Supporting Information

Understanding the synthesis mechanism, chemical structures and optical properties of aromatic carbon nitride

Yunhu Wang[1,#], Fangxu Dai[1,2,#], Yafei Tao, Kai Zhang[1], Bingjie Li[1], Mingming Zhang[1,3], Kang Liu[1], Jixiang Xu[1], Lei Wang[1], Jun Xing[1,*]

[1]Key Laboratory of Eco-chemical Engineering, Ministry of Education, College of Chemistry and Molecular Engineering, Qingdao University of Science & Technology, 266042 Qingdao, China.

[2]School of Pharmacy, Jining Medical University, 276800 Rizhao, China.

[3]College of Sino-German Science and Technology, Qingdao University of Science & Technology, Qingdao 266042, China.

[#]These authors contribute equally.

*Correspondence: xingjun@qust.edu.cn

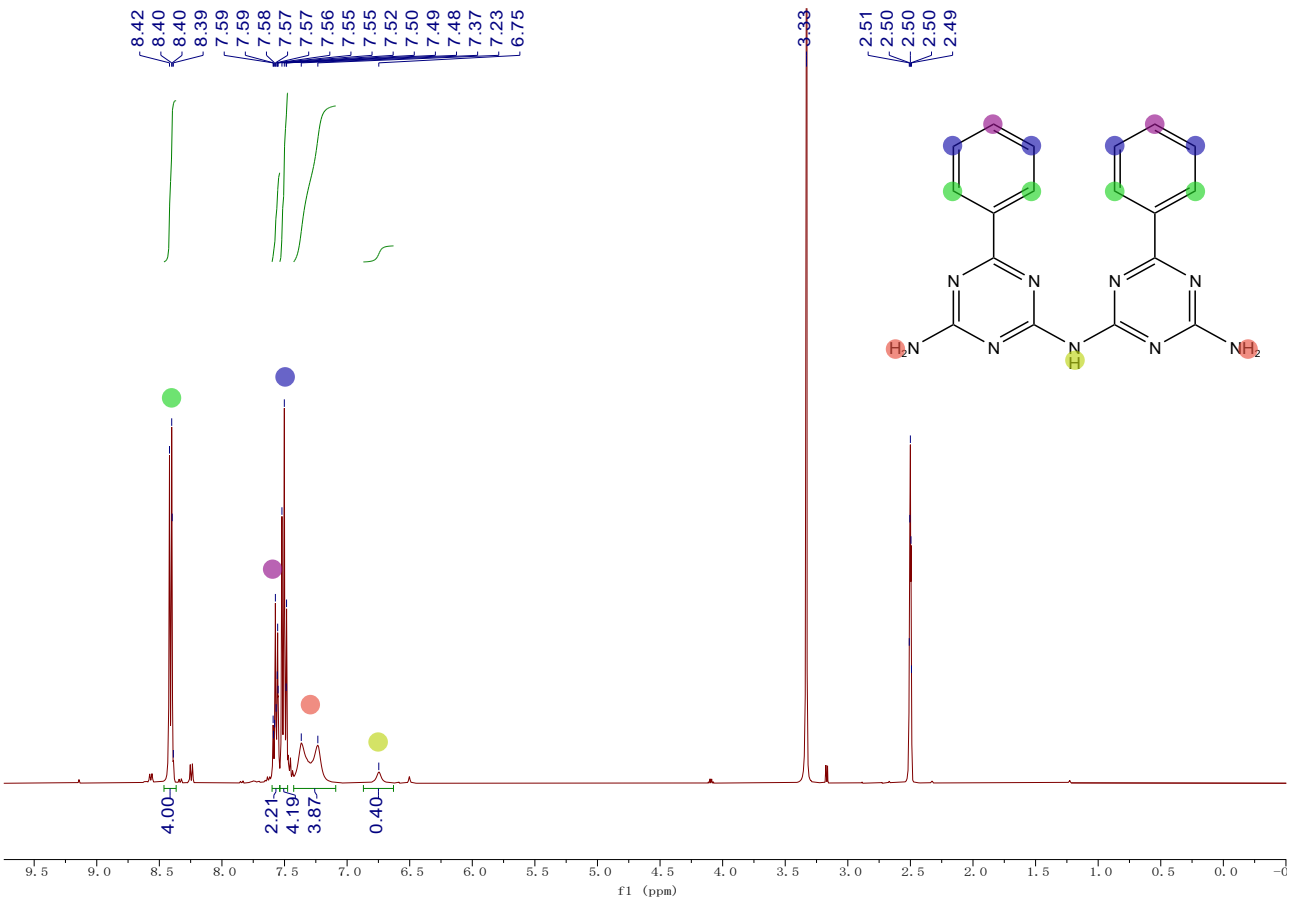

Figure S1. [1]H NMR spectrum of DPT dimer.

[1]H NMR (400 MHz, DMSO-d6) δ 8.44 – 8.37 (m, 4H), 7.62 – 7.53 (m, 2H), 7.50 (t, J = 7.4 Hz, 4H), 7.30 (d, J = 52.9 Hz, 4H), 6.75 (s, 1H).

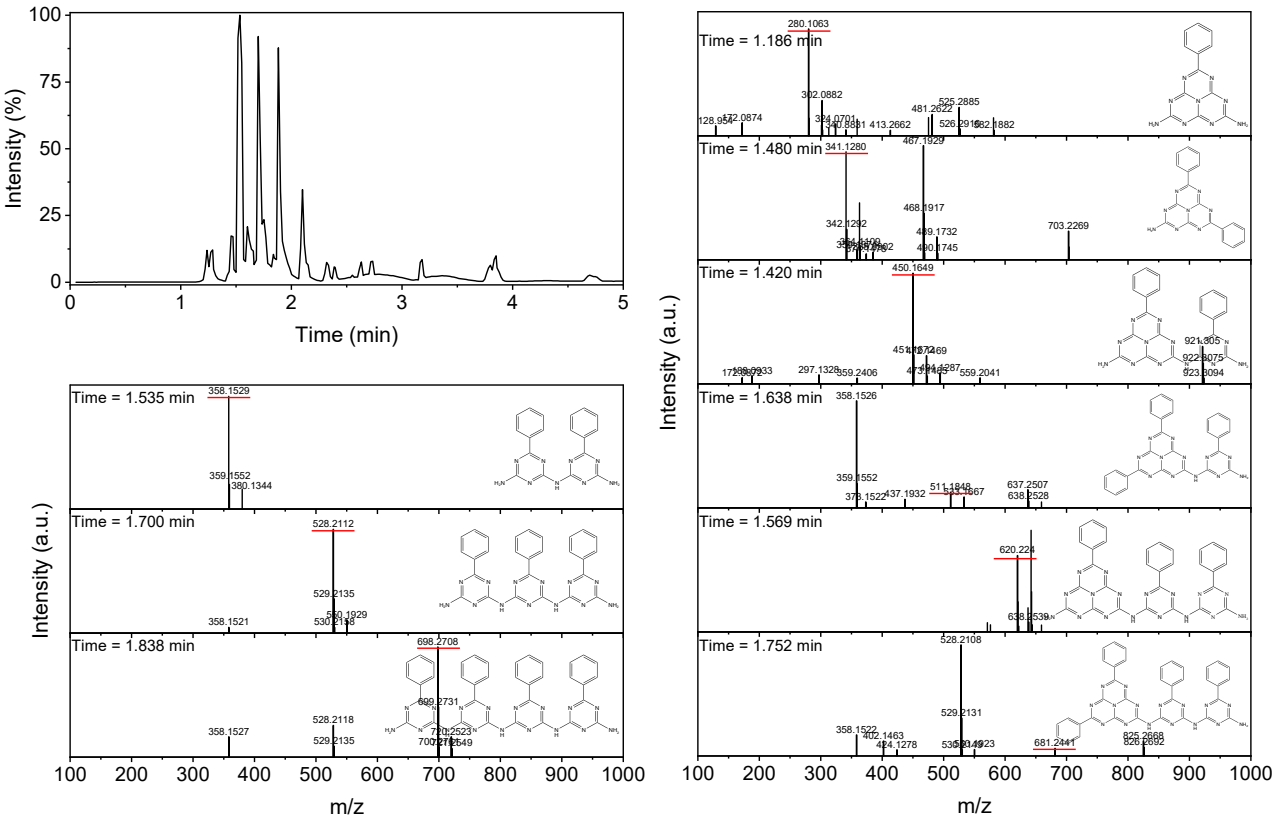

Figure S2. LC-MS spectra of DPT multimer (inset: the molecular structures of intermediates).

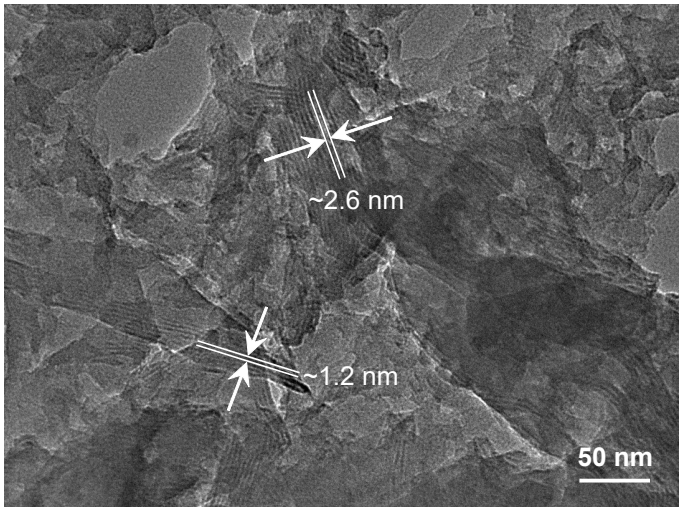

Figure S3. TEM image of PhCN.

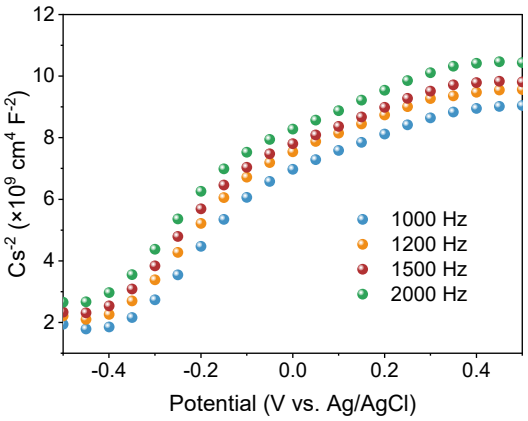

Figure S4. M–S plots of PhCN at different frequencies.

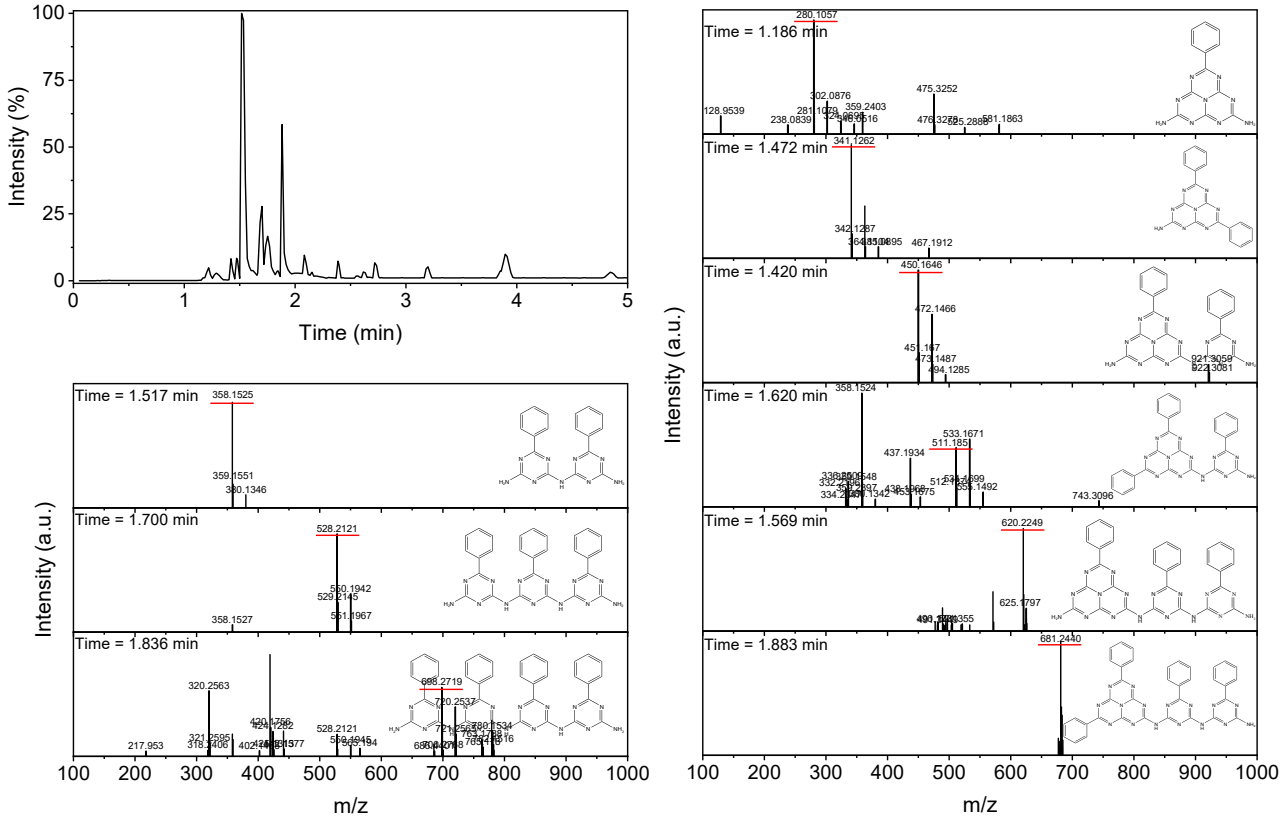

Figure S5. LC-MS spectra of the supernatant of DMF washed PhCN (inset: the molecular structures of intermediates).

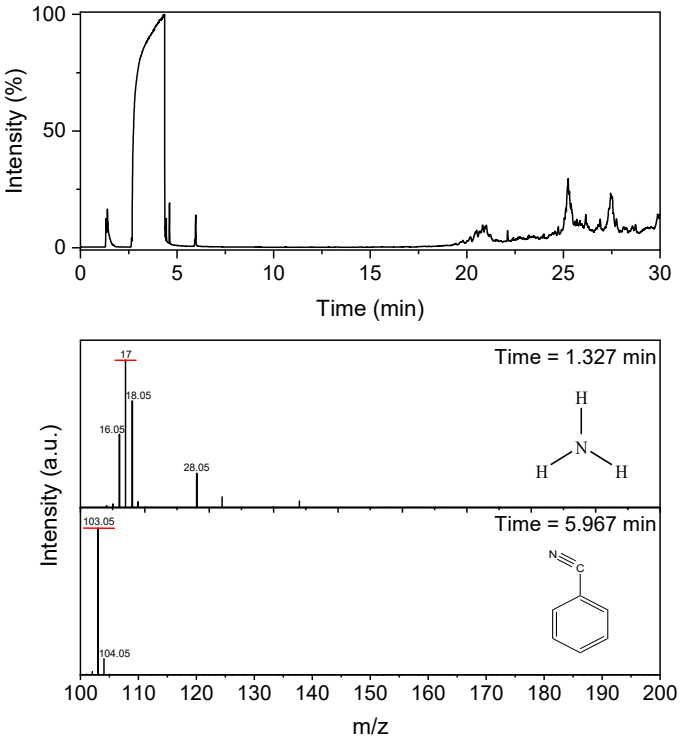

Figure S6. GC-MS spectra of exhaust gas (inset: the molecular structures of volatile gases).

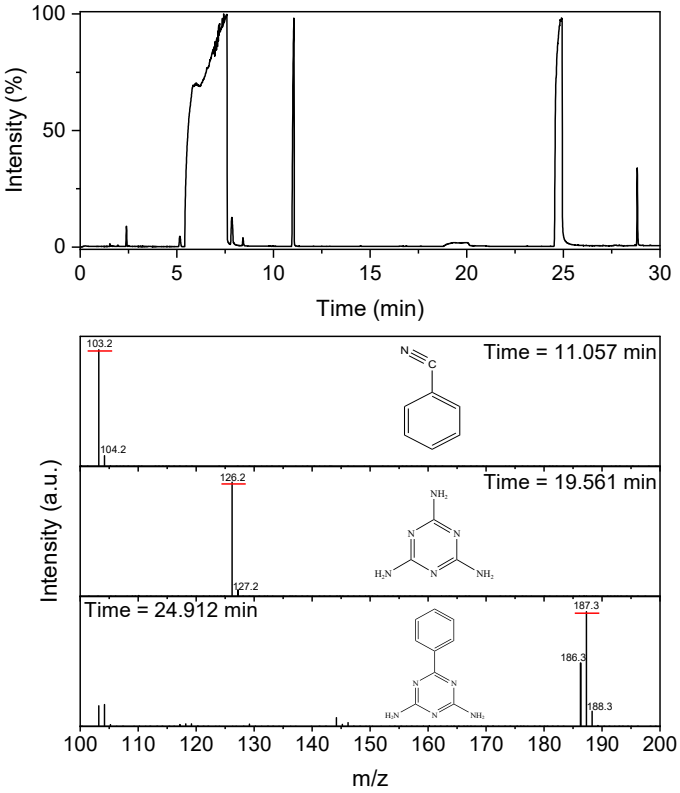

Figure S7. GC-MS spectra of downstream deposit in the tuber furnace (inset: the molecular structures of volatile compounds).

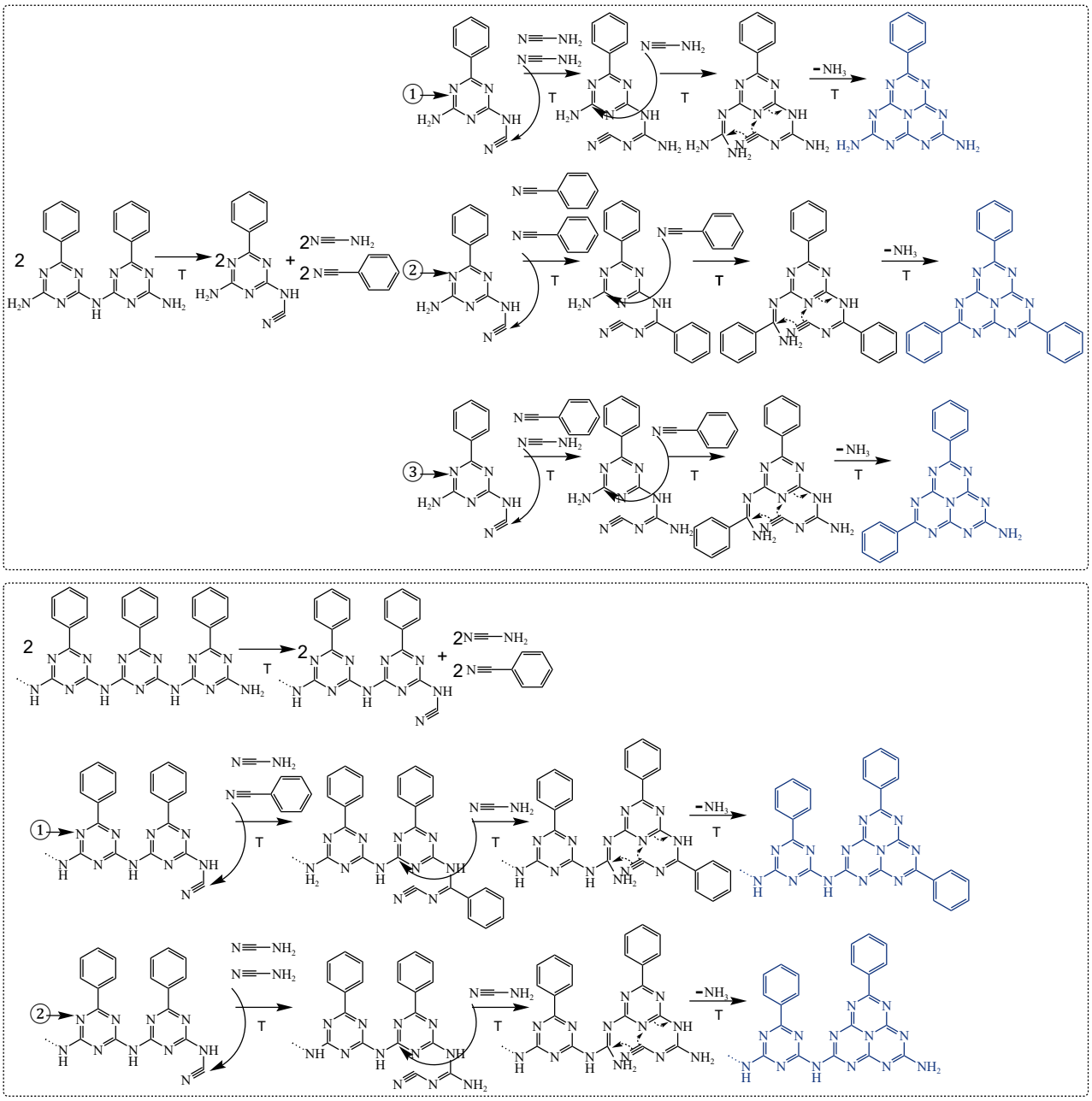

Figure S8. Schematic diagram of ring-opening isomerization reaction.

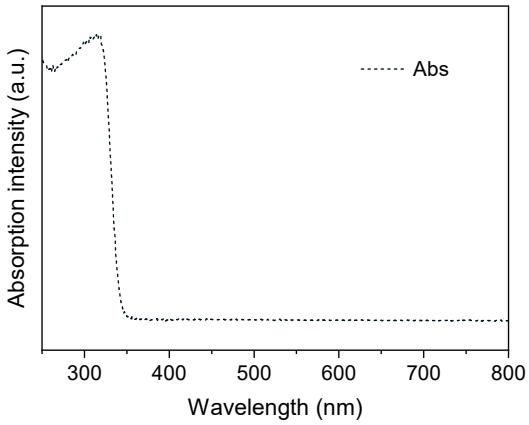

Figure S9. UV-vis absorption spectrum of DPT monomer.

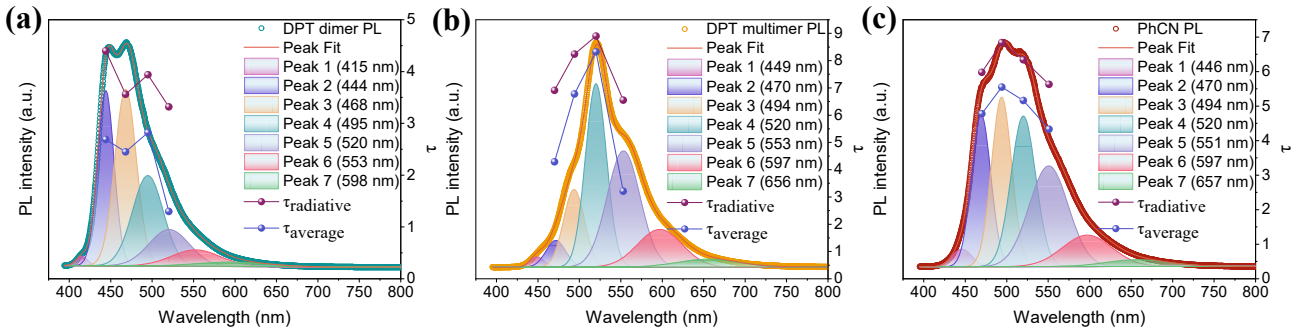

Figure S10. The positive correlation graph between PL spectra and PL lifetimes of (a) DPT dimer, (b) DPT multimer, and (c) PhCN.

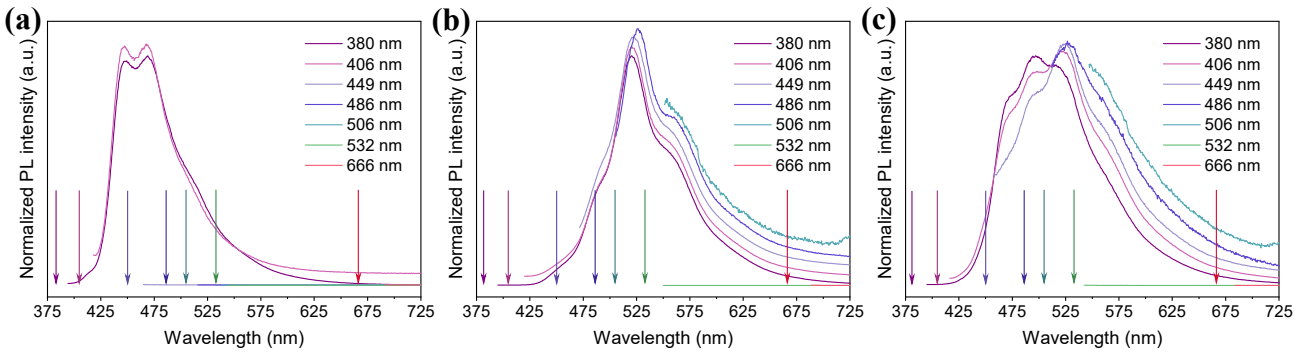

Figure S11. Normalized PL spectra of (a) DPT dimer, (b) DPT multimer, and (c) PhCN under different excitation lights.

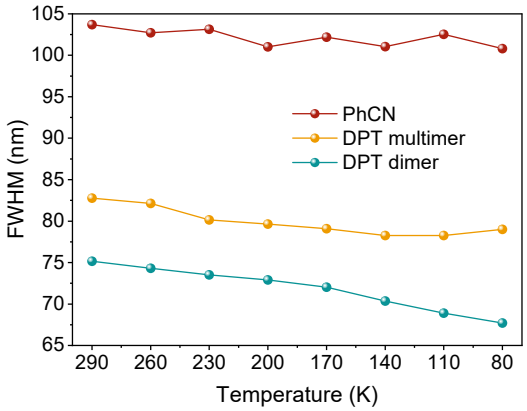

Figure S12. The FWHM of DPT dimer, DPT multimer, and PhCN at different temperatures.

Table S1. Fitted peak, FWHM and element content of C 1s spectra of DPT monomer, DPT dimer, DPT multimer, and PhCN.

		DPT monomer	DPT dimer	DPT multimer	PhCN
C1	Peak BE (eV)	285.1	285.2	285.2	285.1
	FWHM (eV)	1.3	1.4	1.3	1.3
C2	Peak BE (eV)	286.4	286.5	286.4	286.5
	FWHM (eV)	1.1	1.2	1.2	1.0
C3	Peak BE (eV)	287.1	287.4	287.4	287.1
	FWHM (eV)	1.1	1.2	1.4	1.4
C4	Peak BE (eV)	289.1	289.1	289.1	289.0
	FWHM (eV)	1.4	1.3	1.3	1.1

Table S2. Fitted peak, FWHM and element content of N 1s spectra of DPT monomer, DPT dimer, DPT multimer, and PhCN.

		DPT monomer	DPT dimer	DPT multimer	PhCN
N1	Peak BE (eV)	398.6	398.8	398.9	398.9
	FWHM (eV)	1.3	1.2	1.2	1.3
	Atomic (%)	61.7	58.1	47.4	63.2
N2	Peak BE (eV)	399.6	399.9	399.9	399.7
	FWHM (eV)	1.5	1.4	1.5	1.5
	Atomic (%)	38.3	42.0	52.6	19.9
N3	Peak BE (eV)	405.0	404.7	404.7	405.0
	FWHM (eV)	3.4	3.4	3.4	3.4
	Atomic (%)	-	-	-	-
N4	Peak BE (eV)	-	-	-	401.0
	FWHM (eV)	-	-	-	1.7
	Atomic (%)	-	-	-	16.9

Table S3. PL fitting data of DPT dimer, DPT multimer, and PhCN.

Samples	Peak fit	Peak center (nm)	Peak area	Peak area percentage (%)
DPT dimer	Peak 1	415	0.71	0.87
	Peak 2	444	19.33	23.63
	Peak 3	468	25.57	31.26
	Peak 4	495	18.76	22.93
	Peak 5	520	9.92	12.13
	Peak 6	553	5.37	6.56
	Peak 7	598	2.13	2.61
DPT multimer	Peak 1	449	0.94	1.15
	Peak 2	470	3.53	4.32
	Peak 3	494	11.00	13.46
	Peak 4	520	25.98	31.78
	Peak 5	553	25.87	31.65
	Peak 6	597	11.21	13.71
	Peak 7	656	3.20	3.91
PhCN	Peak 1	446	2.33	2.13
	Peak 2	470	19.66	17.96
	Peak 3	494	22.96	20.97
	Peak 4	520	24.88	22.73
	Peak 5	551	26.45	24.16
	Peak 6	597	10.41	9.51
	Peak 7	657	2.78	2.54

Table S4. PL lifetime of DPT dimer, DPT multimer, and PhCN.

Samples	Emission wavelength (nm)	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	τ_{ave} (ns)
DPT dimer	444	1.09	4.40	-	2.69
	468	0.81	3.56	-	2.45
	495	0.81	3.94	-	2.82
	520	0.34	3.32	-	1.30
DPT multimer	470	0.31	1.76	6.91	4.29
	494	1.62	8.24	-	6.78
	520	0.91	8.90	-	8.32
	553	0.14	6.55	-	3.21
PhCN	470	0.99	5.98	-	4.78
	494	1.05	6.84	-	5.55
	520	0.95	6.34	-	5.16
	551	0.91	5.63	-	4.33