Electronic Supplementary Information

Color-tunable Single Molecule White Light Emitter with High Luminescent Efficiency and Ultra-long Room Temperature Phosphorescence

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Materials and Methods

General Information. All of the chemicals were obtained from commercial sources and used without further purification. The UV-Vis absorption spectra were measured with a Perkin Elmer Lambda 900 Spectrometer. Powder X-ray diffraction (PXRD) measurements were performed on a Bruker D8 Avance X-ray powder diffractometer with the Cu Kα (1.5418 Å) source. NMR measurements were carried out on a Bruker DMX500 spectrometer using tetramethylsilane (TMS) as an internal standard. The elemental analysis was determined using a Vario EL III CHNOS elemental analyzer. Fluorescence spectra for the solid samples were recorded at room temperature on an Edinburgh Model FS5 instrument, and emission quantum yields were recorded on the integrating sphere SC-30. The calibration of quantum yields for the powdery (crystalline) samples is conducted with a matched integrating sphere. At first, the emission of the blank integrating sphere was measured, and then the emission of the integrating sphere containing the powdery (crystalline) samples was measured. Finally, the quantum yields could be obtained according to the calibration. Luminescence lifetimes (τ)

were examined using an Edinburgh Model FLS920 phosphorimeter. The power of UV lamp used for photographs is 16 W.

X-ray Crystallography. Crystallographic data were collected on a multiwire proportional diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) using phi and omega scans. The intensity data were integrated by using the SAINT program.[1] An empirical absorption correction was applied using the SADABS program.[2] The structures were solved by direct method and the non-hydrogen atoms were located from the trial structures and then refined anisotropically with SHELXTL using full-matrix least-squares procedures based on F^2 values.[3] The positions of the non-hydrogen atoms were refined with anisotropic displacement factors.

Theoretical calculations

All calculations were performed using the Gaussian 09 series of programs.[4] The commonly used Becke's three parameter exchange functional combined with the LYP4 correlation functional (B3LYP) was used for the calculations. The geometries of **P1**, **P2** and **P3** for calculations were taken from the X-ray diffraction data and no further geometry optimization was conducted in order to maintain the specific molecular configuration and corresponding intermolecular locations. The optimized excited-state geometries of **P1**, **P2** and **P3** were calculated by time-dependent density functional theory (TD-DFT) at the B3LYP/6-31G(d) level.

Synthesis
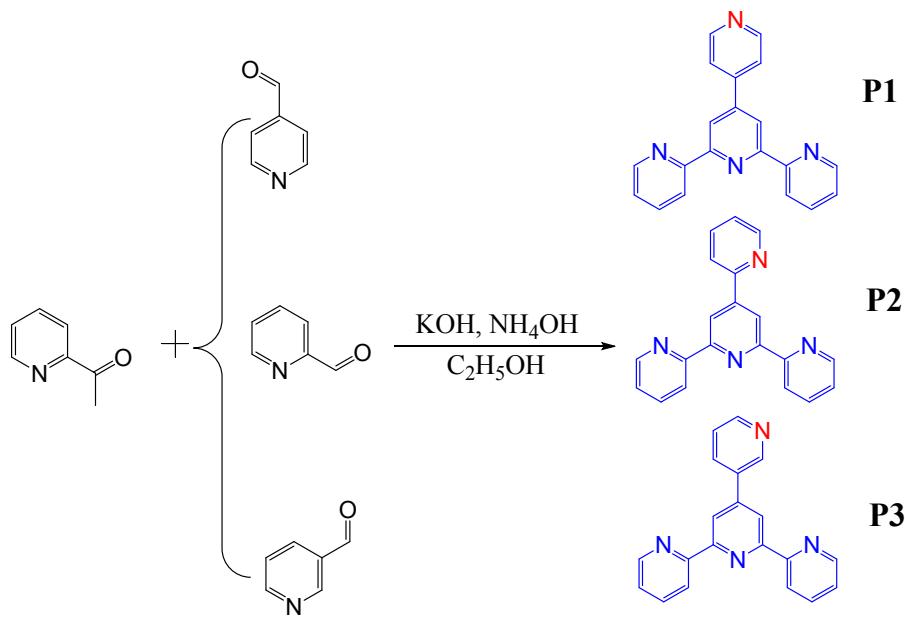
Scheme 1 The synthetic route of **P1**, **P2** and **P3**

4'-(Pyridin-4-yl)-2,2':6',2''-terpyridine (**P1**): In a 250 mL round bottom flask, 2-Acetylpyridine (2.62 g, 21.6 mmol), NH_3 (aqueous) (15 mL) and KOH (2.3 g, 41.0 mmol) were respectively added to a solution of 4-pyridinecarboxadehyde (1.14 g, 10.6 mmol) in EtOH (100 mL). The solution was refluxed for 24 h. After cooling down to the room temperature, the solution was evaporated to dryness under reduced pressure to give the crude product. The crude product was washed by cool methanol twice and then recrystallized by ethanol. A pure white solid was obtained. ^{1}H NMR: (400 MHz, DCM) δ 8.80 (6 H, m), 8.70 (2 H, d), 8.07 (2 H, m), 7.96 (2 H, d) and 7.56 (2 H, d). ^{13}C NMR: (400 MHz, DCM) δ: 156.4, 155.7, 150.5, 149.2, 147.4, 146.1, 137.0, 124.2, 121.8, 121.4, 118.7. Elemental Analysis: C, 77.40; H, 4.55; N, 18.05, found: C, 77.60; H, 4.75; N, 17.65 MS: m/z Calcd. for $C_{20}H_{14}N_4$: 310.12, found $[M+Na]^+$ 333.05.

4'-(Pyridin-2-yl)-2,2':6',2''-terpyridine (**P2**): In a 250 mL round bottom flask, 2-acetylpyridine (2.62 g, 21.6 mmol), NH_3 (aqueous) (15 mL) and KOH (2.3g, 41.0 mmol) were respectively added to a solution of 4-pyridinecarboxadehyde (1.14 g, 10.6 mmol) in EtOH

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(100 mL). The solution was refluxed for 24 h. After cooling down to the room temperature, the solution was evaporated to dryness under reduced pressure to give the crude product. The crude product was washed by cool methanol twice and then recrystallized by ethanol. A pure white solid was obtained. ^{1}H NMR: (400 MHz, DCM) δ 9.15 (2 H, s), 8.85 (1 H, d), 8.78 (2 H, d), 8.71 (2 H, d), 8.13 (1 H, d), 7.91 (3 H, m) and 7.40 (3 H, m). ^{13}C NMR: (400 MHz, DCM) δ: 156.1, 155.1, 150.0, 149.2, 148.7, 136.9, 123.8, 121.3, 118.7. Elemental Analysis: C, 77.40; H, 4.55; N, 18.05, found: C, 77.55; H, 4.68; N, 17.77 MS: m/z Calcd. for $C_{20}H_{14}N_4$: 310.12, found $[M+Na]^+$ 333.05.

4'-(Pyridin-3-yl)-2,2':6',2''-terpyridine (P3): In a 250 mL round bottom flask, 2-acetylpyridine (2.62 g, 21.6 mmol), NH_3 (aqueous) (15 mL) and KOH (2.3g, 41.0 mmol) were respectively added to a solution of 4-pyridinecarboxadehyde (1.14 g, 10.6 mmol) in EtOH (100 mL). The solution was refluxed for 24 h. After cooling down to the room temperature, the solution was evaporated to dryness under reduced pressure to give the crude product. The crude product was washed by cool methanol twice and then recrystallized by ethanol. A pure white solid was obtained. ^{1}H NMR: (400 MHz, DCM) δ 9.16 (1 H, s), 8.10 (7 H, m), 8.22 (1 H, d), 7.94 (2 H, m), 7.49 (1 H, m), 7.42 (2 H, m). ^{13}C NMR: (400 MHz, DCM) δ: 156.2, 155.8, 150.1, 149.2, 148.4, 147.2, 137.0, 134.7, 134.3, 124.1, 123.7, 121.4, 118.8. Elemental Analysis: C, 77.40; H, 4.55; N, 18.05, found: C, 77.45; H, 4.80; N, 17.75 MS: m/z Calcd. for $C_{20}H_{14}N_4$: 310.12, found $[M+Na]^+$ 333.05.

Table S1. Single crystal data and refinement results of **P1**, **P2** and **P3**

	P1	**P2**	**P3**
formula	$C_{20}H_{14}N_4$	$C_{20}H_{14}N_4$	$C_{20}H_{14}N_4$
fw (g/mol)	310.35	310.35	310.35
color	white	light yellow	white
T (K)	100	300	100
Crystal system	orthorhombic	monoclinic	orthorhombic
Space group	$P\ bcn$	$P\ 1\ 21/c1$	$P\ bcn$
Z	4	4	4
a [Å]	10.9973(5)	8.3024(6)	16.4088(8)
b [Å]	11.3955(5)	16.0020(10)	11.2036(5)
c [Å]	12.0267(5)	11.5519(8)	7.9268(4)
α [°]	90	90	90
β [°]	90	94.915(6)	90
γ [°]	90	90	90
V [Å^3]	1507.18(11)	1529.08(18)	1457.24(12)
Density (calcd.)[g·cm^{-3}]	1.368	1.348	1.415
μ [mm^{-1}]	0.084	0.083	0.087
θ-range [°]	2.565 to 30.822	2.168 to 30.538	2.197 to 30.303
Index range	-15≤h≤13	-10≤h≤10	-20≤h≤20
	-15≤k≤13	-19≤k≤19	-12≤k≤15
	-16≤l≤11	-13≤l≤13	-10≤l≤9
Reflections collected	6735	17756	8436
Unique reflections	3659	5404	4080
Observed reflections ($I > 2\sigma(I)$)	1877	2647	1815
parameters refined	111	199	217
Final R_1 values ($I > 2\sigma(I)$)	0.0395	0.0975	0.0371
Final w$R(F^2)$ values (I $> 2\sigma(I)$)	0.0999	0.2125	0.0948
Final R_2 values (all data)	0.0472	0.1563	0.0465
Final w$R(F^2)$ values (all data)	0.1043	0.2338	0.0993
GOOF (goodness of fit)	1.097	1.018	1.043
CCDC number	2007820	2007821	2007822

$R_1 = \Sigma(||F_0| - |F_c||)/\Sigma|F_0|$;

$wR_2 = [\Sigma w(|F_0^2| - |F_c^2|)^2/\Sigma w|F_0^2|^2]^{1/2}$
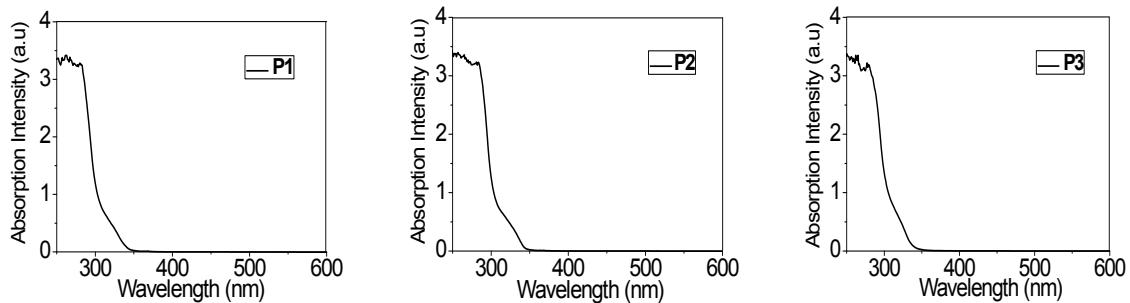
Fig. S1 UV-vis absorption spectra of **P1**, **P2** and **P3** (CH$_2$Cl$_2$, 2x10^{-5} mol/L).
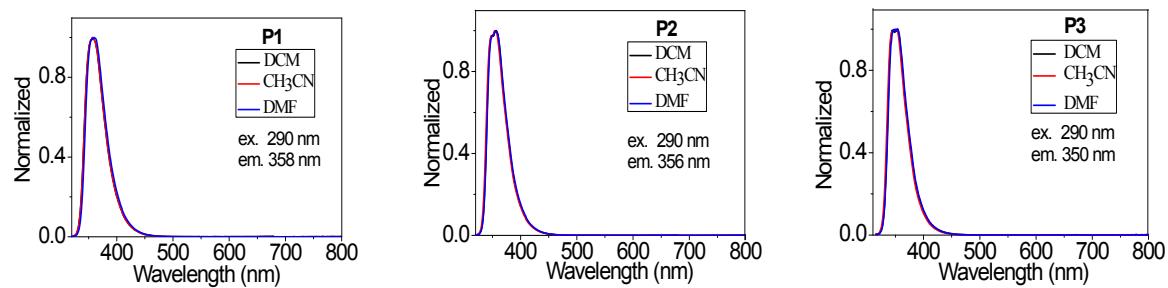
Fig. S2 Photoluminescence spectra of **P1**, **P2** and **P3** in the dilute solutions of different solvents (2x10^{-5} mol/L). (excitation wavelength = ex, emission wavelength = em).
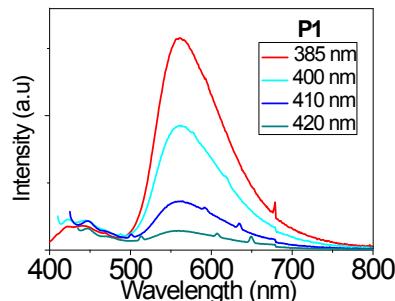
Fig. S3 The excitation wavelength-dependent photoluminescence spectra for **P1** (Excitation wavelength is ranging from 385 nm to 420 nm). When the excitation wavelength is increased to 420 nm, the emission intensity obviously decays.
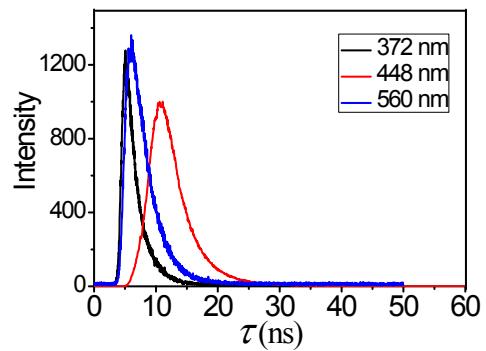
Fig. S4 The time-resolved photoluminescence decay curves of **P1** at three emission peaks 372 nm (λ_{ex} = 340 nm, 2.10 ns), 448 nm (λ_{ex} = 400 nm, 3.82 ns) and 560 nm (λ_{ex} = 340 nm, 2.77 ns).
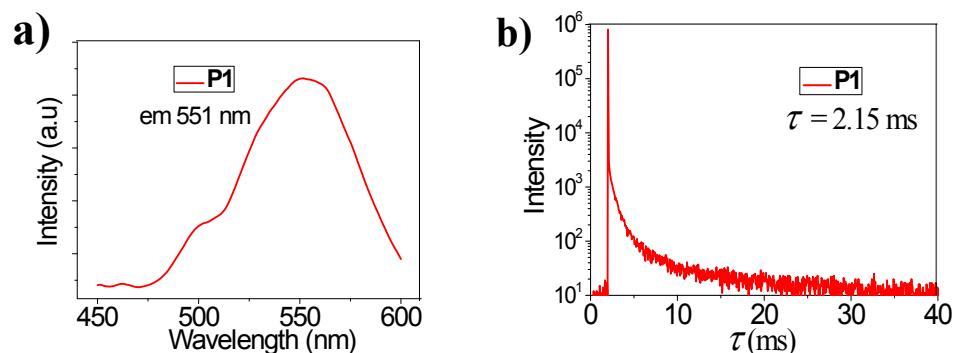
Fig. S5 a) The phosphorescence emission spectra of **P1** (λ_{ex} = 358 nm, λ_{em} = 551 nm); b) the corresponding phosphorescence decay curves of **P1**.
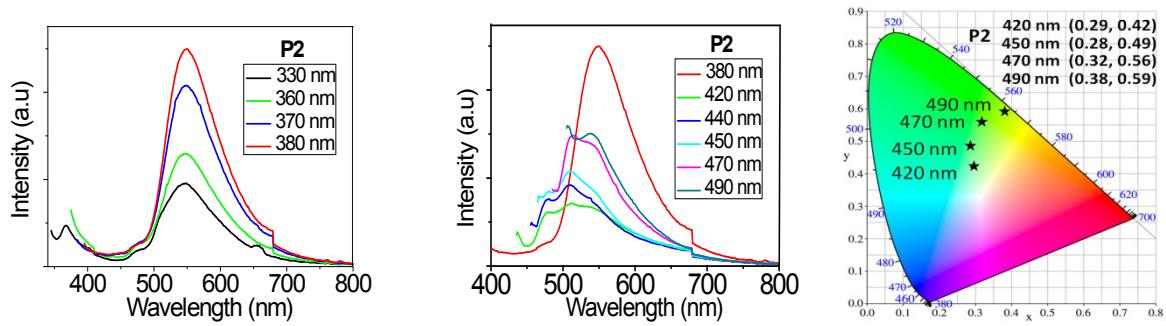
Fig. S6 The excitation wavelength-dependent photoluminescence spectra ranging from 330 nm to 490 nm for **P2** and the CIEx,y coordinates of **P2** under several different excitation wavelengths.
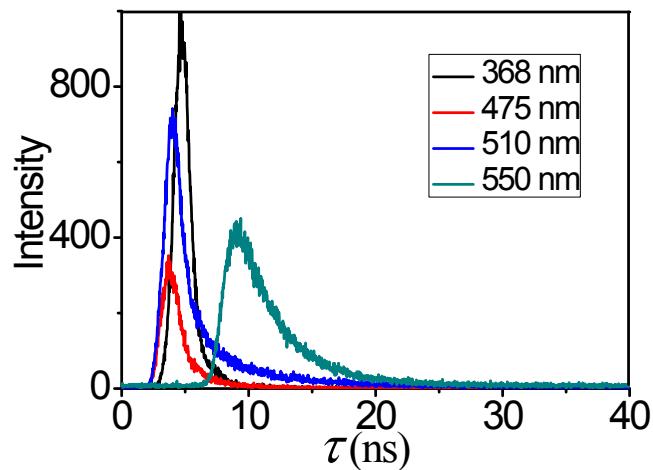
Fig. S7 The time-resolved photoluminescence decay curves of **P2** at four emission peaks 368 nm (λ_{ex} = 340 nm, 0.84 ns), 475 nm (λ_{ex} = 450 nm, 1.30 ns) 510 nm (λ_{ex} = 450 nm, 3.44 ns), and 550 nm (λ_{ex} = 380 nm, 3.41 ns).
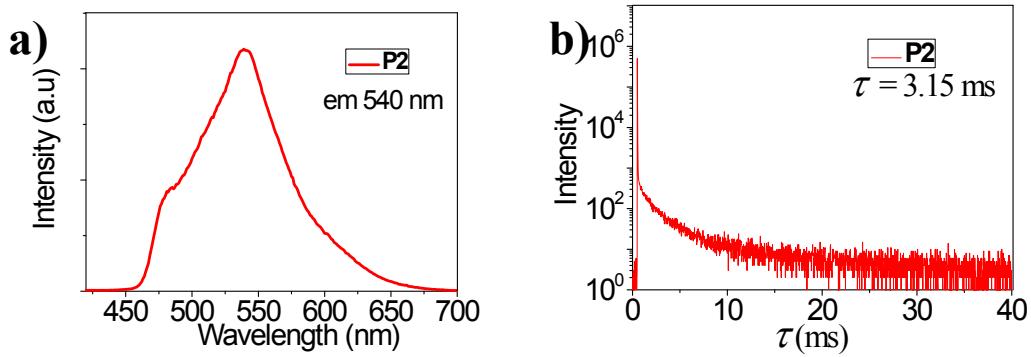
Fig. S8 a) The phosphorescence emission spectra of **P2** (λ_{ex} = 380 nm, λ_{em} = 540 nm); b) the corresponding phosphorescence decay curves of **P2**.
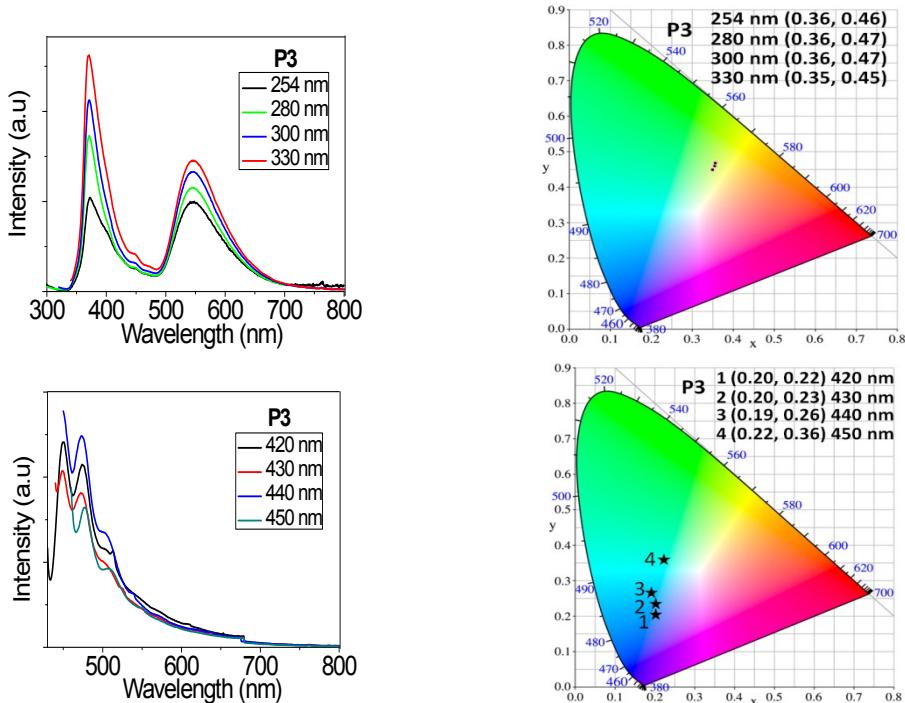
Fig. S9 The excitation wavelength-dependent photoluminescence spectra and the corresponding CIEx,y coordinates of **P3**.
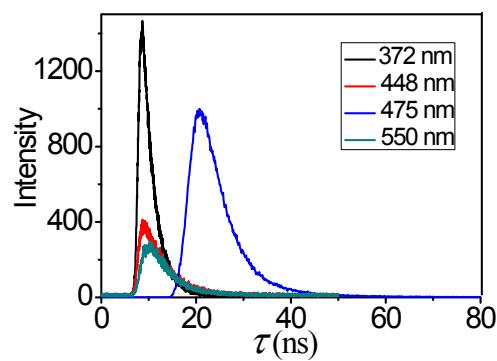
Fig. S10 The transient photoluminescence decay curves of the emission peaks 372 nm (λ_{ex} = 340 nm, 2.48 ns), 448 nm (λ_{ex} = 380 nm, 4.7 ns), 475 nm (λ_{ex} = 380 nm, 5.6 ns), and 550 nm (λ_{ex} = 380 nm, 4.5 ns) for **P3**.
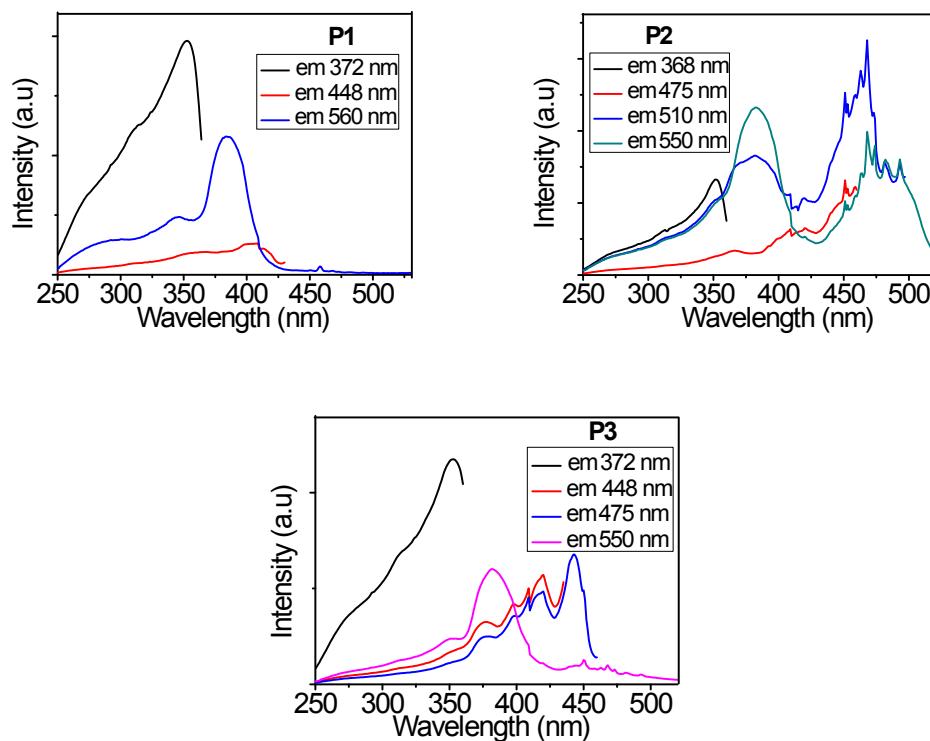
Fig. S11 the corresponding excitation spectra of the different emission peaks of compounds **P1**, **P2** and **P3**
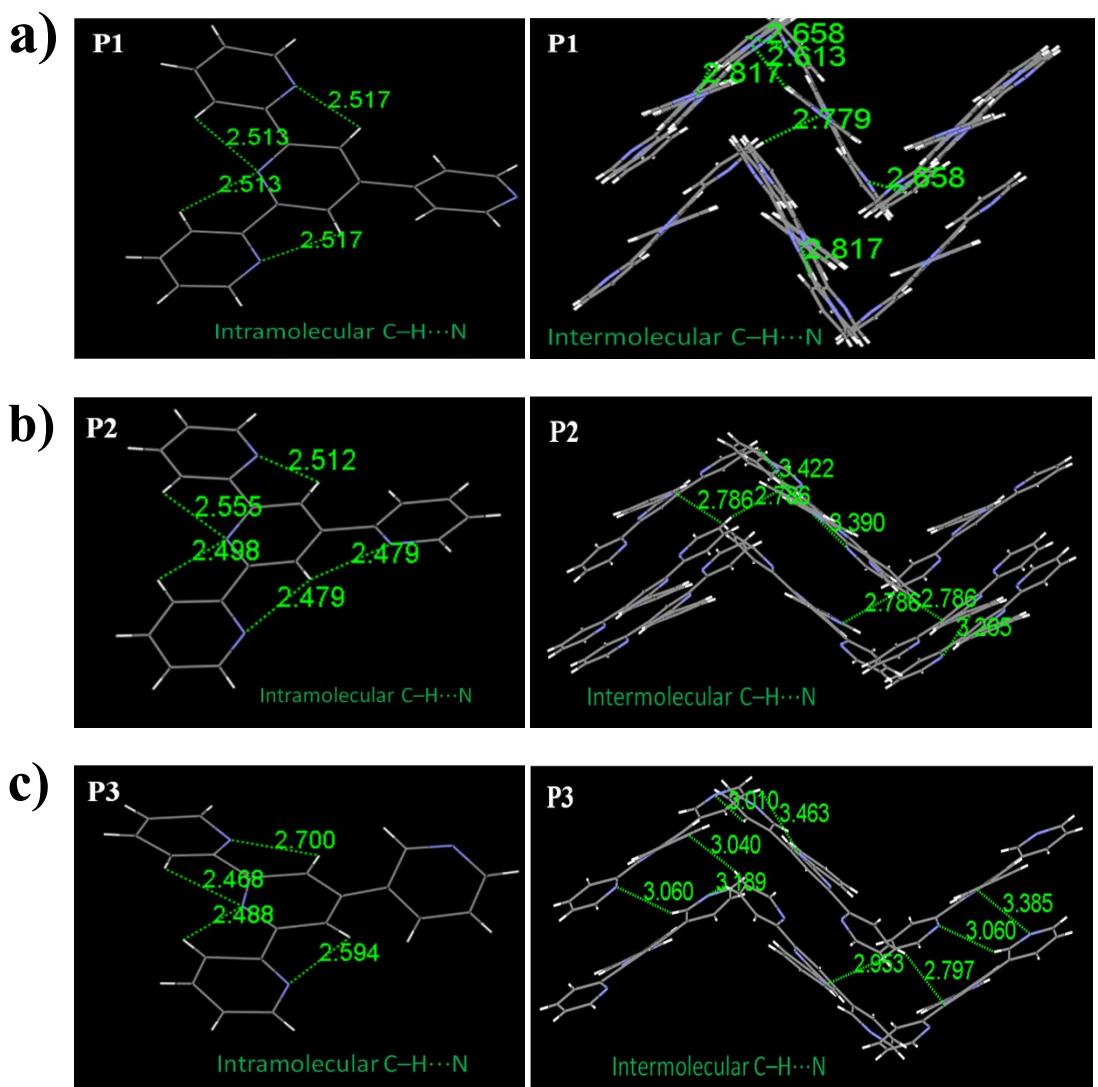
Fig. S12 Numerous intramolecular C–H⋯N interactions and intermolecular C–H⋯N interactions in (a) **P1**, (b) **P2**, (c) **P3** crystals.
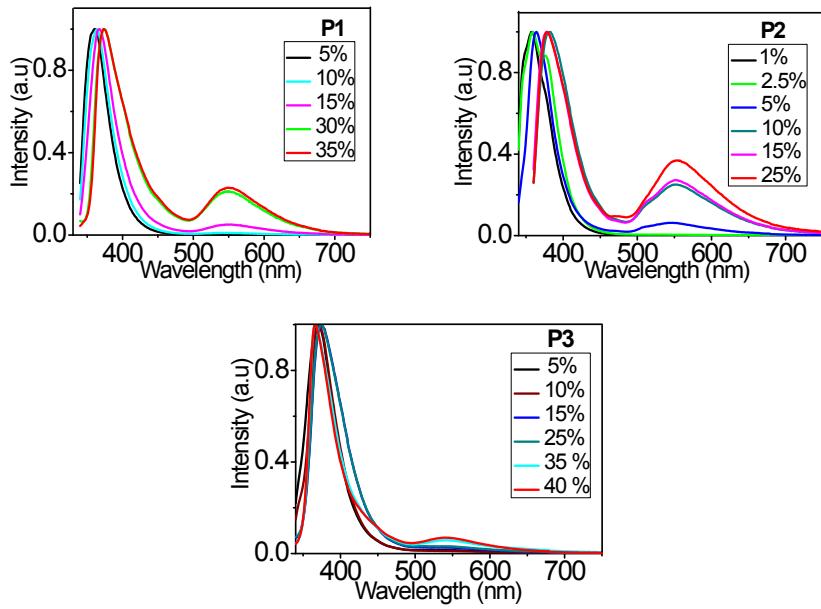
Fig. S13 Emission spectra of **P1**, **P2** and **P3** with increasing concentrations in PMMA films upon excitation at 330 nm.
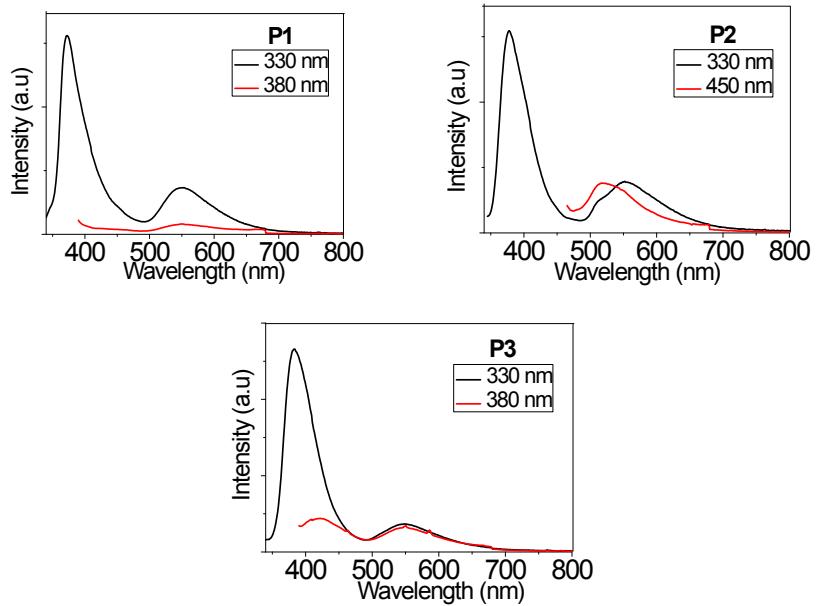
Fig. S14 Excitation wavelength-dependent emissions of doped films of **P1** (35%wt), **P2** (25%wt) and **P3** (40%wt).
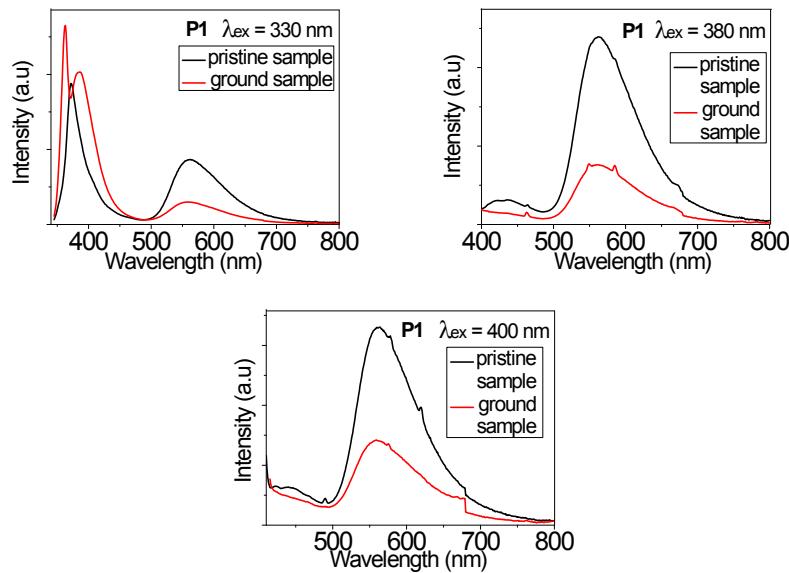
Fig. S15 Emission spectra of both the pristine samples and the ground samples for **P1** under different excitation wavelengths.
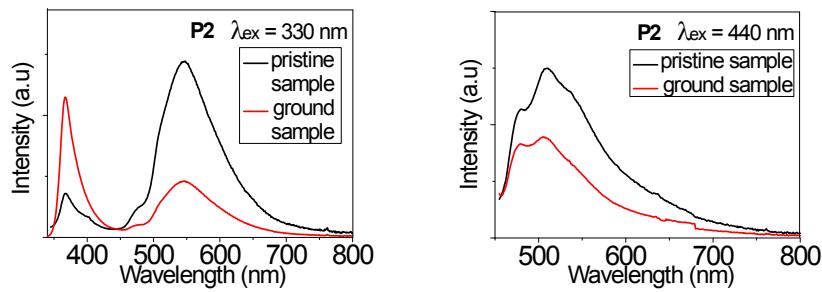
Fig. S16 Emission spectra of both the pristine samples and the ground samples for **P2** under different excitation wavelengths.
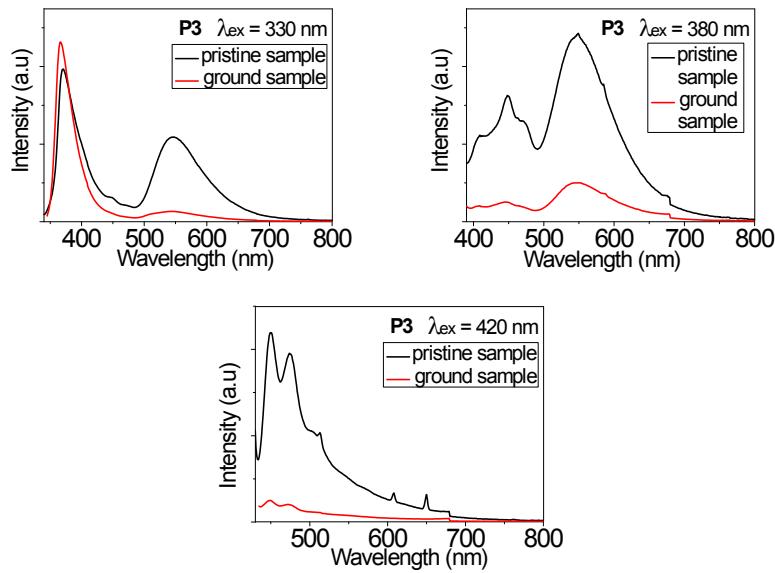
Fig. S17 Emission spectra of both the pristine samples and the ground samples for **P3** under different excitation wavelengths.
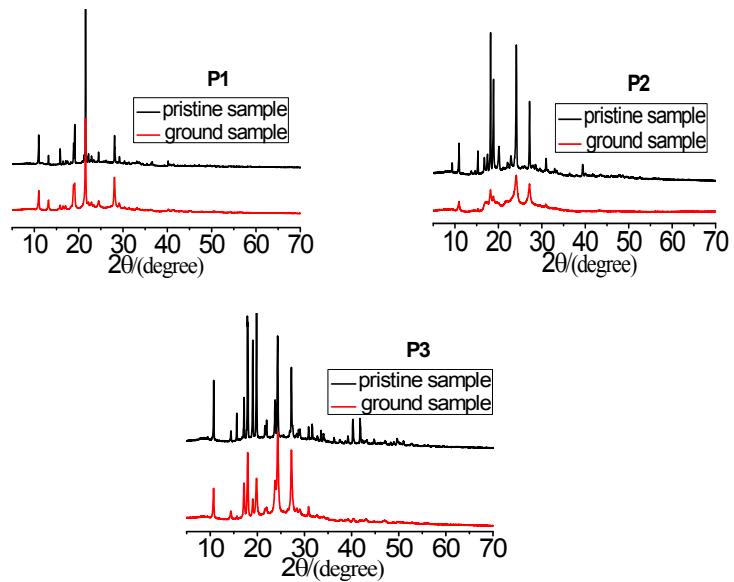
Fig. S18 X-ray powder diffractions of both the pristine samples and the ground samples for **P1**, **P2** and **P3**.
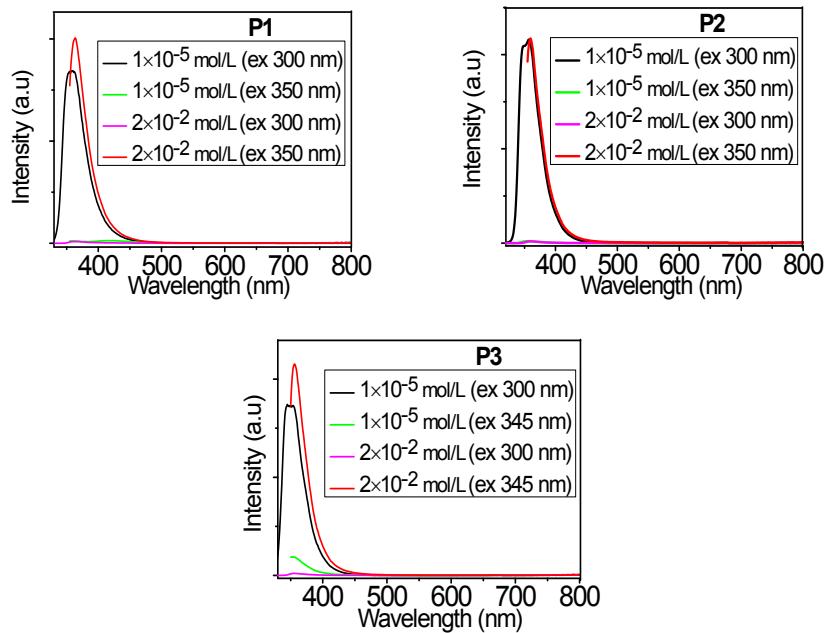
Fig. S19 Emission spectra of compounds **P1**, **P2** and **P3** irradiated by different excitation wavelengths at different concentrations in CH_2Cl_2.
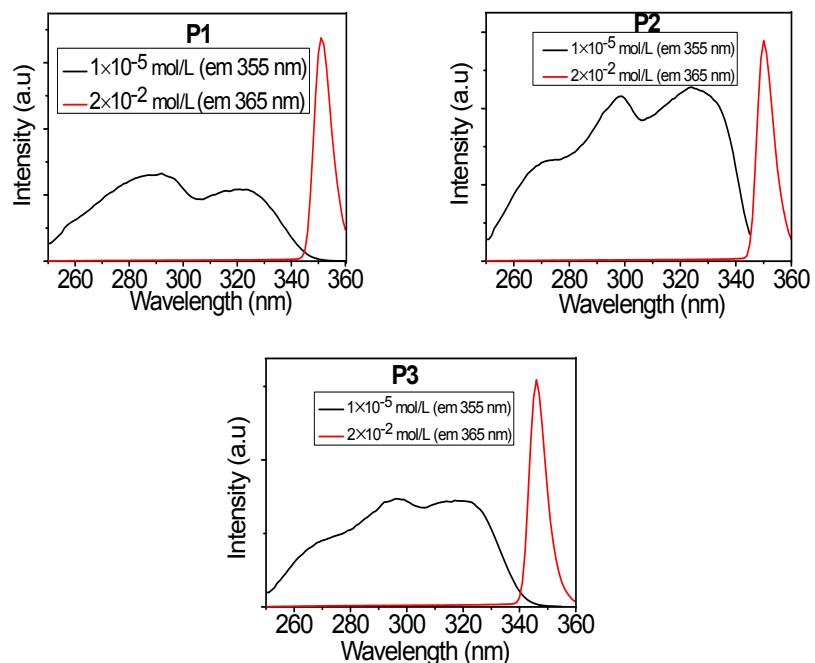
Fig. S20 Fluorescence excitation spectra of **P1**, **P2** and **P3** at different concentrations in CH_2Cl_2.
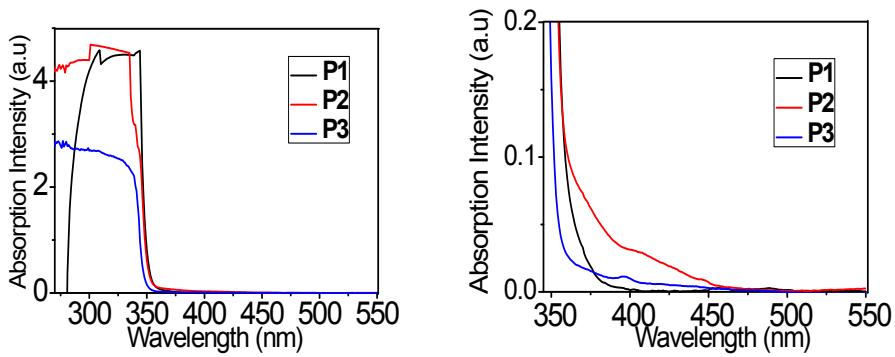
Fig. S21 The UV-Vis absorption spectra of **P1**, **P2** and **P3** at 2×10^{-2} mol/L in CH$_2$Cl$_2$.
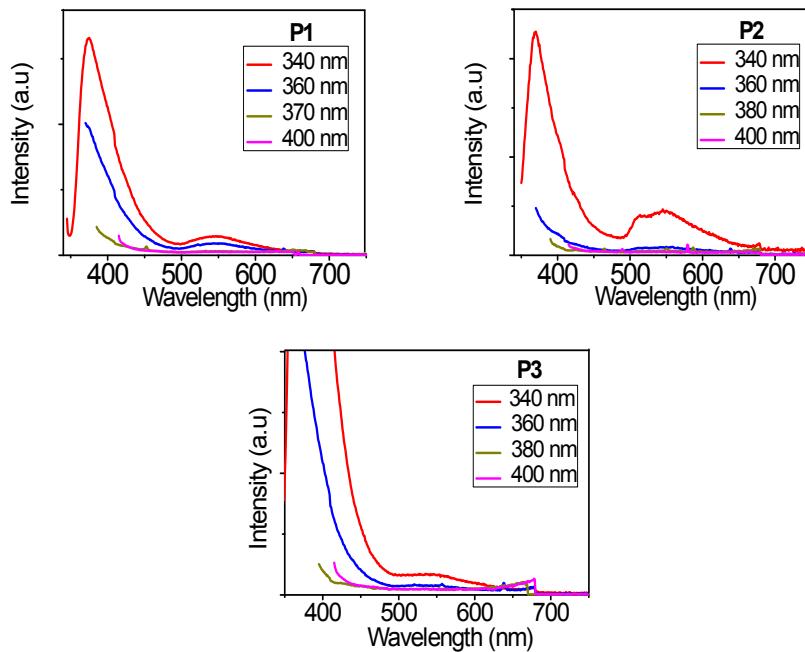
Fig. S22 Emission spectra of thin films of **P1**, **P2** and **P3** under different excitation wavelengths.

Table S2. The singlet and triplet excited state transition configurations for the dimer of **P1** from single crystal by TD-DFT calculations at the B3LYP/6-31G(d) level.

Excited state	Energy	Orbitals	Transition
T₁	2.8007 eV	158 ->167	-0.10679
		159 ->163	-0.17841
		159 ->164	0.13147
		160 ->163	0.16258
		160 ->164	-0.18289
		161 ->165	-0.26915
		161 ->166	0.20587
		162 ->165	0.2422
		162 ->166	-0.28529
T₂	2.8054 eV	159 ->163	0.15221
		159 ->164	0.19314
		160 ->163	0.17186
		160 ->164	0.13698
		161 ->165	0.21043
		161 ->166	0.2718
		162 ->165	0.28631
		162 ->166	0.2356
T₃	3.3015 eV	159 ->166	0.13006
		160 ->165	0.15868
		161 ->163	-0.10789
		161 ->164	0.29006
		161 ->167	0.13091
		162 ->163	0.34707
		162 ->164	-0.10347
		162 ->167	-0.14311
T₄	3.3072 eV	159 ->165	0.13296
		160 ->166	0.15477
		161 ->163	0.29958
		161 ->164	0.10909
		161 ->168	-0.1221
		162 ->163	0.10629
		162 ->164	0.32398
		162 ->168	-0.15584
T₅	3.4615 eV	153 ->173	0.12252
		155 ->174	0.17959
		156 ->163	-0.12701
		157 ->163	0.19273
		157 ->173	-0.14343
		158 ->163	-0.10422

		158 ->164	0.25035
		158 ->174	-0.10741
		159 ->164	0.12624
		160 ->163	0.14536
		160 ->167	0.13096
		161 ->166	-0.13497
		162 ->165	-0.15135
T$_6$	3.4664 eV	153 ->174	-0.13549
		155 ->173	-0.17362
		156 ->164	-0.13711
		156 ->174	0.10486
		157 ->164	0.20282
		157 ->174	0.12338
		158 ->163	0.23131
		159 ->163	0.14141
		160 ->164	0.14122
		160 ->168	0.11633
		161 ->165	-0.12255
		162 ->166	-0.14911
T$_7$	3.9734 eV	139 ->163	-0.10593
		141 ->166	-0.16576
		142 ->165	-0.17788
		144 ->170	0.1167
		145 ->169	-0.12257
		147 ->171	0.15485
		148 ->172	-0.11711
		155 ->173	-0.11425
		157 ->169	-0.1126
		159 ->172	0.12038
		160 ->169	0.10378
		161 ->165	-0.11997
		161 ->171	-0.11216
		161 ->177	0.14785
		162 ->166	-0.12965
		162 ->178	-0.15095
T$_8$	3.9784 eV	141 ->165	-0.16366
		142 ->166	-0.1736
		144 ->169	0.13541
		145 ->167	-0.10077
		147 ->170	0.14855
		148 ->171	0.15276
		157 ->173	-0.12153
		159 ->169	0.1368
		161 ->166	-0.12495
		161 ->178	-0.14348
		162 ->165	-0.14283
		162 ->177	0.15678
T$_9$	4.0098 eV	141 ->164	0.14226
		142 ->163	0.16622
		145 ->166	-0.10277
		148 ->169	0.10186

		158 ->165	0.1073
		161 ->163	0.2695
		161 ->175	0.13799
		162 ->163	-0.11824
		162 ->164	0.30327
		162 ->167	-0.10084
		162 ->176	-0.15104
T$_{10}$	4.0312 eV	141 ->163	0.14806
		142 ->164	0.16018
		144 ->170	0.1092
		147 ->169	0.10636
		161 ->164	0.25993
		161 ->176	-0.13628
		162 ->163	0.29933
		162 ->164	0.11644
		162 ->175	0.15406
S1	4.3648 eV	161 ->164	0.38325
		162 ->163	0.5153
S2	4.3786 eV	161 ->163	0.42308
		162 ->164	0.47366
S3	4.7308 eV	161 ->166	0.38275
		162 ->164	-0.12126
		162 ->165	0.50501
S4	4.7903 eV	143 ->163	-0.12497
		143 ->164	0.10386
		146 ->163	0.13538
		146 ->164	-0.14075
		151 ->165	-0.11904
		151 ->166	0.10309
		152 ->166	-0.11908
		153 ->163	-0.1651
		153 ->164	0.16885
		154 ->163	0.27009
		154 ->164	-0.19996
		154 ->167	-0.13328
		155 ->163	0.11357
		156 ->163	-0.19128
		156 ->164	0.17902
S5	4.7957 eV	143 ->163	-0.11372
		143 ->164	-0.13522
		146 ->163	-0.13434
		146 ->164	-0.11825
		151 ->166	-0.12164
		152 ->165	-0.11252
		152 ->166	-0.11238
		153 ->163	0.18333
		153 ->164	0.15849
		154 ->163	0.22481
		154 ->164	0.23815

		154 ->168	-0.13351
		155 ->163	0.10045
		155 ->164	0.11821
		156 ->163	0.20288
		156 ->164	0.16118
S6	4.8147 eV	159 ->163	0.10604
		161 ->165	0.38298
		162 ->163	0.10183
		162 ->166	0.47316
S7	4.9111 eV	151 ->163	-0.17083
		151 ->167	0.19425
		152 ->164	-0.14668
		152 ->167	-0.17619
		153 ->165	-0.10002
		153 ->166	0.23838
		154 ->165	0.32924
		154 ->166	-0.1308
		155 ->165	0.11839
		156 ->165	-0.1086
		156 ->166	0.23096
S8	4.9143 eV	151 ->164	0.14319
		151 ->168	-0.18293
		152 ->163	0.16667
		152 ->168	-0.18125
		153 ->165	-0.22741
		153 ->166	-0.10989
		154 ->165	-0.13086
		154 ->166	-0.32147
		155 ->166	-0.1205
		156 ->165	-0.23343
		156 ->166	-0.10023
		162 ->166	0.11309
S9	5.0279 eV	148 ->163	0.11172
		149 ->163	-0.11146
		149 ->164	0.24754
		149 ->167	-0.11915
		150 ->163	0.23018
		151 ->165	0.20448
		152 ->166	0.2023
		154 ->167	0.12258
S10	5.0295 eV	148 ->164	-0.10371
		149 ->163	-0.22454
		150 ->163	-0.15869
		150 ->164	-0.27465
		150 ->168	-0.16194
		151 ->166	-0.19292
		152 ->165	-0.19902
		154 ->168	-0.1088

Table S3. The singlet and triplet excited state transition configurations for the dimer of **P2** from single crystal by TD-DFT calculations at the B3LYP/6-31G(d) level.

Excited state	Energy	Orbitals	Transition
T_1	2.9260 eV	159 ->164 160 ->163 161 ->166 162 ->165	-0.26583 -0.28912 0.30103 0.32848
T_2	2.9281 eV	159 ->163 160 ->164 161 ->165 162 ->166	-0.27165 -0.2802 0.33593 0.29297
T_3	3.4014 eV	155 ->166 158 ->165 160 ->165 161 ->164 161 ->168 162 ->163 162 ->167	0.13613 0.14367 -0.12203 0.35646 0.11002 0.38349 0.11432
T_4	3.4150 eV	155 ->165 158 ->166 160 ->166 161 ->163 161 ->167 162 ->164 162 ->168	0.16526 0.11338 -0.10706 0.37867 0.1099 0.36417 0.11488
T_5	3.6455 eV	145 ->168 146 ->169 155 ->164 158 ->163 159 ->164 159 ->173 160 ->163 160 ->167 160 ->172 161 ->166 162 ->165	-0.13719 -0.13506 0.13441 0.18646 0.22178 -0.10722 0.18487 -0.1073 -0.14099 0.15503 0.17893
T_6	3.6515 eV	145 ->167 145 ->169 146 ->168 155 ->163 158 ->164 159 ->163	0.10576 0.13625 0.13083 -0.13925 -0.1825 -0.21587

		159 ->164	0.11197
		159 ->167	0.11562
		159 ->172	0.14317
		160 ->164	-0.19152
		160 ->173	0.10701
		161 ->165	-0.1764
		162 ->166	-0.15964
T$_7$	3.8573 eV	149 ->163	0.12059
		149 ->164	-0.12909
		150 ->163	0.17154
		150 ->164	-0.17681
		156 ->163	-0.23172
		156 ->164	0.22472
		157 ->163	0.29621
		157 ->164	-0.29974
T$_8$	3.8580 eV	149 ->163	0.15773
		149 ->164	0.15098
		150 ->163	-0.14825
		150 ->164	-0.14793
		156 ->163	0.29921
		156 ->164	0.27997
		157 ->163	0.24937
		157 ->164	0.22465
T$_9$	4.1021 eV	149 ->163	0.13108
		149 ->164	0.10647
		150 ->163	-0.1248
		150 ->164	-0.10215
		153 ->163	0.12293
		153 ->165	0.10903
		153 ->167	0.10979
		153 ->170	0.10122
		154 ->163	-0.13092
		154 ->164	-0.10085
		154 ->165	-0.11621
		154 ->167	-0.11561
		154 ->170	-0.10609
		156 ->165	-0.19441
		156 ->166	-0.1765
		156 ->170	-0.11868
		157 ->165	-0.15006
		157 ->166	-0.13816
T$_{10}$	4.1064eV	149 ->163	0.10111
		150 ->163	0.14041
		150 ->164	-0.12331
		153 ->163	-0.11998
		153 ->164	0.10098
		153 ->165	0.11371
		153 ->167	-0.11311
		153 ->170	0.10352
		154 ->163	-0.12235
		154 ->164	0.10229

		154 ->165	0.11646
		154 ->167	-0.11301
		154 ->170	0.10455
		156 ->165	-0.15566
		156 ->166	0.13875
		157 ->165	0.19252
		157 ->166	-0.17198
		157 ->170	0.11248
S1	4.4404 eV	161 ->163	0.47662
		162 ->164	0.45344
S2	4.4709 eV	156 ->164	-0.15424
		157 ->163	-0.16867
		161 ->164	0.41139
		162 ->163	0.43694
S3	4.5120 eV	149 ->164	0.16927
		150 ->163	-0.19384
		154 ->165	0.10852
		156 ->163	0.41083
		157 ->164	0.39394
S4	4.5183 eV	149 ->163	0.14737
		150 ->164	-0.17281
		153 ->165	-0.10082
		156 ->164	0.35182
		156 ->165	0.10632
		157 ->163	0.38054
		161 ->164	0.17993
		162 ->163	0.18721
S5	4.7629 eV	149 ->163	-0.12024
		149 ->164	-0.10215
		150 ->163	0.11918
		150 ->164	0.10148
		153 ->163	-0.15177
		153 ->164	-0.12746
		153 ->167	-0.11009
		154 ->163	0.15946
		154 ->164	0.13343
		154 ->167	0.11467
		156 ->165	0.26264
		156 ->166	0.23763
		157 ->165	0.20713
		157 ->166	0.18732
S6	4.7650 eV	150 ->163	0.12987
		150 ->164	-0.11951
		153 ->163	-0.14813
		153 ->164	0.13532
		153 ->167	-0.11276
		154 ->163	-0.15049
		154 ->164	0.13509
		154 ->167	-0.11358
		156 ->165	-0.2136

Excited state	Energy	Orbitals	Transition
		156 ->166	0.18752
		157 ->165	0.26687
		157 ->166	-0.23722
S7	4.8980 eV	153 ->166	-0.138
		154 ->165	0.13876
		158 ->163	0.11016
		160 ->163	-0.10568
		161 ->166	0.3348
		162 ->165	0.44603
S8	4.9204 eV	150 ->164	0.12204
		153 ->165	-0.20504
		154 ->166	0.20396
		156 ->165	-0.10436
		157 ->166	-0.1069
		157 ->167	0.10165
		161 ->165	0.34582
		162 ->166	0.31133
S9	4.9679 eV	149 ->164	-0.16859
		150 ->163	0.18795
		150 ->167	0.12373
		153 ->166	-0.2787
		153 ->167	0.1127
		154 ->165	0.28392
		156 ->166	-0.11716
		156 ->167	0.12717
		157 ->165	-0.1223
		161 ->166	-0.16166
		162 ->165	-0.22365
S10	4.9830 eV	149 ->163	0.15081
		149 ->167	0.10086
		150 ->164	-0.15667
		153 ->165	0.2393
		154 ->166	-0.23495
		157 ->167	-0.1099
		161 ->165	0.2994
		162 ->166	0.26647

Table S4. The singlet and triplet excited state transition configurations for the dimers of **P3** from single crystal by TD-DFT calculations at the B3LYP/6-31G(d) level.

Excited state	Energy	Orbitals	Transition
T_1	2.2659 eV	143 ->163	0.10133
		159 ->168	0.10643
		161 ->163	0.32356
		161 ->164	0.13169
		162 ->163	0.49318
		162 ->164	

		162 <-163	0.1648
			0.11193
T$_2$	2.3839 eV	160 ->165	0.15441
		161 ->163	-0.17857
		161 ->164	0.41467
		162 ->163	0.10929
		162 ->164	-0.31898
T$_3$	2.8801 eV	144 ->164	0.11154
		153 ->164	-0.15623
		153 ->165	-0.14932
		153 ->166	-0.10385
		160 ->164	-0.16458
		160 ->167	-0.12739
		160 ->169	-0.10374
		161 ->165	-0.26981
		161 ->166	-0.17238
		162 ->165	0.26001
		162 ->166	0.11724
T$_4$	3.0358 eV	148 ->166	-0.10042
		148 ->168	0.11301
		154 ->163	-0.10253
		154 ->165	-0.20674
		154 ->166	0.25972
		154 ->168	-0.15634
		159 ->163	0.10402
		160 ->163	-0.14611
		160 ->168	-0.17837
		161 ->165	-0.10765
		162 ->165	-0.15568
		162 ->166	0.23691
T$_5$	3.0630 eV	154 ->163	0.1657
		154 ->166	-0.10667
		159 ->163	0.21603
		159 ->166	0.12563
		159 ->168	0.11656
		160 ->163	-0.16771
		160 ->165	0.15476
		160 ->166	-0.17042
		160 ->168	-0.10451
		161 ->168	0.12214
		162 ->167	-0.10621
		162 ->168	0.25153
T$_6$	3.2136 eV	153 ->164	0.16954
		158 ->165	-0.15215
		159 ->164	-0.10085
		159 ->165	0.13285

		160 ->165	0.22329
		160 ->166	0.15435
		160 ->169	-0.11132
		161 ->164	-0.13642
		161 ->167	0.13092
		161 ->169	0.18633
		162 ->167	-0.10099
		162 ->169	-0.14477
T_7	3.6218 eV	143 ->163	-0.10642
		155 ->163	-0.15172
		157 ->163	0.40821
		157 ->164	0.12802
		157 ->166	0.11565
		158 ->163	0.21024
		159 ->163	-0.16025
		162 ->175	-0.12042
T_8	3.7130 eV	143 ->163	-0.1339
		154 ->163	-0.13628
		154 ->168	0.10126
		155 ->163	0.10961
		156 ->171	0.1314
		157 ->163	-0.25208
		158 ->164	-0.12938
		158 ->165	0.16057
		159 ->164	-0.11697
		161 ->175	-0.1138
		162 ->175	-0.15724
T_9	3.7134 eV	156 ->167	0.11479
		156 ->169	0.13454
		156 ->170	0.12253
		156 ->171	0.17965
		157 ->163	0.15392
		158 ->163	0.12224
		158 ->164	-0.14224
		158 ->165	0.17967
		158 ->171	-0.11373
		159 ->164	-0.13569
		159 ->165	0.179
		159 ->171	-0.1157
		162 ->175	0.11582
T_{10}	3.8105 eV	142 ->164	-0.14092
		144 ->167	-0.10863
		146 ->164	0.18261
		146 ->167	-0.41549
		146 ->168	-0.13602
		146 ->169	0.20179
		147 ->167	0.11473
		153 ->169	0.13834
		161 ->176	0.10943

S1	3.9100 eV	155 ->163	-0.22189
		157 ->163	0.52489
		157 ->164	0.18195
		157 ->175	0.10066
		158 ->163	0.23776
		159 ->163	-0.1467
S2	4.0527 eV	156 ->163	-0.13324
		156 ->164	0.33878
		156 ->169	-0.11122
		157 ->164	-0.12432
		158 ->163	-0.16874
		158 ->164	0.40947
		159 ->163	-0.10964
		159 ->164	0.26372
S3	4.2595 eV	157 ->163	-0.12362
		161 ->163	0.26575
		161 ->164	0.18232
		162 ->163	0.54425
S4	4.2791 eV	156 ->164	0.18715
		156 ->167	0.11813
		156 ->169	0.13265
		156 ->171	0.10378
		156 ->177	0.10528
		157 ->165	-0.10505
		158 ->165	0.37703
		158 ->166	0.19583
		159 ->165	0.28255
		159 ->166	0.13468
		160 ->165	0.12098
S5	4.3696 eV	161 ->163	0.2464
		161 ->164	-0.36722
		161 ->165	-0.24604
		162 ->164	0.36952
		162 ->165	0.14724
		162 ->166	0.13346
S6	4.4255 eV	156 ->164	-0.13714
		156 ->165	0.41382
		156 ->166	0.20116
		158 ->165	0.13461
		158 ->166	0.10481
		158 ->169	0.11999
		158 ->171	0.11382
		159 ->167	0.10814
		159 ->169	0.11553
		159 ->171	0.11242
		161 ->165	0.14093
		162 ->165	-0.1346
S7	4.4741 eV	155 ->163	0.14605
		155 ->168	0.12313
		157 ->165	-0.30989

		157 ->166	0.35784
		157 ->168	0.14163
		158 ->165	-0.14826
		158 ->166	0.14774
		162 ->165	-0.13784
S8	4.4979 eV	156 ->165	0.1239
		157 ->165	-0.10174
		159 ->164	0.12644
		160 ->164	0.11161
		161 ->164	0.1995
		161 ->165	-0.3106
		161 ->166	-0.17543
		162 ->163	0.12875
		162 ->164	-0.13718
		162 ->165	0.35662
S9	4.5439 eV	157 ->163	-0.15642
		157 ->166	-0.10401
		159 ->163	-0.31711
		160 ->163	0.3199
		160 ->164	0.12059
		161 ->165	-0.17924
		162 ->163	-0.13282
		162 ->164	-0.13609
		162 ->165	-0.11161
		162 ->166	0.20766
S10	4.6210 eV	155 ->163	0.25588
		155 ->165	-0.2028
		155 ->166	0.20581
		155 ->168	0.20478
		155 ->171	0.11382
		157 ->166	-0.10647
		157 ->168	0.1083
		157 ->171	0.10831
		159 ->163	-0.10958
		160 ->163	0.14142
		161 ->165	0.14572
		162 ->165	0.16605
		162 ->166	-0.16449

Table S5. The selected calculated spin orbital coupling (SOC) coefficient for the dimer of **P1** in different transition paths.

Transition	SOC (cm^{-1})	Transition	SOC (cm^{-1})
$S_0 \rightarrow T_3$	28.08	$S_5 \rightarrow T_1$	2.25
$S_0 \rightarrow T_5$	3.33	$S_5 \rightarrow T_{10}$	5.21
$S_0 \rightarrow T_7$	41.13	$S_6 \rightarrow T_2$	2.94

$S_1 \rightarrow T_1$	2.21	$S_6 \rightarrow T_8$	2.99
$S_1 \rightarrow T_4$	7.73	$S_6 \rightarrow T_{10}$	1.59
$S_1 \rightarrow T_9$	2.03	$S_7 \rightarrow T_5$	1.97
$S_1 \rightarrow T_{10}$	3.97	$S_7 \rightarrow T_7$	3.52
$S_2 \rightarrow T_1$	8.14	$S_8 \rightarrow T_{10}$	2.12
$S_2 \rightarrow T_4$	4.28	$S_9 \rightarrow T_1$	4.48
$S_2 \rightarrow T_9$	3.51	$S_9 \rightarrow T_9$	2.98
$S_2 \rightarrow T_{10}$	3.15	$S_9 \rightarrow T_{10}$	1.93
$S_4 \rightarrow T_2$	5.13	$S_{10} \rightarrow T_8$	4.44
$S_4 \rightarrow T_8$	3.60		

Table S6. The selected calculated spin orbital coupling (SOC) coefficient for the dimer of **P2** in different transition paths.

Transition	SOC (cm^{-1})	Transition	SOC (cm^{-1})
$S_0 \rightarrow T_4$	6.69	$S_6 \rightarrow T_2$	2.68
$S_0 \rightarrow T_5$	25.72	$S_6 \rightarrow T_3$	1.94
$S_0 \rightarrow T_6$	12.10	$S_6 \rightarrow T_8$	2.74
$S_0 \rightarrow T_7$	40.45	$S_6 \rightarrow T_9$	1.80
$S_1 \rightarrow T_1$	6.63	$S_6 \rightarrow T_{10}$	2.48
$S_1 \rightarrow T_9$	3.95	$S_7 \rightarrow T_4$	1.78
$S_1 \rightarrow T_{10}$	4.59	$S_7 \rightarrow T_7$	3.56
$S_3 \rightarrow T_1$	4.29	$S_8 \rightarrow T_4$	6.72
$S_3 \rightarrow T_3$	7.28	$S_8 \rightarrow T_5$	3.71
$S_3 \rightarrow T_{10}$	5.75	$S_8 \rightarrow T_6$	2.09
$S_4 \rightarrow T_2$	4.93	$S_8 \rightarrow T_7$	2.72
$S_4 \rightarrow T_3$	1.97	$S_9 \rightarrow T_1$	3.53
$S_4 \rightarrow T_8$	3.83	$S_9 \rightarrow T_9$	2.87
$S_5 \rightarrow T_1$	3.16	$S_9 \rightarrow T_{10}$	2.26
$S_5 \rightarrow T_3$	4.52	$S_{10} \rightarrow T_8$	1.70
$S_5 \rightarrow T_{10}$	3.88	$S_{10} \rightarrow T_{10}$	4.20

Table S7. The calculated spin orbital coupling (SOC) coefficient for the dimer of **P3** in different transition paths.

Transition	SOC (cm^{-1})	Transition	SOC (cm^{-1})
$S_0 \rightarrow T_4$	4.16	$S_6 \rightarrow T_3$	2.20
$S_0 \rightarrow T_5$	11.55	$S_7 \rightarrow T_4$	2.43
$S_0 \rightarrow T_6$	20.44	$S_7 \rightarrow T_7$	2.98
$S_0 \rightarrow T_7$	44.21	$S_8 \rightarrow T_2$	2.16
$S_1 \rightarrow T_1$	5.50	$S_8 \rightarrow T_3$	1.58
$S_1 \rightarrow T_8$	3.67	$S_8 \rightarrow T_2$	2.16
$S_3 \rightarrow T_2$	5.04	$S_8 \rightarrow T_3$	1.58
$S_3 \rightarrow T_9$	1.81	$S_8 \rightarrow T_{10}$	4.81
$S_3 \rightarrow T_{10}$	4.99	$S_9 \rightarrow T_4$	2.28
$S_4 \rightarrow T_3$	2.74	$S_9 \rightarrow T_5$	1.68
$S_4 \rightarrow T_8$	1.83	$S_9 \rightarrow T_6$	1.82
$S_5 \rightarrow T_1$	1.77	$S_9 \rightarrow T_7$	2.02
$S_5 \rightarrow T_3$	5.45	$S_{10} \rightarrow T_4$	4.77
$S_5 \rightarrow T_{10}$	1.63	$S_{10} \rightarrow T_5$	2.39
$S_6 \rightarrow T_2$	2.37	$S_{10} \rightarrow T_7$	3.57

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