

Supporting information

Construction and Function of High Efficient Supramolecular Luminescent System

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Table S1. Summary of intermolecular interactions in C1 crystal.

Orientation of interaction	$d(\text{Å})$	$A(\text{deg})$
I π - π	3.65	
II π - π	3.67	
III C-H...F	2.72	120.05
IV C-H...F	2.65	121.98
V C-H...F	2.85	125.89
VI C-H...F	2.81	128.10
VII C-I...N	3.00	174.27

Table S2. Summary of intermolecular interactions in C2 crystal.

Orientation of interaction	$d(\text{Å})$	$A(\text{deg})$
I C-H...F	2.49	157.86
II C-H...F	2.92	143.79
III C-H...F	2.79	127.68
IV C-I...N	2.84	173.03
V C-H...I	2.85	165.67
VI C-H... π	2.77	147.84
VII C-H... π	2.78	147.84

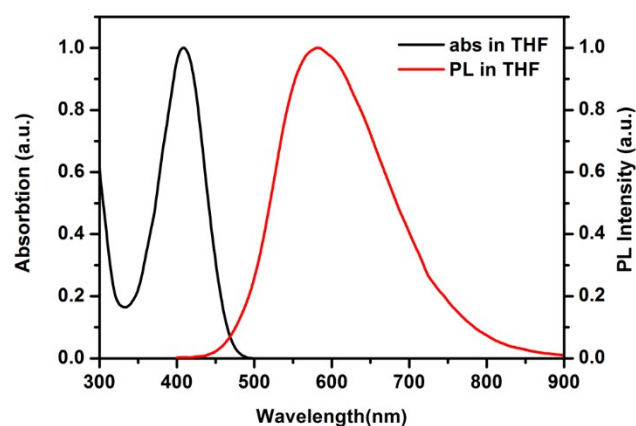


Figure S1. Absorption and PL spectra of BP4VA in THF.

Table S3. Crystal data and structure refinements of C1 and C2 crystals.

	C1	C2
Sum formula	C ₂₀ H ₁₀ F ₃ I ₃ N	C ₄₀ H ₂₀ F ₆ I ₆ N ₂
formula wt	701.99	1403.98
<i>T</i> , K	293(2) K	293(2) K
crystal system	monoclinic	triclinic
space group	P 21/c	P -1
<i>a</i> , Å	8.6902(17)	5.1420(10)
<i>b</i> , Å	13.870(3)	12.724(3)
<i>c</i> , Å	17.377(4)	16.436(3)
α ,deg	90.00	109.15(3)
β ,deg	102.80(3)	96.00(3)
γ ,deg	90.00	93.79(3)
<i>V</i> ,Å ³	2042.5(7)	1004.5(4)
<i>Z</i>	4	1
F(000)	1292	646
density, Mg/m ³	2.283	2.321
Absorption coefficient, mm ⁻¹	4.622	4.699
θ range, deg	3.00 - 27.48	3.21 - 27.48
no. of reflcns collected	18046	9853
no. of unique reflcns	4648	4537
<i>R</i> (int)	0.0363	0.0224
Good-of-fit on F ²	1.035	1.065
<i>R</i> 1 [<i>I</i> > 2 σ (<i>I</i>)]	0.0462	0.0354
<i>wR</i> 2 [<i>I</i> > 2 σ (<i>I</i>)]	0.1237	0.0787
<i>R</i> 1 (all data)	0.0646	0.0447
<i>wR</i> 2 (all data)	0.1414	0.0815