

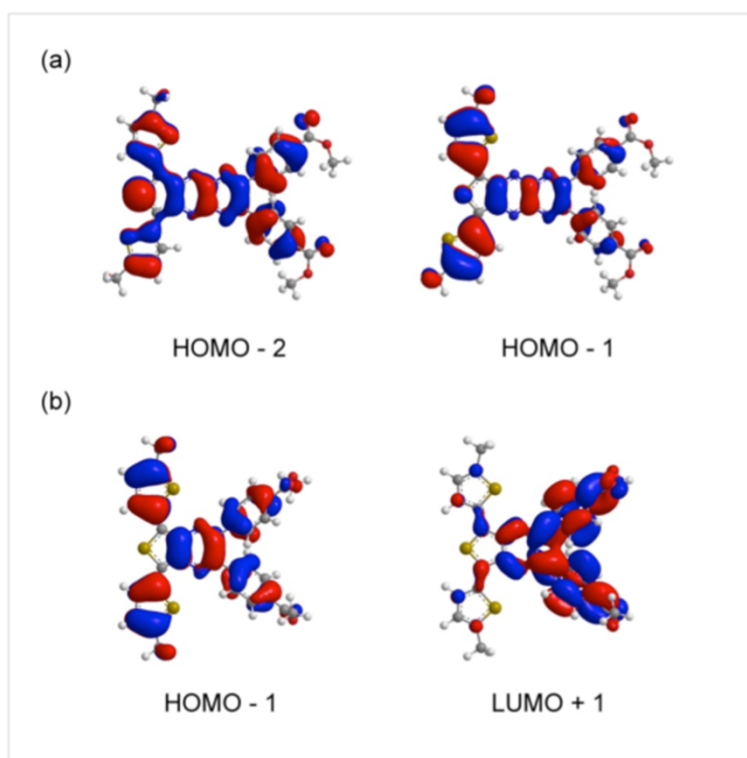
Electronic Supplementary Information

**A new route to the synthesis of near-infrared absorbing pyrazinopyrazine  
bridged dyes with intramolecular charge transfer character**

*Liang Zhang, Kin Cheung Lo, Wai Kin Chan\**

*Department of Chemistry, The University of Hong Kong*

*Pokfulam Road, Hong Kong, China*



**Figure S1.** Spatial plots (isovalue = 0.02) of the molecular orbitals of (a) **5** and (b) **6** in toluene from TDDFT calculations.

**Table S1.** Shift in absorption energy (in eV) for compounds **5** and **6** in DMF and toluene. The first number corresponds to the shift of the higher energy absorption band and the second number corresponds to the shift of the lower energy band.

Compound	Experimental Results obtained from UV-vis absorption spectra (eV)	TDDFT results (eV)
<b>5</b>	0.063, 0.086	-0.009, 0.019
<b>6</b>	0.020, 0.021	0.019, 0.020

**Table S2.** Selected electronic excitations of **6** in toluene (Key: H – HOMO; L – LUMO).

No.	Vertical excitation wavelength $\lambda$ (nm)	$f$	Excitation	Configuration interaction (CI) coefficient
1	584	0.363	H $\rightarrow$ L	0.70
2	345	0.649	H – 1 $\rightarrow$ L H $\rightarrow$ L + 1 H $\rightarrow$ L + 5	0.33 0.57 -0.17

**Table S3.** Selected electronic excitations of **6** in DMF.

No.	$\lambda$ (nm)	$f$	Excitation	CI coefficient
1	578	0.358	H $\rightarrow$ L	0.70
2	343	0.690	H – 1 $\rightarrow$ L H $\rightarrow$ L + 1 H $\rightarrow$ L + 5	0.36 0.56 -0.17

**Table S4.** Selected electronic excitations of **5** in toluene.

No.	$\lambda$ (nm)	$f$	Excitation	CI coefficient
1	870	0.183	H $\rightarrow$ L	0.70
2	397	0.980	H – 2 $\rightarrow$ L H – 1 $\rightarrow$ L	0.30 0.60

**Table S5.** Selected electronic excitations of **5** in DMF.

No.	$\lambda$ (nm)	$f$	Excitation	CI coefficient
1	859	0.179	H $\rightarrow$ L	0.70
3	398	0.991	H - 9 $\rightarrow$ L	0.12
			H - 2 $\rightarrow$ L	0.27
			H - 1 $\rightarrow$ L	0.62

**Table S6.** Cartesian coordinates of the optimized geometry of **6**.

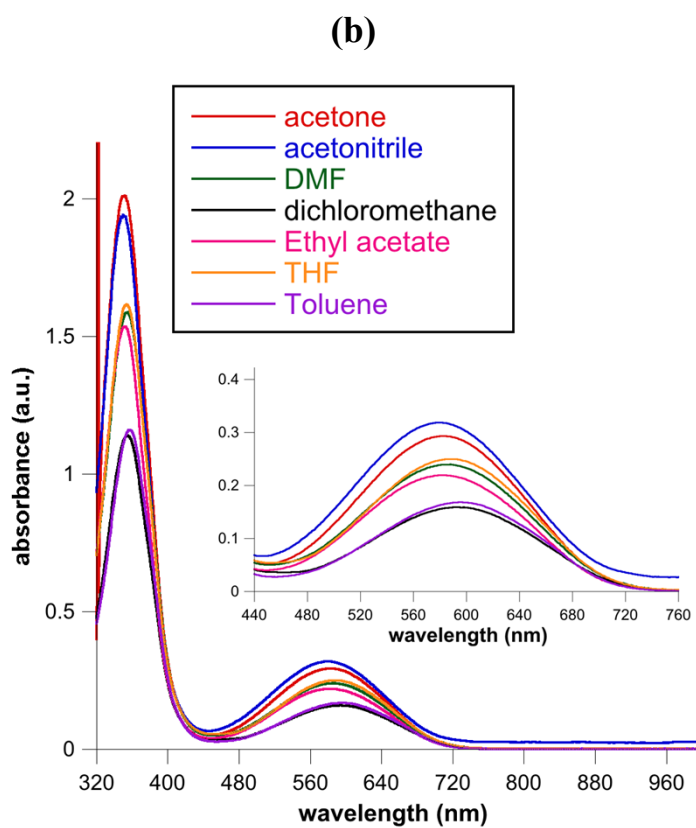
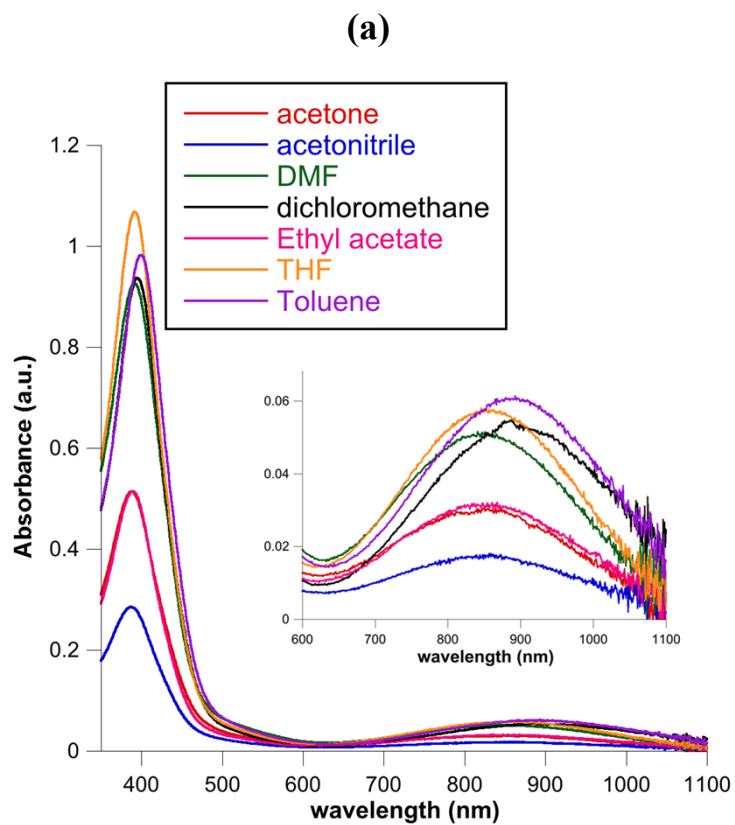
Atom	X (Å)	Y (Å)	Z (Å)
C(1)	-2.3399	0.7181	-0.0328
C(2)	-2.3399	-0.7181	0.0328
N(3)	-1.1755	1.4103	-0.0120
N(4)	-1.1755	-1.4103	0.0120
C(5)	-0.0504	0.7322	0.0279
C(6)	-0.0504	-0.7322	-0.0279
C(7)	1.1836	-1.5495	-0.1824
C(8)	1.1836	1.5495	0.1824
C(9)	1.2983	-2.7577	0.5176
C(10)	2.4188	-3.5635	0.3631
C(11)	3.4372	-3.1986	-0.5243
C(12)	3.3000	-2.0199	-1.2646
C(13)	2.2004	-1.1939	-1.0800
C(14)	1.2983	2.7577	-0.5176
C(15)	2.4188	3.5636	-0.3631
C(16)	3.4372	3.1986	0.5243
C(17)	3.3000	2.0199	1.2646
C(18)	2.2004	1.1939	1.0800
C(19)	4.6094	-4.0861	-0.8230
C(20)	4.6094	4.0861	0.8230
O(21)	5.0371	4.2204	1.9387
O(22)	5.1748	4.7953	-0.1907
O(23)	5.0371	-4.2203	-1.9387
O(24)	5.1748	-4.7953	0.1906
C(25)	5.1615	4.3367	-1.5511
C(26)	5.1615	-4.3367	1.5511
C(27)	-3.6149	1.2852	-0.0631
S(28)	-4.7968	0.0000	0.0000
C(29)	-3.6149	-1.2852	0.0631
C(30)	-4.0135	2.6641	-0.1158

C(31)	-4.0135	-2.6640	0.1158
C(32)	-5.2908	3.1748	-0.2251
C(33)	-5.3404	4.5900	-0.2335
C(34)	-4.1103	5.1828	-0.1338
C(35)	-5.2908	-3.1747	0.2250
C(36)	-5.3404	-4.5900	0.2335
C(37)	-4.1103	-5.1828	0.1338
S(38)	-2.8480	3.9819	-0.0243
C(39)	-3.7845	6.6445	-0.1141
S(40)	-2.8480	-3.9819	0.0243
C(41)	-3.7845	-6.6445	0.1141
H(42)	0.4951	-3.0593	1.1778
H(43)	2.4825	-4.4957	0.9107
H(44)	4.0614	-1.7685	-1.9924
H(45)	2.1175	-0.2826	-1.6587
H(46)	0.4951	3.0593	-1.1778
H(47)	2.4826	4.4957	-0.9107
H(48)	4.0614	1.7685	1.9924
H(49)	2.1175	0.2825	1.6587
H(50)	6.1495	4.5597	-1.9537
H(51)	4.9755	3.2640	-1.6184
H(52)	4.4095	4.8756	-2.1314
H(53)	6.1494	-4.5597	1.9537
H(54)	4.9755	-3.2641	1.6185
H(55)	4.4095	-4.8757	2.1313
H(56)	-6.1702	2.5480	-0.3015
H(57)	-6.2598	5.1562	-0.3142
H(58)	-6.1702	-2.5480	0.3015
H(59)	-6.2598	-5.1562	0.3142
H(60)	-4.7036	7.2291	-0.1880
H(61)	-3.2745	6.9355	0.8093
H(62)	-3.1375	6.9290	-0.9497
H(63)	-4.7036	-7.2291	0.1879
H(64)	-3.2745	-6.9355	-0.8093
H(65)	-3.1375	-6.9290	0.9498

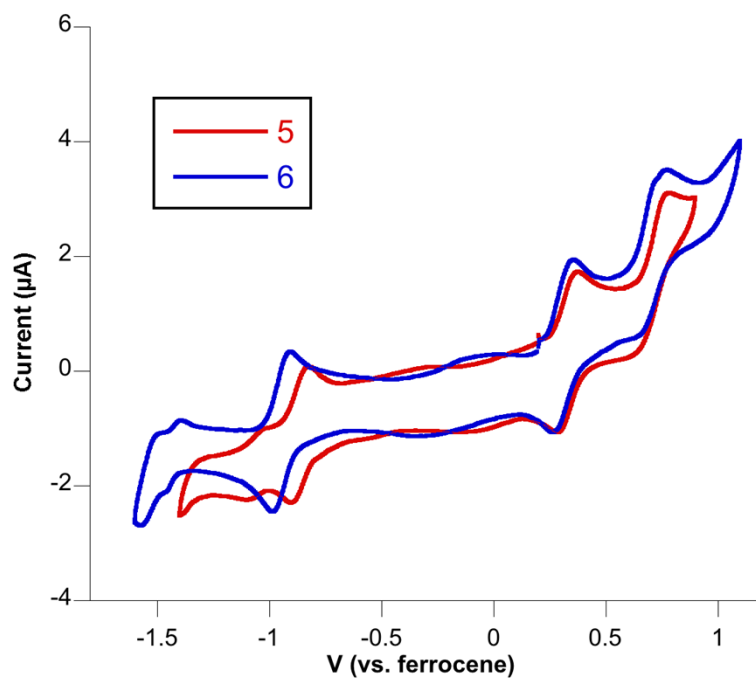
**Table S6.** Cartesian coordinates of the optimized geometry of **5**.

Atom	X (Å)	Y (Å)	Z (Å)
C(1)	-0.7581	-0.7831	-0.0639
C(2)	-0.7828	0.6593	0.0843
N(3)	0.4330	-1.4499	-0.0440
N(4)	0.3886	1.3624	0.0771
C(5)	1.5409	-0.7630	0.0433
C(6)	1.5173	0.7081	0.0049
C(7)	2.7361	1.5436	-0.1671
C(8)	2.7835	-1.5586	0.2298
C(9)	2.8309	2.7636	0.5148
C(10)	3.9279	3.5946	0.3297
C(11)	4.9535	3.2281	-0.5486
C(12)	4.8616	2.0107	-1.2308
C(13)	3.7630	1.1824	-1.0510
C(14)	3.7885	-1.1595	1.1204
C(15)	4.9144	-1.9500	1.3155
C(16)	5.0602	-3.1578	0.6267
C(17)	4.0371	-3.5797	-0.2303
C(18)	2.9155	-2.7894	-0.4298
C(19)	6.2164	4.0262	-0.6974
C(20)	6.2090	-4.0946	0.8691
O(21)	6.0500	-5.2841	0.9412
O(22)	7.4517	-3.5798	1.0558
O(23)	7.2954	3.4970	-0.7468
O(24)	6.1410	5.3810	-0.7319
N(25)	-1.9135	1.3474	0.1759
C(26)	-3.0455	0.6305	0.0966
C(27)	-3.0186	-0.8166	-0.0975
N(28)	-1.8687	-1.5011	-0.1673
C(29)	-4.3503	1.1540	0.1680
S(30)	-5.4875	-0.1485	-0.0119
C(31)	-4.2942	-1.3999	-0.1801
C(32)	-4.7645	2.5165	0.3473
C(33)	-4.6590	-2.7752	-0.3588
S(34)	-6.4652	2.9699	0.4285
C(35)	-6.0725	4.6600	0.6382
C(36)	-4.7150	4.8348	0.6426
C(37)	-3.9714	3.6389	0.4803
C(38)	-5.9294	-3.3139	-0.4334

C(39)	-5.9419	-4.7168	-0.6137
C(40)	-4.6906	-5.2719	-0.6797
S(41)	-3.4550	-4.0515	-0.5166
C(42)	-7.1498	5.6883	0.7846
C(43)	-4.3258	-6.7131	-0.8606
C(44)	7.8629	-2.3244	0.4899
C(45)	4.9717	6.0760	-1.1952
H(46)	2.0322	3.0498	1.1871
H(47)	3.9958	4.5184	0.8910
H(48)	5.6639	1.7216	-1.8982
H(49)	3.7016	0.2543	-1.6049
H(50)	3.6868	-0.2382	1.6797
H(51)	5.6660	-1.6349	2.0285
H(52)	4.1309	-4.5385	-0.7249
H(53)	2.1185	-3.1193	-1.0838
H(54)	-4.2572	5.8091	0.7609
H(55)	-2.8936	3.5787	0.4574
H(56)	-6.8285	-2.7151	-0.3601
H(57)	-6.8491	-5.3025	-0.6924
H(58)	-6.7007	6.6763	0.9026
H(59)	-7.8057	5.7194	-0.0910
H(60)	-7.7788	5.4981	1.6598
H(61)	-5.2312	-7.3160	-0.9540
H(62)	-3.7227	-6.8700	-1.7602
H(63)	-3.7521	-7.0966	-0.0112
H(64)	8.8809	-2.4753	0.1316
H(65)	7.2254	-2.0228	-0.3418
H(66)	7.8647	-1.5425	1.2519
H(67)	5.3374	6.9227	-1.7754
H(68)	4.3454	5.4447	-1.8266
H(69)	4.3860	6.4467	-0.3515



**Figure S2.** UV-vis absorption spectra of (a) compound **5**; and (b) compound **6** in solvents with different polarities.



**Figure S3.** Cyclic voltammograms of compounds **5** and **6** measured in dichloromethane with tetrabutylammonium tetrafluoroborate as the electrolyte (conc. = 0.1 M). Scan rate = 20 mV/s.



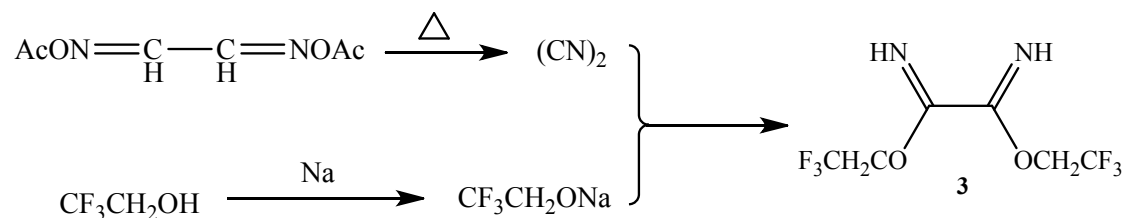
## Experimental Section

**Materials.** All solvents and chemicals were used as received unless otherwise specified. 2-(Tributyl-stannyl)pyridine and tin(II) chloride were obtained from Alfa Aesar. Pd(PPh<sub>3</sub>)<sub>4</sub> was obtained from Apollo. PdBr<sub>2</sub> were obtained from Strem. *p*-Toluenesulfonic acid was obtained from Lancaster Synthesis. 2,2,2-Trifluoroethanol was obtained from Sigma Aldrich. Compounds **2a** and **2b** were synthesized by the reduction of the corresponding dinitro substituted terthiophene derivatives using tin(II) chloride as the reducing agent.

## Instruments

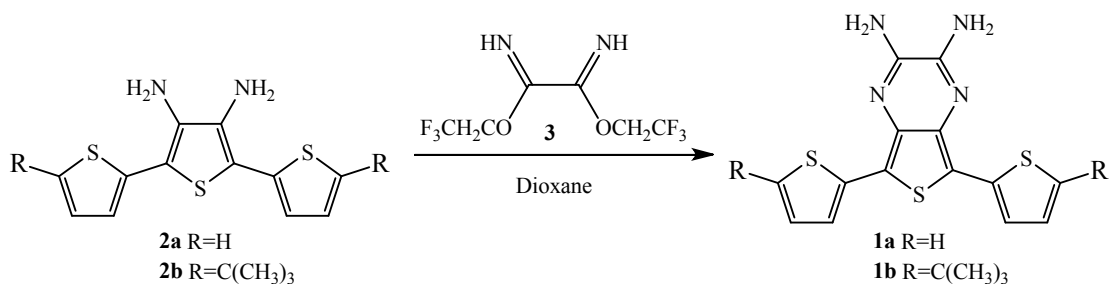
<sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on Bruker DPX 300 MHz, Bruker Avance 400 MHz, Bruker DRX 500 MHz and Bruker Avance 600 MHz spectrometers. <sup>1</sup>H and <sup>13</sup>C NMR signals are reported in ppm. <sup>1</sup>H signals are referenced to the residual proton of a deuterated solvent 7.26 ppm for CDCl<sub>3</sub>, 2.50 ppm for d<sub>6</sub>-DMSO and 4.79 ppm for D<sub>2</sub>O. <sup>13</sup>C NMR signals are referenced to the solvent signal CDCl<sub>3</sub> at 77.0 ppm, 39.5 ppm for d<sub>6</sub>-DMSO. Cyclic voltammety was performed by e-corder 401 potentiostat. UV-vis absorption spectra were recorded on VARIAN CARY 50 Bio. EIMS was recorded on DFS HRMS; ESI was recorded on LCQ Classic Finnigan.

## Synthesis



**Bis(2,2,2-trifluoroethyl) oximidate 3.** Diacetylglyoxim<sup>1</sup> (50 mmol, 8.6 g) was introduced into a three-necked 250 mL round bottom flask equipped with N<sub>2</sub> inlet and N<sub>2</sub> outlet. The N<sub>2</sub> outlet was connected to three traps before exiting to a bleach bubbler. The first trap was cooled by ice-water bath and the second and third ones were cooled to -78 °C. A slow

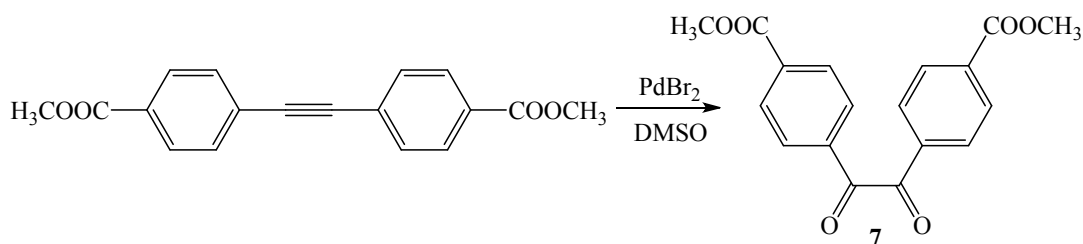
stream of N<sub>2</sub> was allowed to flow through the system. The flask was heated to 160 °C when an exothermic reaction occurred. The temperature was allowed to increase slowly. The first trap contained acetic acid while the other two traps contained cyanogen. In another 100 mL 2-necked round bottom flask, sodium (8.7 mmol, 200 mg) was added to trifluoroethanol (20 mL) at room temperature. The resulting sodium trifluoroethoxide solution was cooled to -50 °C. The trapped liquid cyanogen was allowed to warm up slowly and the cyanogen gas was carried with a N<sub>2</sub> stream to the sodium trifluoroethoxide solution. After addition, the reaction was stirred at room temperature for 1 h. Cold water was added and the mixture was extracted with dichloromethane three times. The combined organic layer was dried over MgSO<sub>4</sub> and the solvent was evaporated to yield the required title compound **3** (6.5g, 53%), which was used for subsequent reactions directly. <sup>1</sup>H NMR (d<sub>6</sub>-DMSO, 400 MHz): δ 9.80 (s, 2H), 4.88-4.78 (m, 4H); <sup>13</sup>C NMR (d<sub>6</sub>-DMSO, 100 MHz): δ 154.9, 127.8, 125.1, 122.3, 119.5, 62.2, 61.9, 61.5, 61.2; MS (ESI): m/z 253.1.



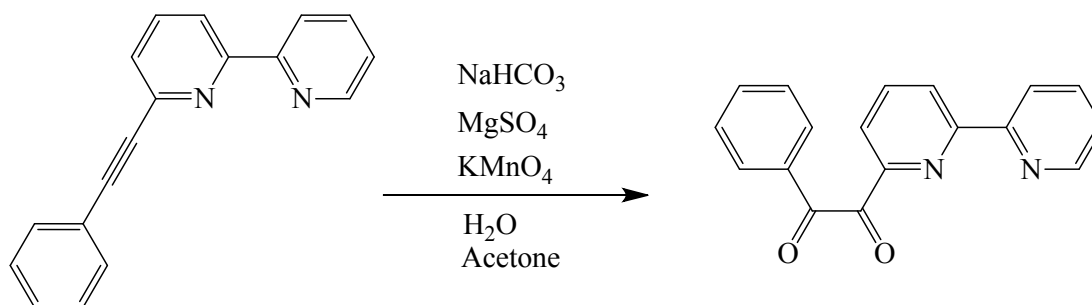
**General procedure for the synthesis of compound 1a-b.** To a solution of degassed dioxane (12 mL), compound **2** (1.41 mmol, 1equiv) and compound **3** (2.12 mmol, 1.5equiv) were added. The mixture was heated at reflux for 5 h. The solvent was evaporated and the residue was subjected directly to silica column chromatography using ethyl acetate/hexane (1:9-3:7) as eluent. The product was purified by recrystallization in hexane.

**1a:** Yield: 65%.  $^1\text{H}$  NMR ( $\text{d}_6\text{-DMSO}$ , 300 MHz):  $\delta$  7.47 (d, 2H,  $J=3.7$  Hz), 7.44 (d, 2H,  $J=5.1$  Hz), 7.07 (dd, 2H,  $J=3.7$  Hz,  $J=5.1$  Hz), 6.78 (s, 4H);  $^{13}\text{C}$  NMR ( $\text{d}_6\text{-DMSO}$ , 100 MHz):  $\delta$  145.5, 135.8, 135.6, 127.1, 124.4, 122.4, 114.3; MS (EI):  $m/z$  329.9 ( $\text{M}^+$ , 100%).

**1b:** Yield: 84%.  $^1\text{H}$  NMR ( $\text{d}_6\text{-DMSO}$ , 400 MHz):  $\delta$  7.24 (d, 2H,  $J=3.7$  Hz), 6.90 (s, 4H), 6.80 (d, 2H,  $J=3.7$  Hz), 1.36 (s, 18H);  $^{13}\text{C}$  NMR ( $\text{d}_6\text{-DMSO}$ , 150 MHz):  $\delta$  155.2, 145.4, 135.4, 132.9, 122.0, 121.7, 114.4, 34.3, 32.3; MS (EI):  $m/z$  442.1 ( $\text{M}^+$ , 100%).



**Diketone 7.** A mixture of bis(4-(methoxycarbonyl)phenyl)acetylene<sup>2</sup> (0.5 mmol, 147 mg) and  $\text{PdBr}_2$ <sup>3</sup> (0.1 mmol, 13 mg) was added into  $\text{DMSO}$  (5 mL). The solution was stirred at 140 °C for 4 h. After cooling to room temperature, water was added and the precipitate was filtered and washed thoroughly by water. Yield: 121 mg (74%).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.18 (d, 4H,  $J=8.6$  Hz), 8.05 (d, 4H,  $J=8.6$  Hz), 3.97 (s, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  192.9, 165.8, 135.8, 135.6, 130.2, 129.9.



**Diketone 8.** NaHCO<sub>3</sub> (0.97 mmol, 82 mg) and MgSO<sub>4</sub> (6.81 mmol, 820 mg) in H<sub>2</sub>O (36 mL) was added to a solution of 6-(phenylethynyl)-2,2'-bipyridine<sup>4</sup> (6.24 mmol, 1.6 g) in acetone (80 mL). KMnO<sub>4</sub> (15.5 mmol, 2.45g) was added in a single portion to the solution with rigorous stirring. The mixture was stirred vigorously at room temperature for 1.5 hours and then quenched by the addition of aqueous NaHSO<sub>3</sub>. After 30 min, the suspension was filtered through celite, and the filtrate was extracted by ethyl acetate three times. The combined organic layer was washed with aqueous K<sub>2</sub>CO<sub>3</sub>, brine, and dried over MgSO<sub>4</sub>. The solvent was evaporated under *vacuo*, yielding the (2,2'-bipyridin)-6-yl-2-phenylethanedione as off-white solid (1.01 mg, 56%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 8.67 (d, 1H, *J*=7.9 Hz), 8.60 (d, 1H, *J*=4.2 Hz), 8.20 (d, 1H, *J*=7.5 Hz), 8.04 (t, 1H, *J*=7.8 Hz), 7.99 (d, 3H, *J*=7.4 Hz), 7.63 (t, 2H, *J*=6.9 Hz), 7.51 (t, 2H, *J*=7.5 Hz), 7.23 (dd, 1H, *J*=4.9 Hz, *J*=6.5 Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz): δ 196.6, 196.5, 156.0, 154.2, 150.8, 148.9, 138.2, 136.9, 134.3, 133.5, 129.2, 128.8, 125.3, 124.2, 122.6, 121.1; MS (EI): *m/z* 288.1 (M<sup>+</sup>, 100%).

**Condensation between diketones and diamines.** The synthesis of **5** is described here as the general procedure. To a degassed solution of ethanol (8 mL), diketones **7** (2.49 mmol, 1.1 equiv), diamines **1** (2.26 mmol, 1 equiv) and *p*-toluenesulfonic acid (0.226 mmol, 0.1 equiv) were added. The mixture was heated under reflux in a N<sub>2</sub> atmosphere overnight. After

cooling, the precipitate was filtered, wash with hot methanol and then with ether to yield the title compound. It was purified by recrystallization with methanol.

**4a.** Yield: 27%. <sup>1</sup>H NMR (d<sub>6</sub>-DMSO, 400 MHz): δ 8.62 (d, 1H, *J*=7.9 Hz), 8.43 (d, 1H, *J*=7.9 Hz), 8.37 (d, 1H, *J*=7.7 Hz), 8.24 (t, 1H, *J*=7.9 Hz), 7.96-7.92 (m, 2H), 7.85-7.79 (m, 2H), 7.72-7.62 (m, 3H), 7.48-7.41 (m, 3H), 7.39 (m, 1H), 7.31-7.24 (m, 2H), 7.20 (d, 8.1 Hz); <sup>13</sup>C NMR (d<sub>6</sub>-DMSO, 150 MHz): δ 160.8, 157.5, 154.4, 153.9, 149.2, 143.8, 143.4, 140.7, 140.6, 138.9, 138.8, 136.9, 133.5, 129.5, 129.2, 128.7, 128.6, 128.1, 128.06, 128.0, 125.8, 125.7, 125.2, 124.4, 123.8, 123.4, 121.3, 120.4; MS (EI): *m/z* 582.2 (M<sup>+</sup>, 100%).

**4b.** Yield: 75%. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 8.59 (m, 1H), 8.45 (d, 1H, *J*=5.2 Hz), 8.42 (d, 1H, *J*=4.1 Hz), 8.06 (t, 1H, *J*=7.8 Hz), 7.96-7.92 (m, 2H), 7.79-7.74 (m, 2H), 7.69-7.65 (m, 2H), 7.55 (m, 1H), 7.37 (m, 3H), 7.24-7.20 (m, 2H), 6.92-6.89 (m, 2H), 1.48 (s, 18H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz): δ 160.8, 160.1, 160.0, 157.4, 155.3, 154.9, 154.5, 148.9, 143.8, 143.4, 141.4, 141.3, 139.3, 138.1, 136.7, 131.7, 131.6, 129.5, 129.4, 128.1, 125.9, 125.8, 125.0, 124.8, 124.5, 123.9, 122.6, 121.7, 121.3, 35.0, 32.4; MS (EI): *m/z* 694.2 (M<sup>+</sup>, 100%). HSMS: Calcd. For C<sub>40</sub>H<sub>34</sub>N<sub>6</sub>S<sub>3</sub>: 694.2007. Found: 694.1988.

**5.** Yield: 77 %. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.04 (d, 4H, *J*=8.4 Hz), 7.75 (d, 2H, *J*=3.8 Hz), 7.70 (d, 4H, *J*=8.4 Hz), 6.90 (d, 2H, *J*=3.8 Hz), 3.95 (s, 6H), 1.47 (s, 18H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ 166.4, 160.3, 158.5, 143.5, 141.6, 141.5, 131.6, 130.1, 129.6, 126.0, 124.8, 122.7, 52.4, 35.0, 32.4; MS (EI): *m/z* 732.2 (M<sup>+</sup>, 100%). HRMS: Calcd. For C<sub>40</sub>H<sub>36</sub>N<sub>4</sub>O<sub>4</sub>S<sub>3</sub>: 732.1899. Found: 732.1920.

**Compound 6.** It was prepared by the same procedure by the reaction between **2b** and **7**. Yield: 75%. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 7.98 (d, 4H, *J*=8.4 Hz), 7.60 (d, 4H, *J*=8.4 Hz), 7.51 (d, 2H, *J*=3.7 Hz), 6.83 (d, 2H, *J*=3.7 Hz), 3.91 (s, 6H), 1.42 (s, 18H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ 166.7, 159.4, 151.2, 143.2, 137.0, 131.5, 130.4, 129.9, 129.4, 125.7, 125.0, 122.2, 52.3, 34.8, 32.4; MS (EI): *m/z* 680.1 (M<sup>+</sup>, 100%). HRMS: Calcd. For C<sub>38</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>S<sub>3</sub>: 680.1837. Found: 680.1821.

### DFT Calculations

The geometric optimization of all the molecules were performed using DFT calculations at the B3LYP/6-311G(d,p) level. The Cartesian coordinates are shown in Tables S1 and S2. Vibrational analysis verified that all the structures were at the minimum of the energy surface. The singlet-singlet transitions were calculated by TDDFT using CAM-B3LYP Coulomb-attenuated functional<sup>5</sup> with the polarizable continuum model<sup>6</sup> using toluene ( $\epsilon = 2.3741$ ) and DMF ( $\epsilon = 37.219$ ). All calculations were performed in Gaussian 09<sup>7</sup> installed in the GRIDPOINT system of the University of Hong Kong. The spatial plots of molecular orbitals were generated by ChemBio3D Ultra 12.0.

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