1.891193
1	-0.577635	3.049778	3.488681
1	-1.399224	5.079108	2.337691
6	0.180792	-0.558792	-0.136423
6	0.859734	0.653746	-0.348811
6	0.954349	-1.720919	0.044776
6	2.249190	0.708113	-0.348802
1	0.304488	1.568119	-0.521790
6	2.340786	-1.674117	0.026828
1	0.442607	-2.667525	0.177771
6	3.014375	-0.454231	-0.161107
1	2.749830	1.657076	-0.507132
1	2.913512	-2.585571	0.159641
7	4.431512	-0.401230	-0.169006
6	5.110166	0.441468	-1.092520
6	4.685197	0.524862	-2.428239
6	6.218149	1.200081	-0.682088
6	5.350651	1.356608	-3.326347
1	3.834512	-0.064083	-2.754160
6	6.888254	2.014546	-1.592519
1	6.548549	1.144679	0.349722
6	6.457779	2.102918	-2.917765
1	7.744131	2.593911	-1.257984
6	5.180681	-1.197782	0.740679
6	6.334202	-1.873995	0.312384
6	4.779590	-1.317835	2.080944
6	7.070468	-2.644865	1.209535
1	6.646580	-1.790210	-0.723014
6	5.512340	-2.105949	2.965890
1	3.893113	-0.792553	2.420074
6	6.663626	-2.770728	2.539249
1	7.960024	-3.161770	0.860935
1	5.187100	-2.188365	3.999083
1	7.235667	-3.378622	3.233307
1	6.978238	2.743954	-3.622556
1	5.008689	1.408423	-4.356101
6	-2.765996	5.246341	-0.022590
1	-3.672258	5.619817	0.469294
1	-2.030050	6.056222	0.000580
1	-3.017131	5.046565	-1.067599

AC-Fl:

6	-5.525165	-0.869589	0.586670
6	-4.566747	-1.820256	0.299427
6	-5.000492	-3.150773	-0.015575
6	-6.342948	-3.541759	-0.046114
6	-7.307761	-2.535048	0.256905
6	-6.897671	-1.250087	0.559017
1	-5.258097	0.153751	0.830722
6	-3.910320	-4.028766	-0.300200
6	-6.599892	-4.904829	-0.382774
1	-8.366071	-2.781487	0.247801
1	-7.645086	-0.495111	0.785556
6	-5.550643	-5.760836	-0.659082
6	-4.189842	-5.338089	-0.623280
1	-7.624007	-5.266084	-0.422220
1	-5.764084	-6.794923	-0.914199
1	-3.398165	-6.046058	-0.848688
6	-3.114062	-1.909187	0.205150
6	-2.715958	-3.188402	-0.153165
6	-0.909120	-2.050547	-0.000252
7	-1.958194	-1.163511	0.300055
7	-1.365644	-3.272907	-0.277795
6	0.523309	-1.736786	0.020070
6	1.102957	-0.702190	0.776091
6	1.385650	-2.570952	-0.718374
6	2.480534	-0.505467	0.786238
1	0.483944	-0.064559	1.395844
6	2.758258	-2.373908	-0.715113
1	0.951230	-3.377870	-1.297455
6	3.331339	-1.335900	0.040107
1	2.906677	0.285861	1.393676
1	3.399239	-3.024390	-1.300553
7	4.736847	-1.142546	0.058562
6	5.275558	0.171251	-0.010352
6	4.758195	1.105887	-0.921441
6	6.338893	0.551142	0.824219
6	5.292515	2.391403	-0.989036
1	3.942803	0.815164	-1.575420
6	6.875233	1.834316	0.739679
1	6.740005	-0.165150	1.533347
6	6.354953	2.763976	-0.162796
1	7.697346	2.111231	1.393448
6	5.609557	-2.262236	0.141501
6	6.788750	-2.304209	-0.620025
6	5.306319	-3.342362	0.986228

6	7.646509	-3.398137	-0.527180
1	7.026243	-1.477502	-1.280922
6	6.161637	-4.439850	1.057418
1	4.400051	-3.315847	1.581679
6	7.338436	-4.474549	0.306895
1	8.554374	-3.413580	-1.123549
1	5.910730	-5.266637	1.715765
1	8.005554	-5.328570	0.370655
1	6.772878	3.764030	-0.223244
6	-1.933348	0.248475	0.528064
6	-1.429335	1.112968	-0.454294
6	-2.471597	0.750555	1.719529
6	-1.467387	2.481731	-0.224360
1	-1.025195	0.698196	-1.372187
6	-2.523958	2.127223	1.941790
1	-2.846483	0.054773	2.462998
6	-0.980673	3.613618	-1.128328
6	-2.022121	2.992171	0.967885
1	-2.947290	2.510067	2.865721
6	-1.358179	4.837982	-0.295776
6	-1.954794	4.457936	0.923030
6	-1.178632	6.184470	-0.594419
6	-2.371684	5.420371	1.844812
6	-1.597305	7.150055	0.328568
1	-0.719286	6.491134	-1.530601
6	-2.188175	6.770009	1.538128
1	-2.831578	5.129773	2.785308
1	-1.461854	8.203931	0.103781
1	-2.507123	7.531219	2.243995
6	0.557230	3.532369	-1.365144
1	0.760694	2.618076	-1.937306
1	0.838986	4.368620	-2.017999
6	-1.690113	3.604137	-2.512947
1	-1.373015	2.700219	-3.048917
1	-1.300344	4.449946	-3.093737
6	-3.219649	3.669484	-2.482707
1	-3.572144	4.582115	-1.993086
1	-3.620326	3.660505	-3.501248
1	-3.647802	2.815187	-1.949882
6	1.427220	3.551238	-0.105576
1	2.485754	3.469704	-0.369339
1	1.291628	4.476818	0.461315
1	1.188989	2.712778	0.555156
1	4.886875	3.099123	-1.706627

AC-mCF3:

6	-5.447149	0.173031	0.307966
6	-4.523842	-0.811144	0.013425
6	-5.009277	-2.113584	-0.342602
6	-6.366644	-2.444980	-0.407021
6	-7.292797	-1.406642	-0.092448
6	-6.833478	-0.149112	0.250298
1	-5.151769	1.183300	0.572765
6	-3.954687	-3.033761	-0.625143
6	-6.676311	-3.787840	-0.777974
1	-8.360236	-1.607236	-0.124474
1	-7.551063	0.631694	0.484645
6	-5.660780	-4.684292	-1.052271
6	-4.284148	-4.322965	-0.980731
1	-7.714367	-4.102373	-0.843358
1	-5.914353	-5.702379	-1.333338
1	-3.519467	-5.059999	-1.206048
6	-3.073699	-0.962480	-0.067080
6	-2.727285	-2.254737	-0.429338
6	-0.868072	-1.238015	-0.135429
7	-1.879204	-0.296636	0.137095
7	-1.376478	-2.420212	-0.472089
6	-1.772546	1.005653	0.702268
6	-2.493545	2.052357	0.128672
6	-1.008074	1.228251	1.854821
6	-2.474051	3.314702	0.726842
1	-3.073157	1.878037	-0.771054
6	-0.967836	2.499770	2.420140
1	-0.458892	0.406067	2.298771
6	-1.707715	3.547511	1.868066
1	-0.371711	2.671211	3.310597
1	-1.694643	4.532554	2.319244
6	0.572099	-0.961993	-0.119706
6	1.131357	0.283047	-0.456082
6	1.452485	-2.017988	0.180473
6	2.508216	0.474548	-0.460380
1	0.490013	1.114048	-0.727552
6	2.827810	-1.836693	0.160416
1	1.034879	-2.992489	0.408263
6	3.381894	-0.581790	-0.151540
1	2.914654	1.446318	-0.717783
1	3.485086	-2.669023	0.386749
7	4.784793	-0.390296	-0.163635
6	5.384877	0.448703	-1.145503
6	4.989422	0.369047	-2.490030
6	6.385872	1.362657	-0.781349

6	5.578176	1.195899	-3.444627
1	4.222470	-0.341849	-2.778741
6	6.981725	2.172190	-1.746350
1	6.691978	1.430829	0.257196
6	6.579699	2.098506	-3.081388
1	7.755440	2.874031	-1.448496
6	5.607403	-1.038898	0.799561
6	6.821870	-1.628309	0.414603
6	5.221375	-1.092996	2.148344
6	7.632058	-2.250516	1.362098
1	7.123201	-1.593731	-0.626872
6	6.029562	-1.733624	3.085170
1	4.287975	-0.632422	2.454035
6	7.240759	-2.312291	2.700974
1	8.568447	-2.701863	1.046912
1	5.715651	-1.766746	4.124584
1	7.871152	-2.804399	3.435034
1	7.041389	2.735717	-3.829248
1	5.261137	1.121709	-4.480877
6	-3.344371	4.392419	0.138965
9	-3.176869	4.497160	-1.197676
9	-4.657589	4.119293	0.344121
9	-3.098840	5.603231	0.678309

AC-pCF3:

6	-5.657033	0.403911	-0.151544
6	-4.788496	-0.668879	-0.167179
6	-5.342999	-1.991566	-0.195055
6	-6.716133	-2.256820	-0.212751
6	-7.585043	-1.125359	-0.199376
6	-7.058960	0.152381	-0.167778
1	-5.300170	1.428584	-0.123411
6	-4.338542	-3.006275	-0.193306
6	-7.096957	-3.632153	-0.234576
1	-8.661720	-1.271219	-0.211132
1	-7.733872	1.003262	-0.154335
6	-6.130526	-4.620117	-0.234426
6	-4.736412	-4.324701	-0.212593
1	-8.150165	-3.899169	-0.249366
1	-6.438106	-5.661722	-0.250303
1	-4.012499	-5.133792	-0.211477
6	-3.349320	-0.908588	-0.161005
6	-3.071624	-2.266779	-0.162463
6	-1.162866	-1.303955	-0.077951
7	-2.123604	-0.274004	-0.097181

7	-1.732681	-2.505745	-0.112615
6	-1.941409	1.128226	0.074908
6	-2.497164	2.012541	-0.856303
6	-1.241967	1.620705	1.181558
6	-2.355242	3.386264	-0.678465
1	-3.026986	1.618229	-1.716838
6	-1.092100	2.994106	1.348608
1	-0.820703	0.927808	1.900683
6	-1.649503	3.879115	0.421951
1	-2.776380	4.074465	-1.403008
1	-0.544692	3.379946	2.201150
6	0.290771	-1.109074	-0.079644
6	0.934717	-0.021922	-0.695553
6	1.097143	-2.102304	0.506969
6	2.320686	0.084937	-0.698435
1	0.354525	0.749412	-1.189115
6	2.481207	-2.009634	0.490829
1	0.614777	-2.963185	0.956459
6	3.120030	-0.907245	-0.105915
1	2.792244	0.937477	-1.174397
1	3.079125	-2.794392	0.941042
7	4.531801	-0.805024	-0.118681
6	5.201978	-0.270534	-1.255774
6	4.823383	-0.652371	-2.552533
6	6.256788	0.641132	-1.093497
6	5.481417	-0.121997	-3.660310
1	4.014831	-1.363606	-2.684019
6	6.920978	1.151627	-2.206973
1	6.550605	0.942763	-0.093687
6	6.535765	0.778619	-3.496084
1	5.176506	-0.427959	-4.656959
1	7.735567	1.855858	-2.064124
6	5.294959	-1.245089	0.999305
6	6.468312	-1.991355	0.808101
6	4.890430	-0.933879	2.307061
6	7.221334	-2.408474	1.903681
1	6.783114	-2.239082	-0.199998
6	5.640399	-1.371098	3.396941
1	3.988843	-0.350444	2.460641
6	6.811515	-2.106357	3.203758
1	8.126656	-2.985464	1.738259
1	5.313324	-1.121871	4.402354
1	7.397022	-2.439368	4.055068
1	7.050919	1.183859	-4.361460
6	-1.542971	5.364818	0.637690
9	-2.608394	5.847039	1.319203

9	-0.440991	5.692090	1.346987
9	-1.490689	6.037746	-0.533292

References:

1. M. J. Frisch, et. al., Gaussian, Inc., Wallingford CT, 2009.
2. (a) R. Bauernschmitt and R. Ahlrichs, Chem. Phys. Lett., 1996, 256, 454–464; (b) G. Scalmani, M. J. Frisch, B. Mennucci, J. Tomasi, R. Cammi and V. Barone, J. Chem. Phys., 2006, 124, 094107.