Electronic Supplementary Information

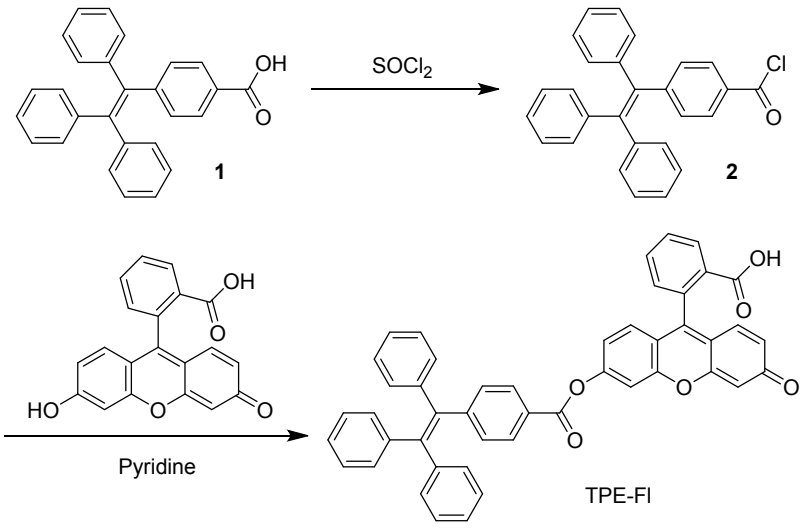
A mechanistic study of AIE processes of TPE luminogens: intramolecular rotation vs. configurational isomerization

Zhiyong Yang,[a,b] Wei Qin,[b] Nelson L. C. Leung,[b] Mathieu Arseneault,[b] Jacky W. Y. Lam,[a,b] Guodong Liang,[b] Herman H. Y. Sung,[b] Ian D. Williams,[b] and Ben Zhong Tang*[,a,b,c]

[a]HKUST Shenzhen Research Institute, Hi-tech Park, Nanshan, Shenzhen 518057, China, E-mail: tangbenz@ust.hk

[b]Department of Chemistry, Division of Biomedical Engineering, Institute for Advanced Study, Division of Life Science, State Key Laboratory of Molecular Neuroscience, Institute of Molecular Functional Materials, The Hong Kong University of Science & Technology (HKUST), Clear Water Bay, Kowloon, Hong Kong, China

[c]Guangdong Innovative Research Team, SCUT–HKUST Joint Research Laboratory, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology (SCUT), Guangzhou 510640, China



Scheme S1. Synthetic route to TPE-Fl.

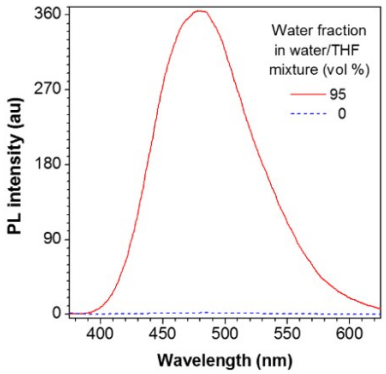


Fig. S1. PL spectra of (*E*)-TPE-FM in pure THF and a THF/water mixture with 95% water fraction. Excitation wavelength (λ_{ex}): 312 nm; luminogen concentration (*c*): ~10 μM. The dilute solution in THF is non-emissive but the nanoaggregates in an aqueous mixture containing a large fraction of water (f_w = 95 vol %) are highly luminescent, indicating distinct AIE activity of (*E*)-TPE-FM.

Table S1. Crystal data and structure refinement for (*E*)-TPE-FM.

Identification code	(*E*)-TPE-FM	
Empirical formula	C28 H22 F2 O2	
Formula weight	428.46	
Temperature	173.00(14) K	
Wavelength	1.5418 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 9.9507(9) Å	α= 90°.
	b = 14.1404(14) Å	β= 90°.
	c = 15.7474(11) Å	γ = 90°.
Volume	2215.8(3) $Å^3$	
Z	4	
Density (calculated)	1.284 Mg/m^3	
Absorption coefficient	0.747 mm^{-1}	
F(000)	896	
Crystal size	0.3 x 0.23 x 0.17 mm^3	
Theta range for data collection	4.20 to 67.49°.	
Index ranges	-11<=h<=9, -16<=k<=15, -18<=l<=18	
Reflections collected	12591	
Independent reflections	3951 [R(int) = 0.0407]	
Completeness to theta = 66.50°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.82430	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3951 / 0 / 291	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.1006	
R indices (all data)	R1 = 0.0465, wR2 = 0.1059	
Absolute structure parameter	0.01(17)	
Largest diff. peak and hole	0.234 and -0.160 $e.Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for (*E*)-TPE-FM single crystal structure.

F(1)-C(14)	1.370(2)	C(1)-C(2)-C(41)	122.31(18)
F(2)-C(24)	1.362(3)	C(21)-C(2)-C(41)	114.90(17)
O(1)-C(34)	1.367(2)	C(12)-C(11)-C(1)	122.22(19)
O(1)-C(37)	1.439(3)	C(12)-C(11)-C(16)	118.29(19)
O(2)-C(44)	1.373(3)	C(16)-C(11)-C(1)	119.45(18)
O(2)-C(47)	1.433(4)	C(13)-C(12)-C(11)	120.6(2)
C(1)-C(2)	1.360(3)	C(14)-C(13)-C(12)	118.78(19)
C(1)-C(11)	1.491(3)	F(1)-C(14)-C(13)	118.82(19)
C(1)-C(31)	1.497(3)	C(15)-C(14)-F(1)	118.7(2)
C(2)-C(21)	1.492(3)	C(15)-C(14)-C(13)	122.5(2)
C(2)-C(41)	1.493(3)	C(14)-C(15)-C(16)	118.1(2)
C(11)-C(12)	1.391(3)	C(15)-C(16)-C(11)	121.77(19)
C(11)-C(16)	1.392(3)	C(22)-C(21)-C(2)	120.65(19)
C(12)-C(13)	1.389(3)	C(26)-C(21)-C(2)	121.01(19)
C(13)-C(14)	1.378(3)	C(26)-C(21)-C(22)	118.3(2)
C(14)-C(15)	1.366(3)	C(23)-C(22)-C(21)	121.0(2)
C(15)-C(16)	1.384(3)	C(24)-C(23)-C(22)	118.9(2)
C(21)-C(22)	1.392(3)	F(2)-C(24)-C(23)	118.7(2)
C(21)-C(26)	1.392(3)	F(2)-C(24)-C(25)	118.9(2)
C(22)-C(23)	1.383(3)	C(23)-C(24)-C(25)	122.3(2)
C(23)-C(24)	1.370(3)	C(24)-C(25)-C(26)	118.0(2)
C(24)-C(25)	1.380(3)	C(25)-C(26)-C(21)	121.5(2)
C(25)-C(26)	1.388(3)	C(32)-C(31)-C(1)	120.19(16)
C(31)-C(32)	1.387(3)	C(32)-C(31)-C(36)	117.95(17)
C(31)-C(36)	1.400(3)	C(36)-C(31)-C(1)	121.85(17)
C(32)-C(33)	1.395(3)	C(31)-C(32)-C(33)	121.73(17)
C(33)-C(34)	1.386(3)	C(34)-C(33)-C(32)	119.12(18)
C(34)-C(35)	1.387(3)	O(1)-C(34)-C(33)	123.88(18)
C(35)-C(36)	1.386(3)	O(1)-C(34)-C(35)	115.94(17)
C(41)-C(42)	1.399(3)	C(33)-C(34)-C(35)	120.17(18)
C(41)-C(46)	1.377(3)	C(36)-C(35)-C(34)	120.05(19)
C(42)-C(43)	1.380(3)	C(35)-C(36)-C(31)	120.92(18)
C(43)-C(44)	1.387(4)	C(42)-C(41)-C(2)	122.47(19)
C(44)-C(45)	1.371(4)	C(46)-C(41)-C(2)	119.77(19)
C(45)-C(46)	1.395(3)	C(46)-C(41)-C(42)	117.75(18)
		C(43)-C(42)-C(41)	120.4(2)
C(34)-O(1)-C(37)	117.61(17)	C(42)-C(43)-C(44)	120.5(2)
C(44)-O(2)-C(47)	116.9(2)	O(2)-C(44)-C(43)	115.6(2)
C(2)-C(1)-C(11)	123.06(17)	C(45)-C(44)-O(2)	124.2(2)
C(2)-C(1)-C(31)	122.37(18)	C(45)-C(44)-C(43)	120.13(19)
C(11)-C(1)-C(31)	114.58(16)	C(44)-C(45)-C(46)	118.8(2)
C(1)-C(2)-C(21)	122.74(17)	C(41)-C(46)-C(45)	122.3(2)

Table S3. Crystal data and structure refinement for (*Z*)-TPE–FM.

Identification code	(*Z*)-TPE-FM	
Empirical formula	C28 H22 F2 O2	
Formula weight	428.46	
Temperature	173.00(14) K	
Wavelength	0.7107 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.9658(5) Å	α= 90°.
	b = 10.8639(5) Å	β= 102.330(5)°.
	c = 10.6141(5) Å	γ = 90°.
Volume	1122.65(9) $Å^3$	
Z	2	
Density (calculated)	1.267 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
F(000)	448	
Crystal size	0.38 x 0.28 x 0.05 mm^3	
Theta range for data collection	3.16 to 25.50°.	
Index ranges	-12<=h<=12, -8<=k<=13, -11<=l<=12	
Reflections collected	5546	
Independent reflections	2867 [R(int) = 0.0351]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.99417	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2867 / 1 / 291	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0557, wR2 = 0.0975	
R indices (all data)	R1 = 0.0716, wR2 = 0.1038	
Largest diff. peak and hole	0.172 and -0.170 $e.Å^{-3}$	

Table S4. Bond lengths [Å] and angles [°] for (*Z*)-TPE–FM single crystal structure.

F(1)-C(34)	1.366(4)	C(1)-C(2)-C(41)	122.3(3)
F(2)-C(44)	1.366(4)	C(21)-C(2)-C(41)	113.0(3)
O(1)-C(10)	1.430(5)	C(12)-C(11)-C(1)	123.3(3)
O(1)-C(14)	1.368(4)	C(16)-C(11)-C(1)	119.9(3)
O(2)-C(20)	1.424(5)	C(16)-C(11)-C(12)	116.8(3)
O(2)-C(24)	1.369(4)	C(13)-C(12)-C(11)	121.5(3)
C(1)-C(2)	1.343(4)	C(14)-C(13)-C(12)	120.1(3)
C(1)-C(11)	1.495(5)	O(1)-C(14)-C(13)	125.8(4)
C(1)-C(31)	1.495(5)	O(1)-C(14)-C(15)	115.0(3)
C(2)-C(21)	1.493(5)	C(13)-C(14)-C(15)	119.1(3)
C(2)-C(41)	1.500(5)	C(16)-C(15)-C(14)	120.4(4)
C(11)-C(12)	1.398(5)	C(15)-C(16)-C(11)	122.0(3)
C(11)-C(16)	1.398(5)	C(22)-C(21)-C(2)	122.8(3)
C(12)-C(13)	1.392(5)	C(26)-C(21)-C(2)	119.6(3)
C(13)-C(14)	1.379(5)	C(26)-C(21)-C(22)	117.6(3)
C(14)-C(15)	1.391(5)	C(23)-C(22)-C(21)	120.6(3)
C(15)-C(16)	1.371(5)	C(22)-C(23)-C(24)	120.8(4)
C(21)-C(22)	1.407(5)	O(2)-C(24)-C(23)	116.2(3)
C(21)-C(26)	1.383(5)	O(2)-C(24)-C(25)	124.3(3)
C(22)-C(23)	1.373(5)	C(25)-C(24)-C(23)	119.5(3)
C(23)-C(24)	1.386(5)	C(24)-C(25)-C(26)	119.5(4)
C(24)-C(25)	1.380(5)	C(21)-C(26)-C(25)	121.9(4)
C(25)-C(26)	1.389(5)	C(32)-C(31)-C(1)	121.0(3)
C(31)-C(32)	1.392(5)	C(32)-C(31)-C(36)	117.6(3)
C(31)-C(36)	1.394(5)	C(36)-C(31)-C(1)	121.4(3)
C(32)-C(33)	1.387(5)	C(33)-C(32)-C(31)	121.6(3)
C(33)-C(34)	1.363(5)	C(34)-C(33)-C(32)	118.1(4)
C(34)-C(35)	1.363(5)	C(33)-C(34)-F(1)	118.6(4)
C(35)-C(36)	1.389(5)	C(33)-C(34)-C(35)	123.2(4)
C(41)-C(42)	1.390(5)	C(35)-C(34)-F(1)	118.2(3)
C(41)-C(46)	1.395(5)	C(34)-C(35)-C(36)	118.2(3)
C(42)-C(43)	1.384(5)	C(35)-C(36)-C(31)	121.3(4)
C(43)-C(44)	1.369(5)	C(42)-C(41)-C(2)	122.3(3)
C(44)-C(45)	1.364(5)	C(42)-C(41)-C(46)	118.5(3)
C(45)-C(46)	1.384(5)	C(46)-C(41)-C(2)	119.1(3)
		C(43)-C(42)-C(41)	121.1(3)
C(14)-O(1)-C(10)	117.3(3)	C(44)-C(43)-C(42)	118.2(3)
C(24)-O(2)-C(20)	117.2(3)	F(2)-C(44)-C(43)	118.0(3)
C(2)-C(1)-C(11)	124.0(3)	C(45)-C(44)-F(2)	119.1(3)
C(2)-C(1)-C(31)	121.3(3)	C(45)-C(44)-C(43)	122.9(3)
C(11)-C(1)-C(31)	114.6(3)	C(44)-C(45)-C(46)	118.7(3)
C(1)-C(2)-C(21)	124.7(3)	C(45)-C(46)-C(41)	120.6(4)