Supporting Information

Cyanophenylcarbazole isomers exhibiting different UV and visible light excitable room temperature phosphorescence

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Table S3b The singlet and triplet excited state transition configurations of the MCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1\text{-}T_n| < 0.3$ eV were highlighted in red. (for the upper interacted pair in Figure 5)

Table S3c The singlet and triplet excited state transition configurations of the OCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1\text{-}T_n| < 0.3$ eV were highlighted in red. (for the upper interacted pair in Figure 5)

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Table S3e The singlet and triplet excited state transition configurations of the 3CN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1\text{-}T_n| < 0.3$ eV were highlighted in red. (for the upper interacted pair in Figure 5)

Table S4a The singlet and triplet excited state transition configurations of the PCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1\text{-}Tn| < 0.3$ eV were highlighted in red. (for the bottom interacted pair in Figure 5)

Table S4b The singlet and triplet excited state transition configurations of the MCN from single crystal revealed by TD-DFT calculations. The matched excited states that

contain the same orbital transition components of S_1 and $|S_1-T_n| < 0.3$ eV were highlighted in red. **(**for the bottom interacted pair in Figure 5**)**

Table S4c The singlet and triplet excited state transition configurations of the OCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1-T_n| < 0.3$ eV were highlighted in red. **(**for the bottom interacted pair in Figure 5**)**

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Table S4e The singlet and triplet excited state transition configurations of the 3CN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1-T_n| < 0.3$ eV were highlighted in red. **(**for the bottom interacted pair in Figure 5**)**

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Measurements

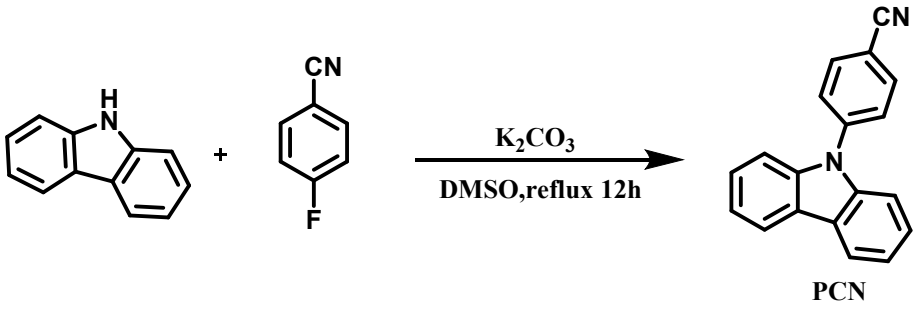
^{1}H and ^{13}C NMR spectra were recorded on a Bruker AC500 spectrometer at 500 MHz and 125 MHz, respectively, using deuterated chloroform ($CDCl_3$) as the solvent and tetramethylsilane (TMS) as the internal standard. UV-visible absorption and photofluorescence and phosphorescence emission spectra were recorded on Hitachi U-4100 and Hitachi F-4600 spectrophotometers, respectively. Differential scanning calorimetry (DSC) curves were determined on a Netzsch DSC (204F1) instrument at a heating rate of 10 ^{o}C min^{-1}. Thermogravimetric analysis (TGA) was performed on a Netzsch (209F1) thermogravimetric analyzer in a nitrogen atmosphere (50 mL min^{-1}) at a heating rate of 10 ^{o}C min^{-1}. Time-resolved spectra were recorded by a Hamamatsu compact fluorescence lifetime spectrometer (FLS-1000). The gas chromatography and mass spectroscopy were recorded by Agilent Technologic 7890A.

The Gaussian 09 program was utilized to perform the TD-DFT calculations. The ground state (S_0) geometry was obtained from the single crystal structure and no further geometry optimization was conducted in order to maintain the specific molecular configuration and corresponding intermolecular locations. The exciton energies of the n-th singlet (S_n) and n-th triplet states (T_n) were obtained on the corresponding ground state structure using TD-B3LYP/6-31G*. The Kohn–Sham frontier orbital analysis and spin density distributions were obtained in order to elucidate the mechanisms of possible singlet–triplet intersystem crossings (ISC). The possible S_1 to T_n ISC channels are believed to share part of the same transition orbital compositions, and the energy levels of possible Tn are considered to lie within the range of $E_{S1} \pm 0.3$ eV. Especially, the major ISC channels are mainly determined based on two elements. First, the ratio of the same transition configuration in S_1 and T_n should be large in all the transition orbital compositions. Secondly, the energy gap between S_1 and the specific T_n state should be small.

Experimental section

1.Synthesis

4-(9H-carbazol-9-yl)benzonitrile (PCN)

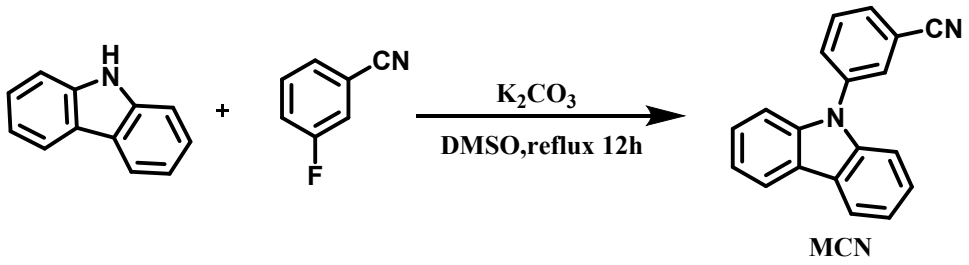


Scheme S1a The Synthetic route of PCN.

In a 100 mL bottom, 9H-carbazole (3 g, 17.94 mmol) and K_2CO_3 (8.22 g, 26.91 mmol) in DMSO (30 ml) was stirred at room temperature for 1 h. 4-Fluorobenzonitrile (2.61 g, 21.5 mmol) was added in the mixture and stirred at 150 °C for 12 h. The reaction mixture was poured into a large amount of ice water and stirred for additional 1 h. After the reaction mixture was extracted with ethyl acetate, the combined organic layer dried with anhydrous $MgSO_4$, filtered and concentrated in vacuo. The crude product was purified by silica-gel column chromatography using petroleum ether/ethyl acetate (10:1 v/v) as the eluent to give the compound as a white solid (4.09 g, Yield 85 %).

^{1}H NMR (500 MHz, Chloroform-*d*): δ 8.14 (d, J = 7.7 Hz, 2H), 7.92–7.86 (m, 2H), 7.75–7.70 (m, 2H), 7.49–7.38 (m, 4H), 7.33 (ddd, J = 8.0, 6.2, 1.9 Hz, 2H).^{13}C NMR (125MHz, Chloroform-*d*): δ 142.05, 139.87, 133.89, 127.08, 126.35, 123.98, 120.97, 120.55, 118.33, 110.45, 109.49.

3-(9H-carbazol-9-yl)benzonitrile (MCN)



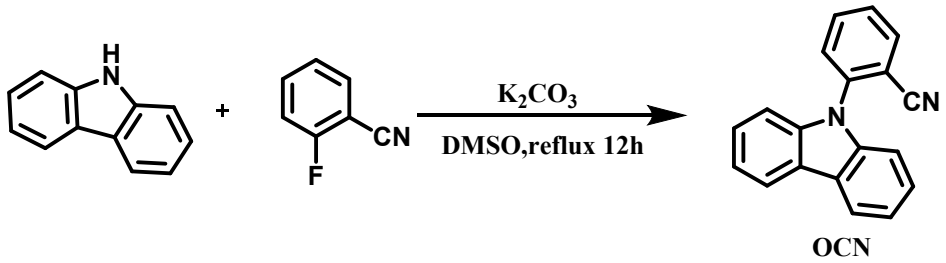
Scheme S1b The Synthetic route of MCN.

NPC-mCN was prepared following the same procedure of NPC-pCN by using 3-fluorobenzonitrile. The eluent is petroleum ether/ethyl acetate (20:1 v/v), yielding a white solid (3.66 g, Yield 76 %).

^{1}H NMR (500 MHz, Chloroform-*d*): δ 8.16 (ddd, J = 7.7, 1.2, 0.7 Hz, 2H), 7.91 (d, J = 3.6 Hz, 1H), 7.88–7.84 (m, 1H), 7.78–7.72 (m, 2H), 7.45 (ddd, J = 8.2, 7.0, 1.2 Hz, 2H), 7.39 (dt, J = 8.3, 0.9 Hz, 2H), 7.34 (ddd, J = 7.9, 7.0, 1.1 Hz, 2H).^{13}C NMR (126 MHz, Chloroform-*d*) : δ 140.21, 138.89, 131.47, 130.93, 130.70, 130.30, 126.29, 123.72,

120.74, 120.52, 117.87, 114.20, 109.23.

2-(9H-carbazol-9-yl)benzonitrile (OCN)



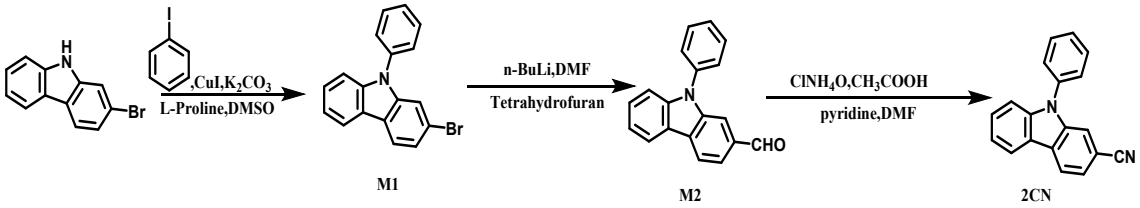
OCN

Scheme S1c The Synthetic route of OCN.

NPC-oCN was prepared following the same procedure of NPC-pCN by using 2-fluorobenzonitrile. The eluent is petroleum ether/ dichloromethane (5:2 v/v), yielding a white solid (3.85 g, Yield 80%).

^{1}H NMR (500 MHz, Chloroform-*d*): δ 8.15 (dt, J = 7.7, 1.0 Hz, 2H), 7.96 (dd, J = 8.1, 1.6 Hz, 1H), 7.84 (td, J = 7.8, 1.6 Hz, 1H), 7.67–7.59 (m, 2H), 7.43 (ddd, J = 8.2, 7.1, 1.2 Hz, 2H), 7.33 (td, J = 7.5, 1.0 Hz, 2H), 7.21 (dd, J = 8.1, 0.9 Hz, 2H).^{13}C NMR (126 MHz, Chloroform-*d*): δ 140.70, 140.60, 134.49, 134.26, 129.67, 128.43, 126.17, 123.87, 120.76, 120.52, 115.98, 112.85, 109.65.

9-phenyl-9H-carbazole-2-carbonitrile (2CN)



M1 M2 2CN

Scheme S1d The Synthetic route of 2CN.

A mixture of iodobenzene (3.11 g, 15.25 mmol), 2-bromocarbazole (2.5 g, 10.16 mmol), CuI (0.94 g, 1.01 mmol), L-proline (0.11 g, 1.01 mmol), and K_2CO_3 (2.20 g, 20.33 mmol) in dimethyl sulfoxide (30 mL) was stirred for 36 hours at 110 °C under nitrogen. After being cooled to room temperature, water was added and extracted with CH_2Cl_2 and dried over anhydrous $MgSO_4$. Solvent was removed, and the residue was purified by column chromatography on silica gel using petroleum ether as the eluent. A white solid (1.80 g, Yield 55%) was obtained, which was regarded as 2-bromo-9-phenyl-9H-carbazole (M1).

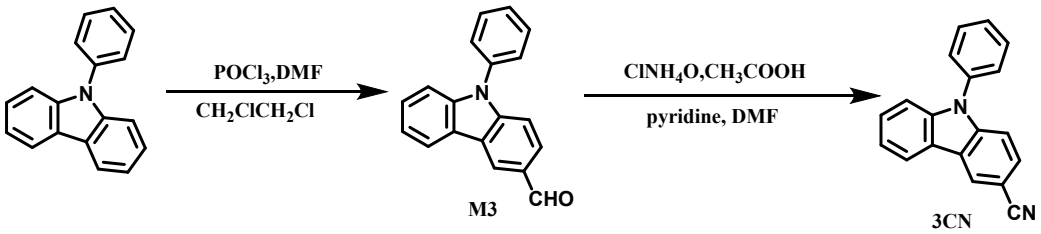
n-BuLi (4.52 mL, 11.19 mmol) was added dropwise to a solution of M1(1.80 g, 5.59 mmol) in anhydrous THF (15 mL) at −78 °C under nitrogen atmosphere. After stirring for 0.5 h, anhydrous DMF (2.61 mL, 33.49 mmol) was added, and the mixture was stirred for an additional 12 h at room temperature. Water and CH_2Cl_2 were added to the mixture, and the organic layer was separated, washed with saturated $NaHCO_3$, and dried over $MgSO_4$. The solvent was removed, and the residue was purified by silica-gel column chromatography using petroleum ether/ethyl acetate (15:1 v/v) to give 9-phenyl-9H-carbazole-2-carbaldehyde (M2) as a white solid (0.82 g, Yield 54%).

A mixture of M2 (0.82 g, 3.01 mmol), hydroxyamine hydrochloride ($ClNH_4O$, 0.26

g, 3.68 mmol), acetic acid (CH_3COOH, 0.62 mL, 10.76 mmol), pyridine (0.41 mL, 5.39 mmol) and DMF (3 mL) was stirred and heated at 140 °C for five hours. The crude product was extracted with dichloromethane and washed with water. The crude product was purified by silica-gel column chromatography using petroleum ether/ dichloromethane (3:2 v/v) as the eluent to give the compound as a white solid (0.65 g, Yield 80 %).

^{1}H NMR (500 MHz, Chloroform-*d*): δ 8.18 (t, J = 8.5 Hz, 2H), 7.65 (dd, J = 16.2, 8.4 Hz, 3H), 7.57–7.47 (m, 5H), 7.42 (d, J = 8.3 Hz, 1H), 7.35 (t, J = 7.4 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*): δ 142.07, 139.84, 136.46, 130.20, 128.32, 127.92, 127.01, 126.68, 122.99, 122.10, 121.13, 120.95, 120.84, 120.00, 114.09, 110.28, 108.32.

9-phenyl-9H-carbazole-3-carbonitrile (3CN)



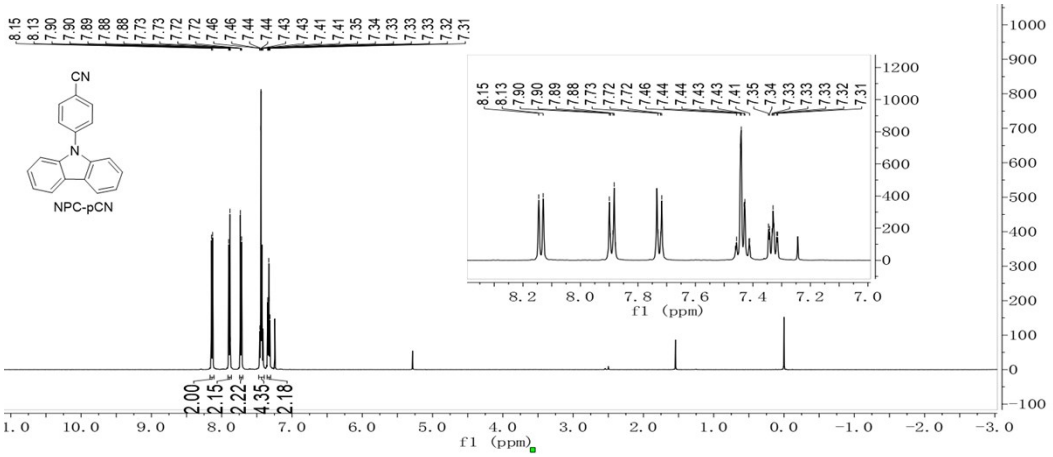
Scheme S1e The Synthetic route of 3CN.

A mixture of phosphoryl chloride (0.42 mL, 4.5 mmol) and anhydrous DMF (1.04 mL, 13.50 mmol) was stirred at 0 °C for 1 h, and then 9-phenyl-9H-carbazole (1.00 g, 4.10 mmol, in 20 mL sym-dichloroethane) was added. The reaction temperature was raised to 90 °C and stirred for 8 h. After cooling, the mixture was poured into ice water and extracted with dichloromethane. The solvent was evaporated, and the crude product was purified by a column chromatography on silica gel using petroleum ether/ethyl acetate (1/3) as the eluent to give the compound as a white solid (0.88 g, Yield 79%).

NPC-3CN was prepared following the same procedure of NPC-2CN by using M3. A white solid was obtained (0.71 g, Yield 82%).

^{1}H NMR (500 MHz, Chloroform-d): δ 8.45 (d, J = 1.5 Hz, 1H), 8.16 (d, J = 7.8 Hz, 1H), 7.68–7.61 (m, 3H), 7.56–7.46 (m, 4H), 7.43–7.34 (m, 3H). ^{13}C NMR (125 MHz, Chloroform-d): δ 142.54, 141.61, 136.40, 130.14, 129.14, 128.40, 127.35, 127.09, 125.23, 123.44, 122.14, 121.20, 120.61, 120.37, 110.47, 110.34, 102.62.

2. Figures



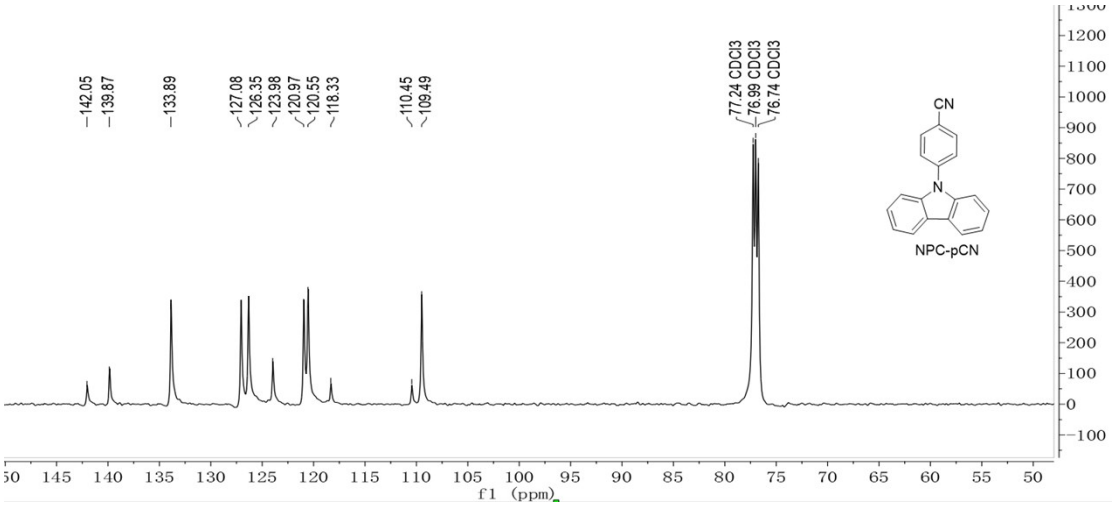


Figure S1a ^{1}H and ^{13}C NMR spectra of PCN in $CDCl_3$.

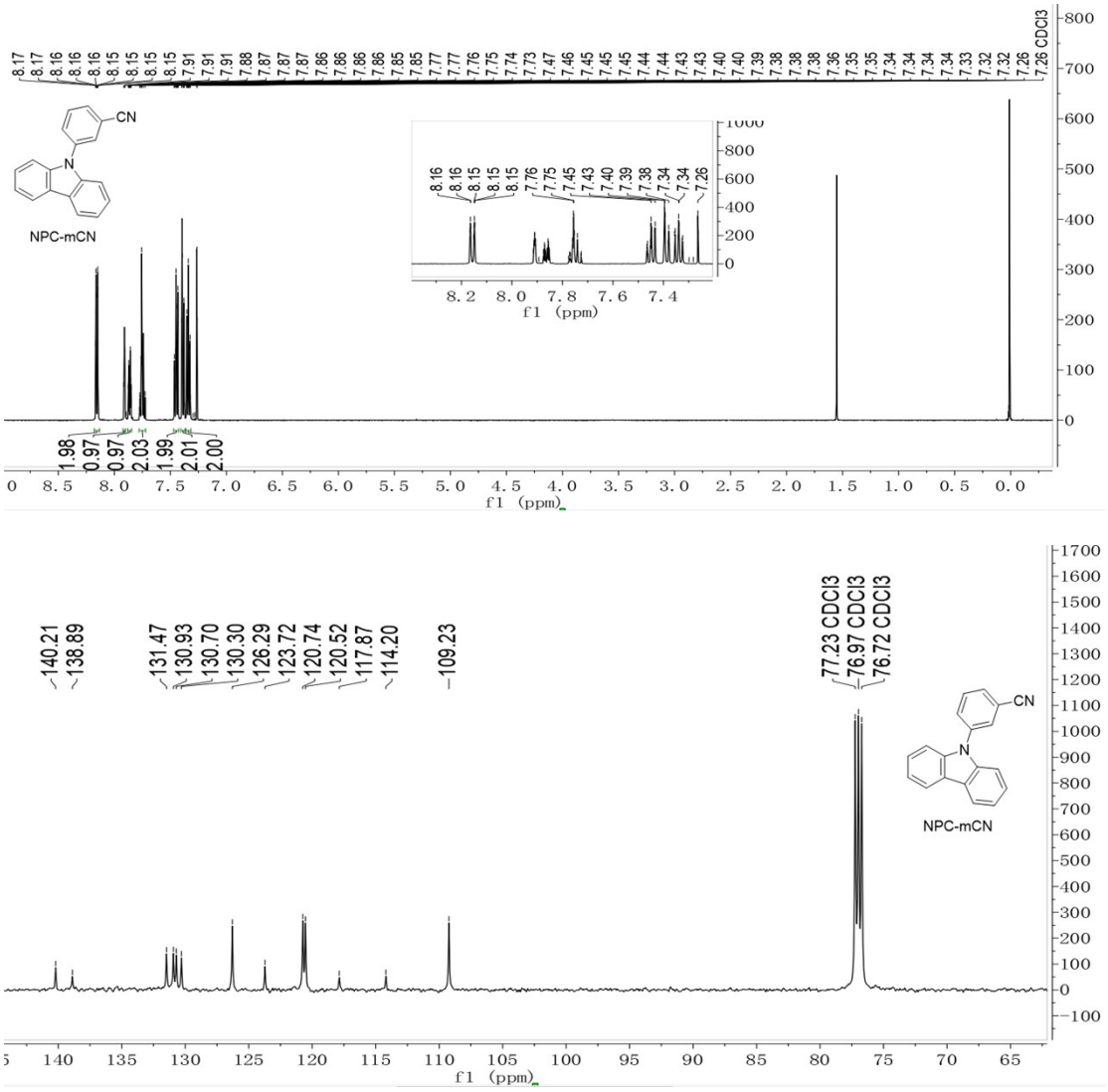


Figure S1b ^{1}H and ^{13}C NMR spectra of MCN in $CDCl_3$.

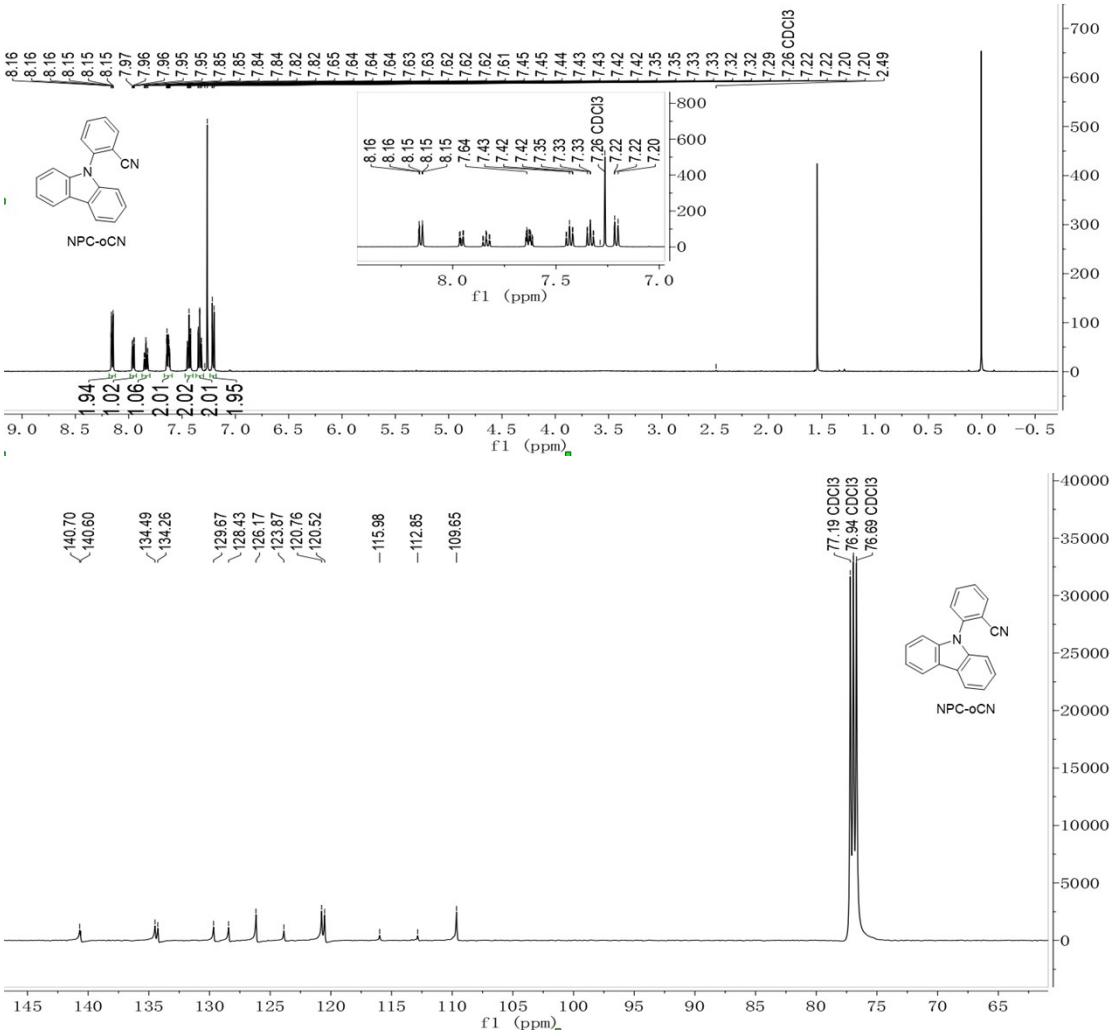
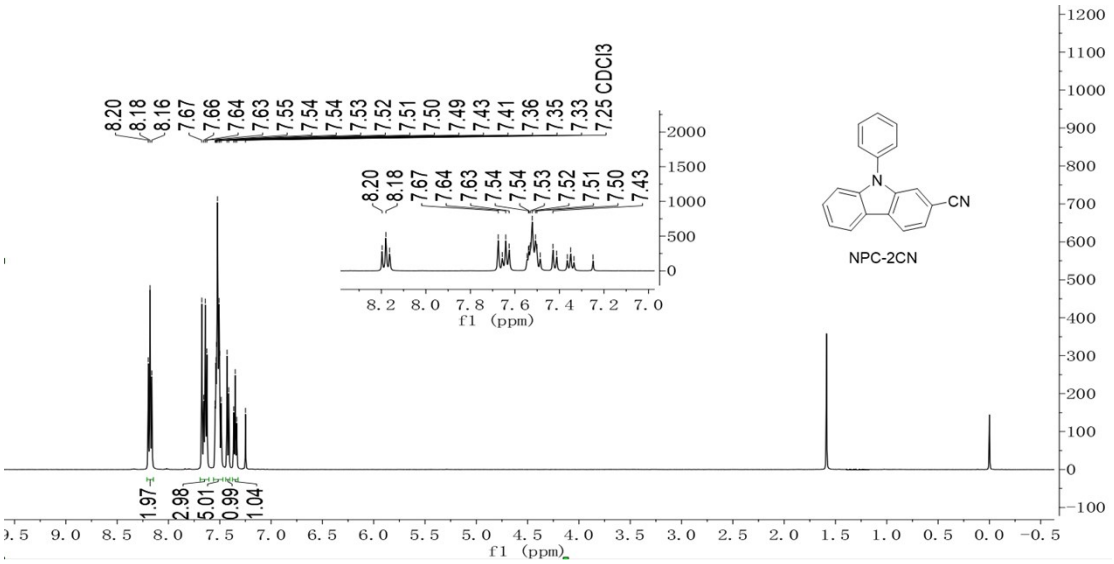


Figure S1c ^{1}H and ^{13}C NMR spectra of OCN in $CDCl_3$.



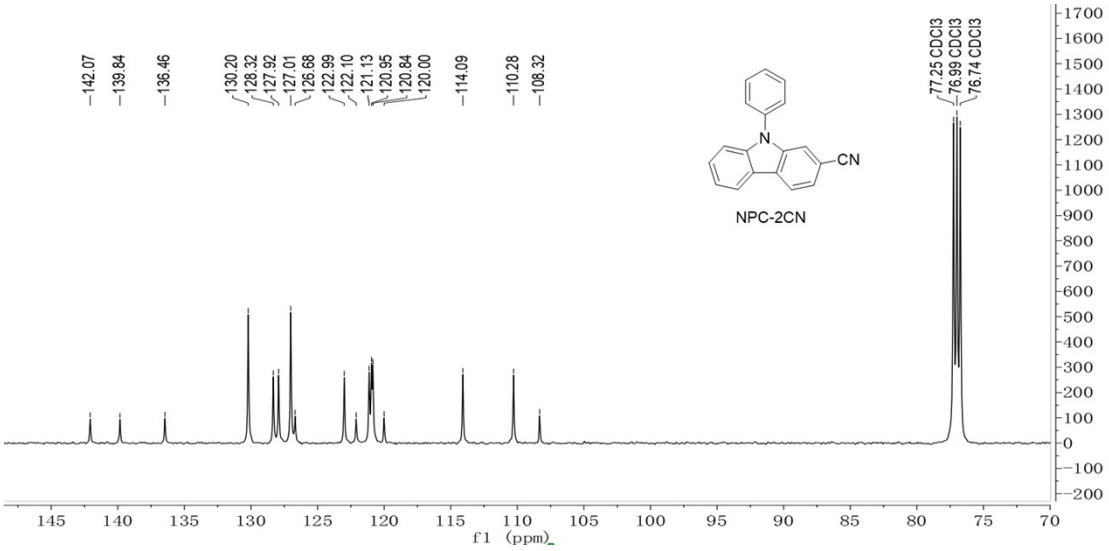


Figure S1d ^{1}H and ^{13}C NMR spectra of 2CN in $CDCl_3$.

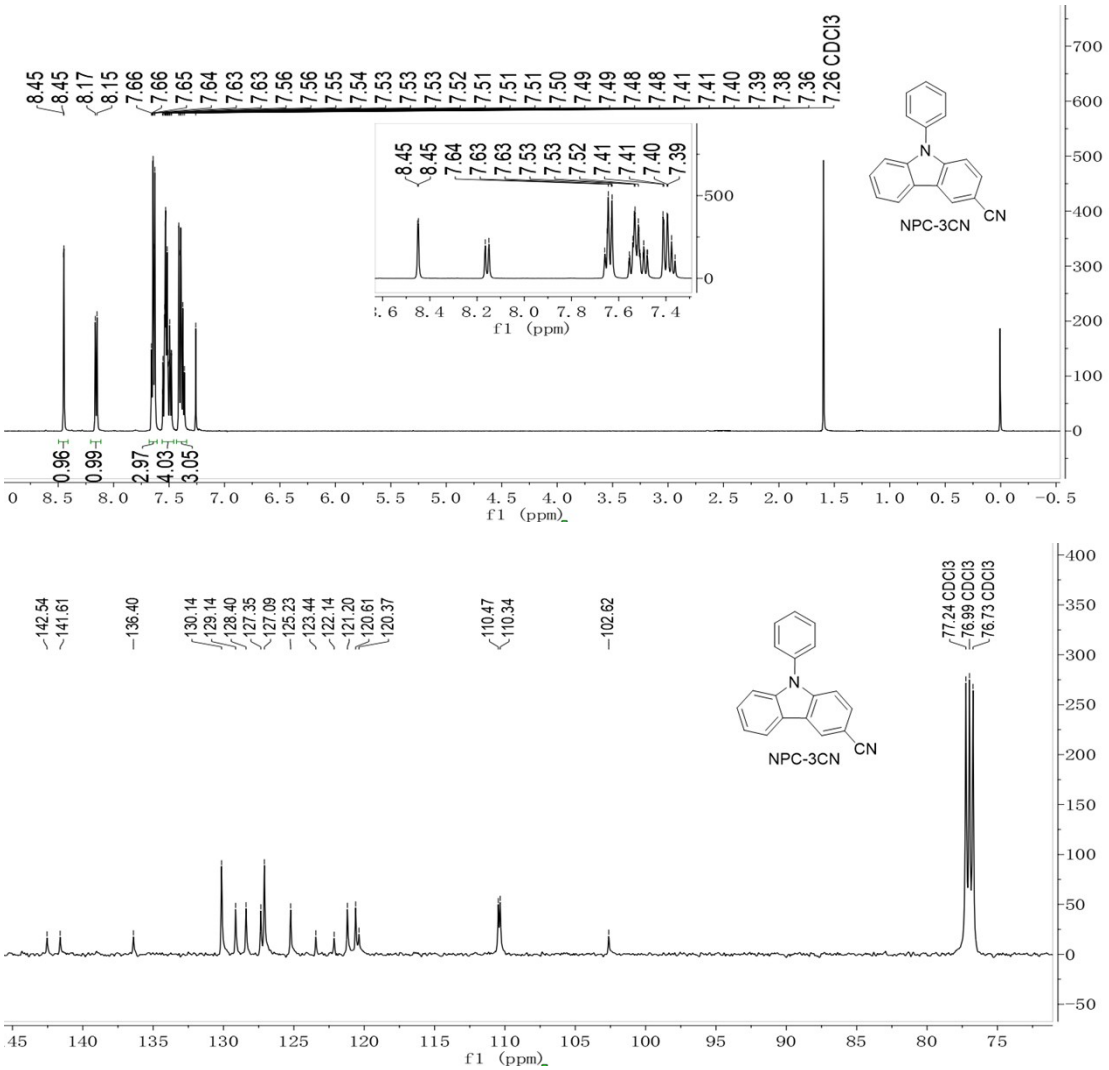


Figure S1e ^{1}H and ^{13}C NMR spectra of 3CN in $CDCl_3$.

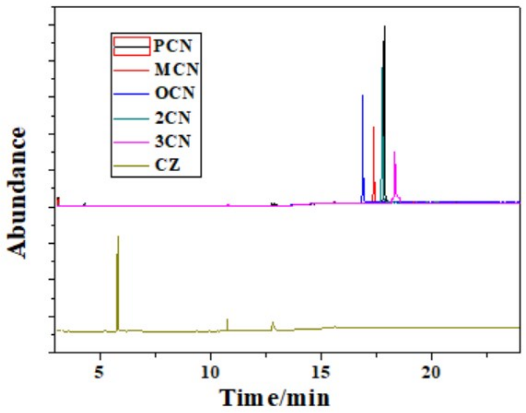


Figure S2 The gas chromatograms of XCN and CZ.

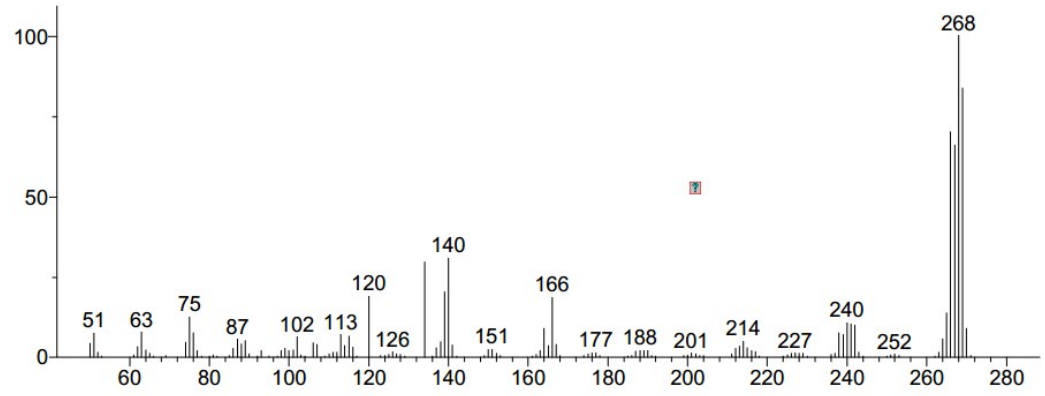


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Figure S3a The mass spectrum of PCN.

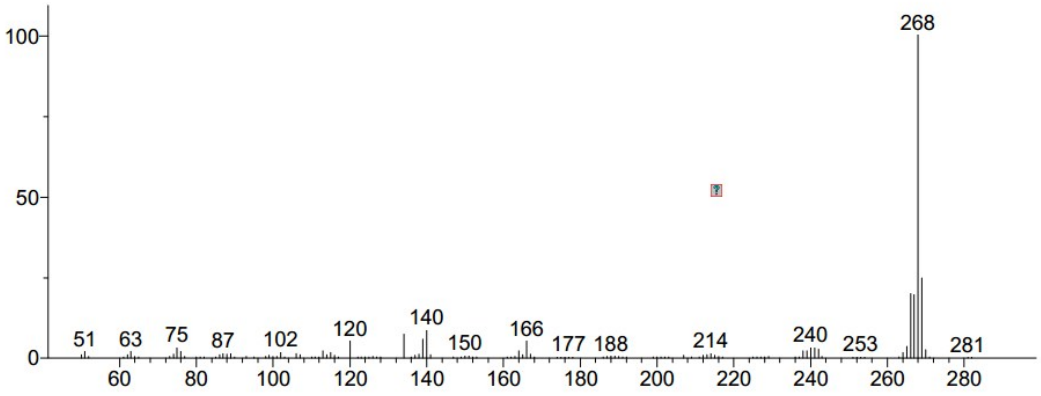

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Figure S3b The mass spectrum of MCN.

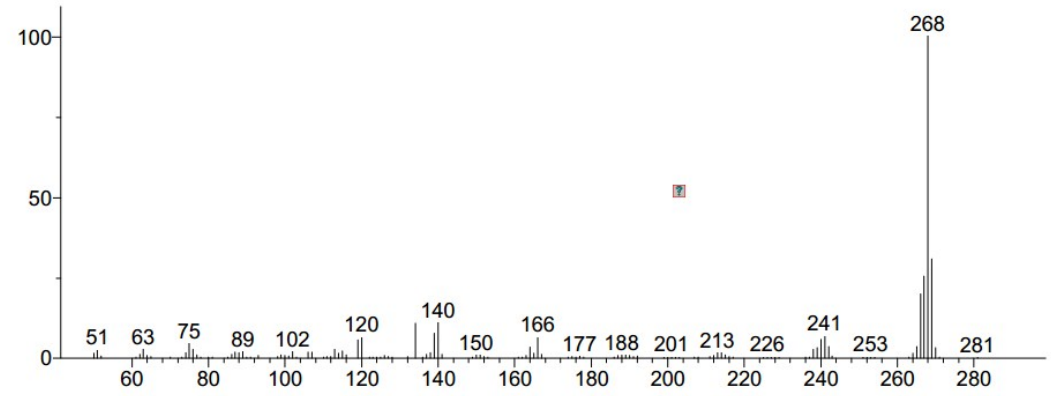

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Figure S3c The mass spectrum of OCN.

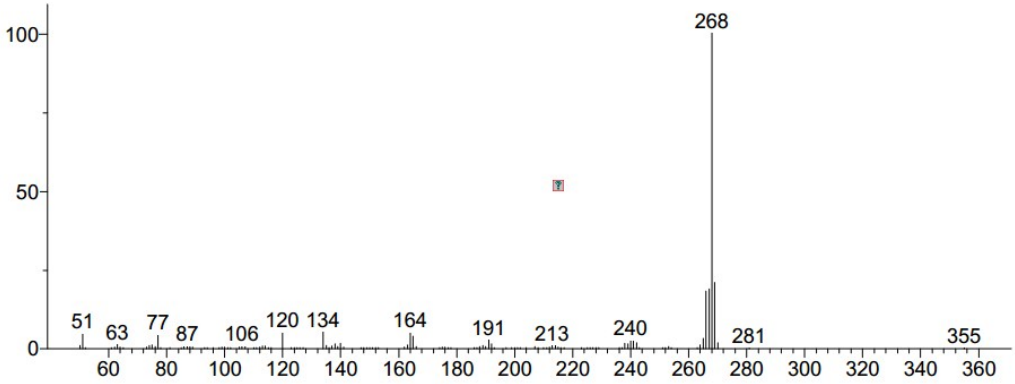

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Figure S3d The mass spectrum of 2CN.

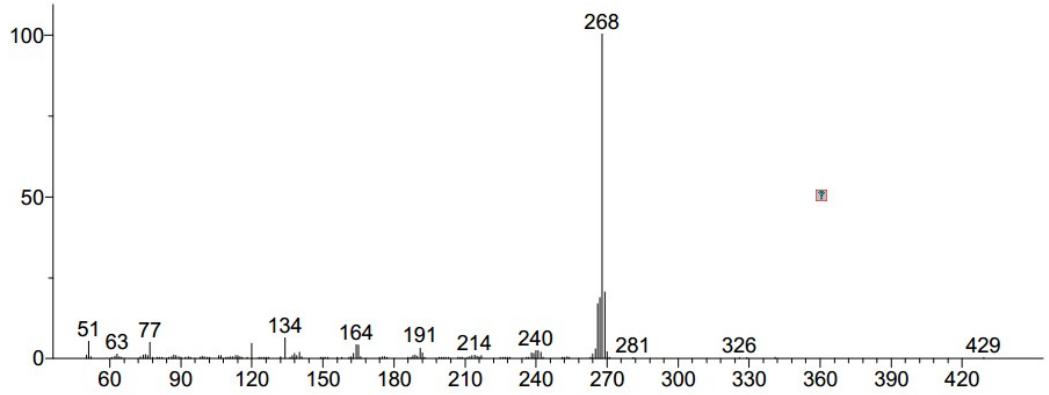

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Figure S3e The mass spectrum of 3CN.

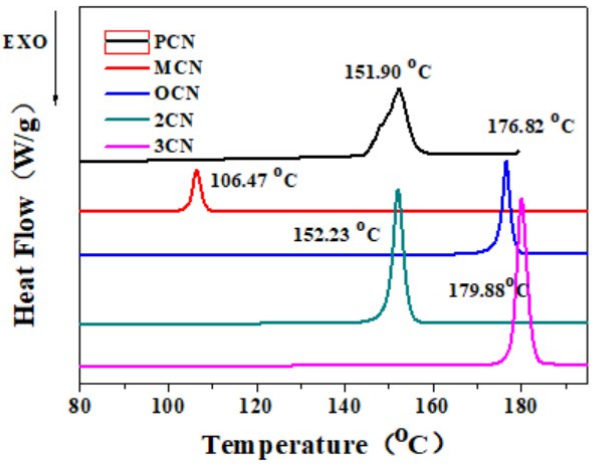


Figure S4 Differential scanning calorimetric (DSC) curves of XCN.

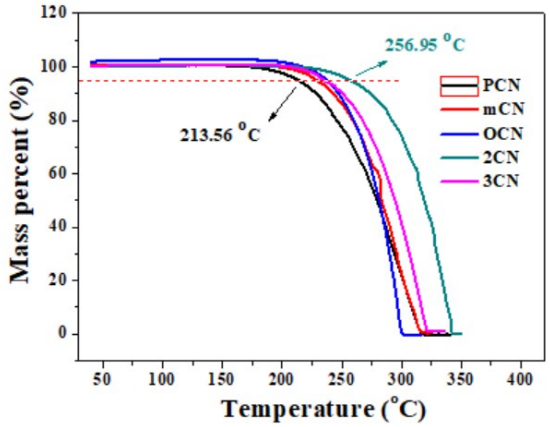


Figure S5 Thermogravimetric analysis (TGA) curves of XCN.

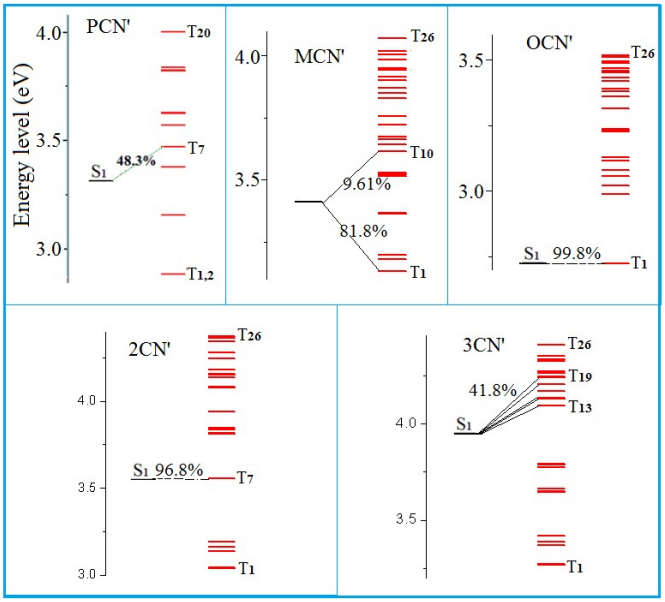


Figure S6 Energy level diagrams and possible ISC channels for XCN crystals based on the bottom interacted pair in Figure 5.

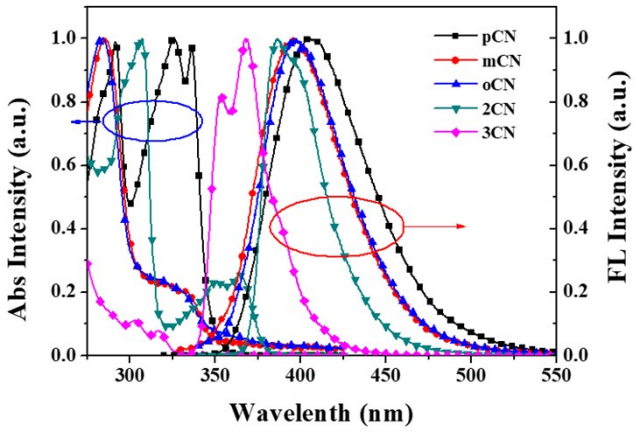


Figure S7 Normalized UV absorption and PL spectra of NPC-XCN in THF (1.0×10^{-5} M) under ambient conditions.

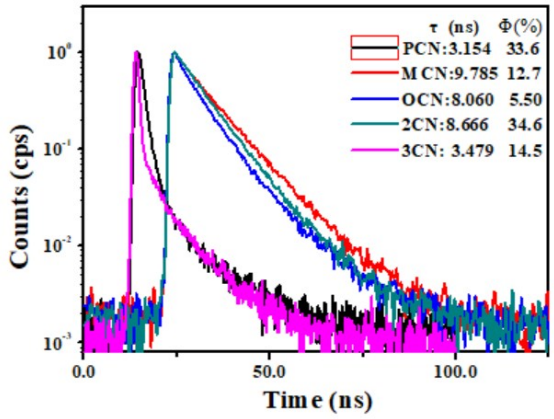


Figure S8 Time-resolved emission decay curves of XCN solution in THF at 298 K. τ is the fluorescence lifetime; Φ represents the fluorescence efficiency.

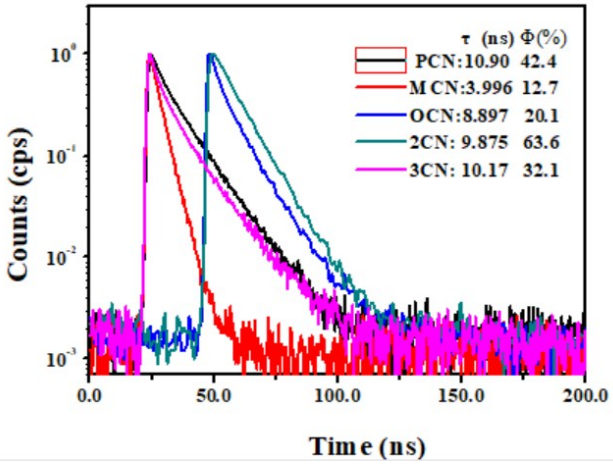


Figure S9 Time-resolved emission decay curves of XCN crystal powder fluorescence at 298 K . τ is the fluorescence lifetime; Φ represents the fluorescence efficiency.

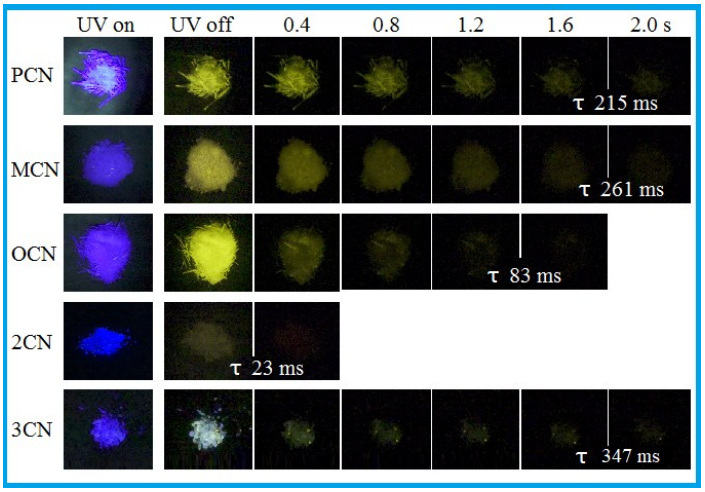


Figure S10 Photoluminescence photos of XCN crystals before and after UV off (365 nm) at room temperature in air, and the corresponding RTP lifetimes (τ) are labeled in the end photos.

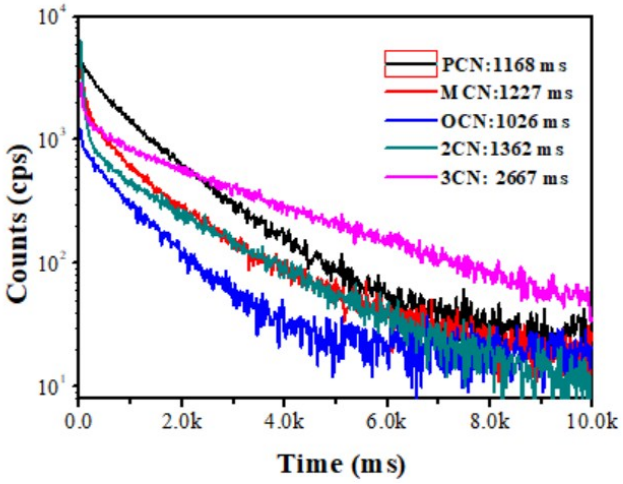


Figure S11 Time-resolved emission decay curves of XCN crystal powder phosphorescence at 78 K.

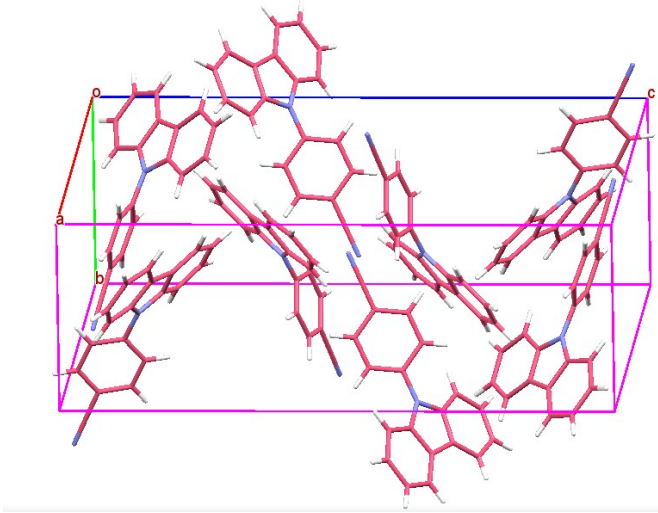


Figure S12a The unit cell of PCN single crystal.

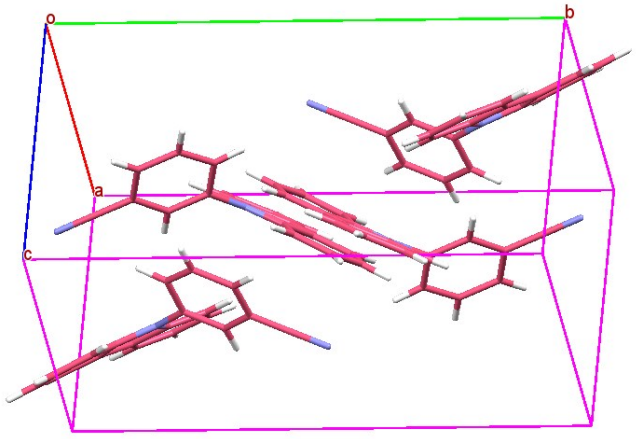


Figure S12b The unit cell of MCN single crystal.

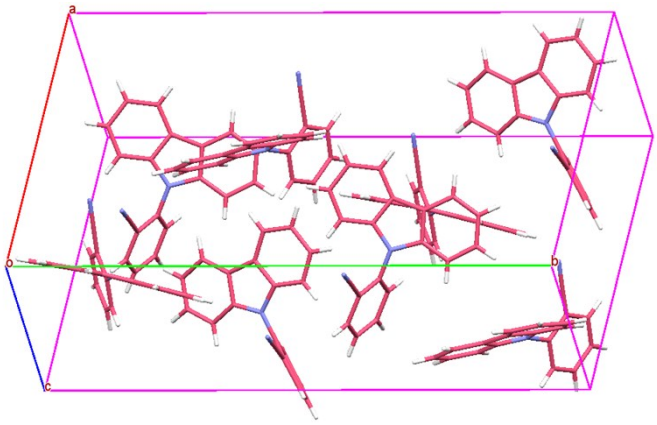


Figure S12c The unit cell of OCN single crystal.

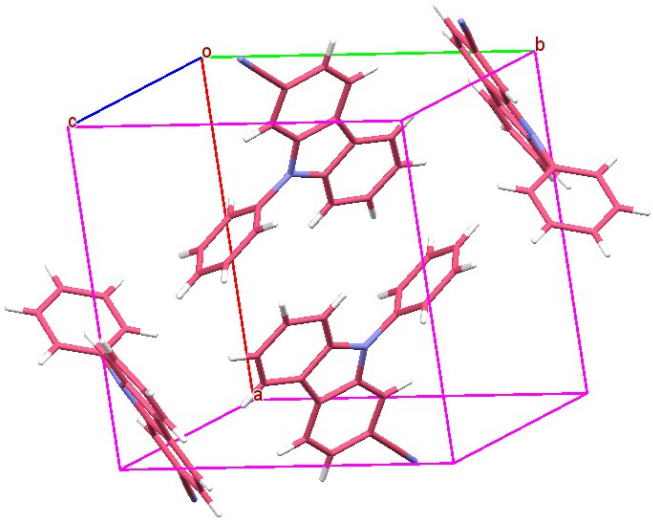


Figure S12d The unit cell of 2CN single crystal.

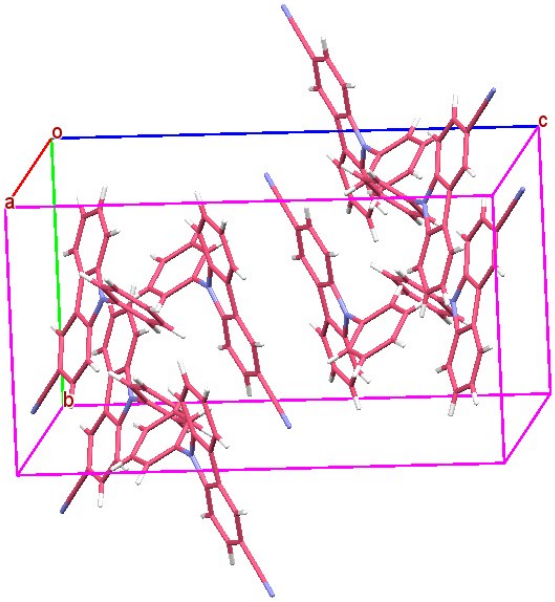


Figure S12e The unit cell of 3CN single crystal.

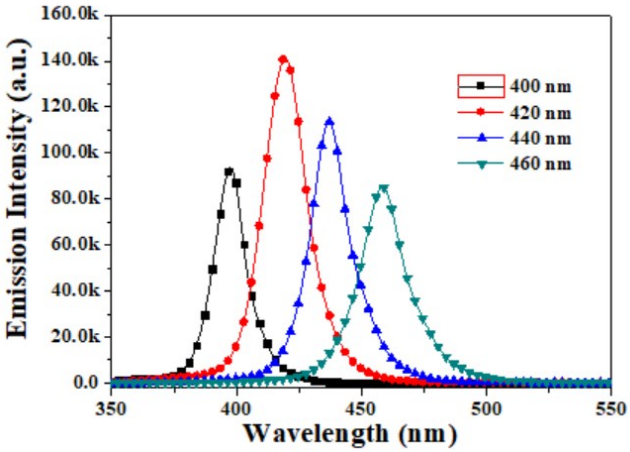


Figure S13 The spectra of 400, 420, 440, and 460 nm visible-light detected by CCD spectrometer.

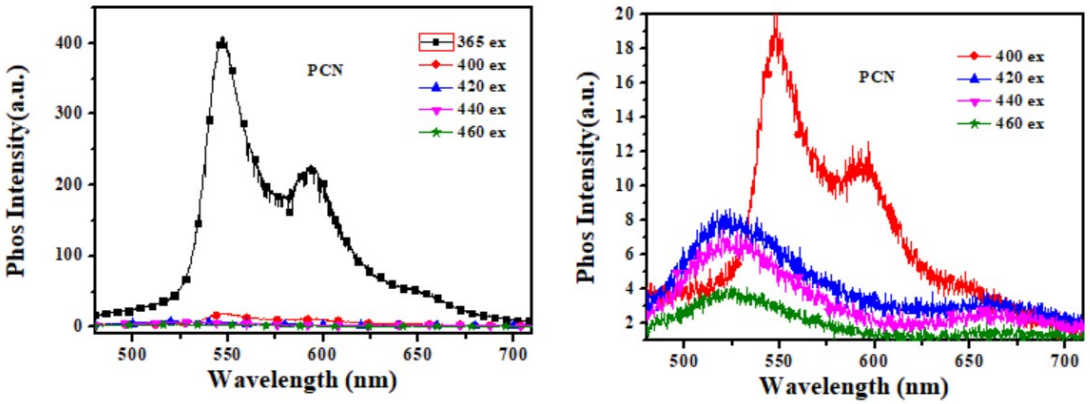


Figure S14a RTP spectra of PCN crystalline powder under the excitation of 365-460 nm. (The right side focuses on the curves of 400-460nm excitation.)

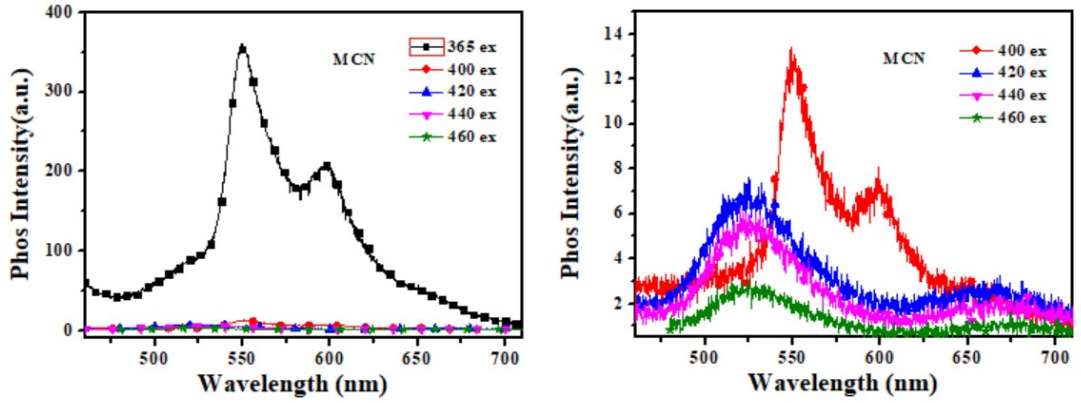


Figure S14b RTP spectra of MCN crystalline powder under the excitation of 365-460 nm. (The right side focuses on the curves of 400-460nm excitation.)

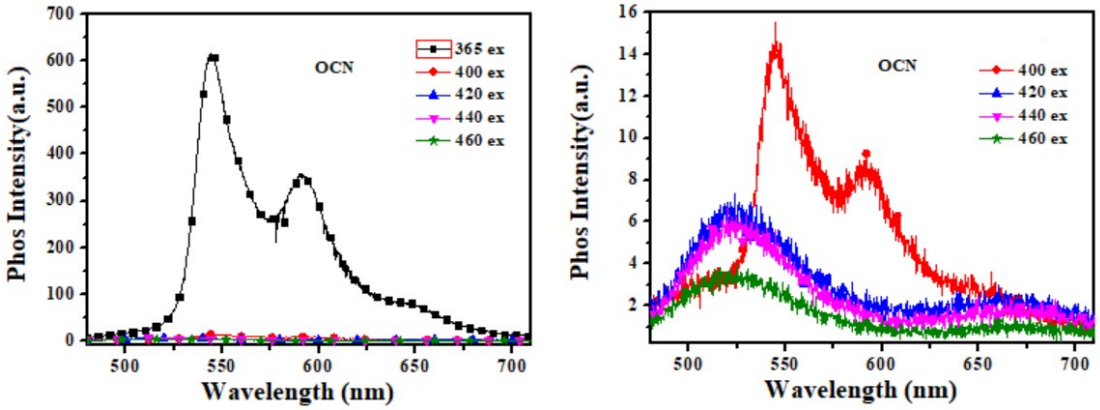


Figure S14c RTP spectra of OCN crystalline powder under the excitation of 365-460 nm. (The right side focuses on the curves of 400-460nm excitation.)

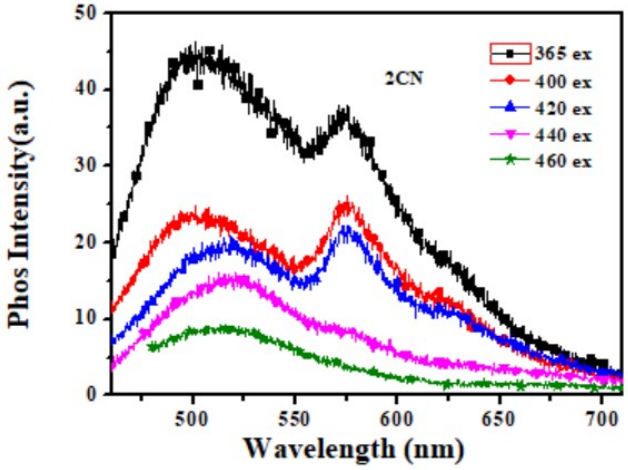


Figure S14d RTP spectra of 2CN crystalline powder under the excitation of 365-460 nm. (The right side focuses on the curves of 400-460nm excitation.)

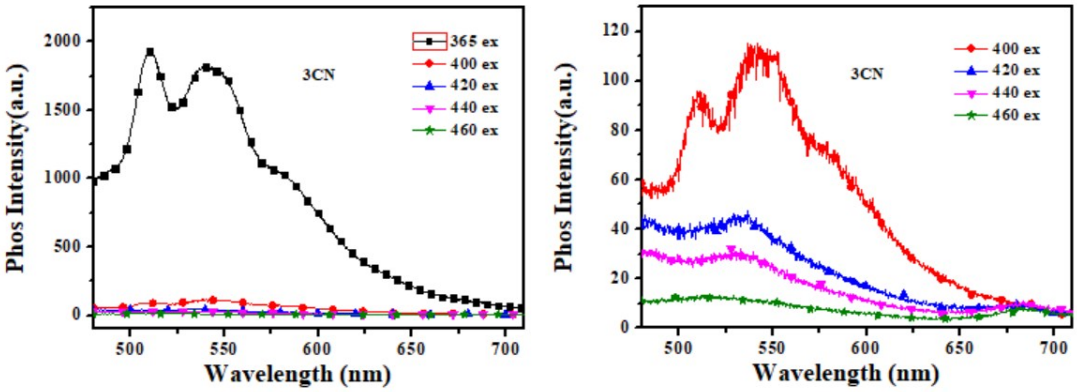


Figure S14e RTP spectra of 3CN crystalline powder under the excitation of 365-460 nm. (The right side focuses on the curves of 400-460nm excitation.)

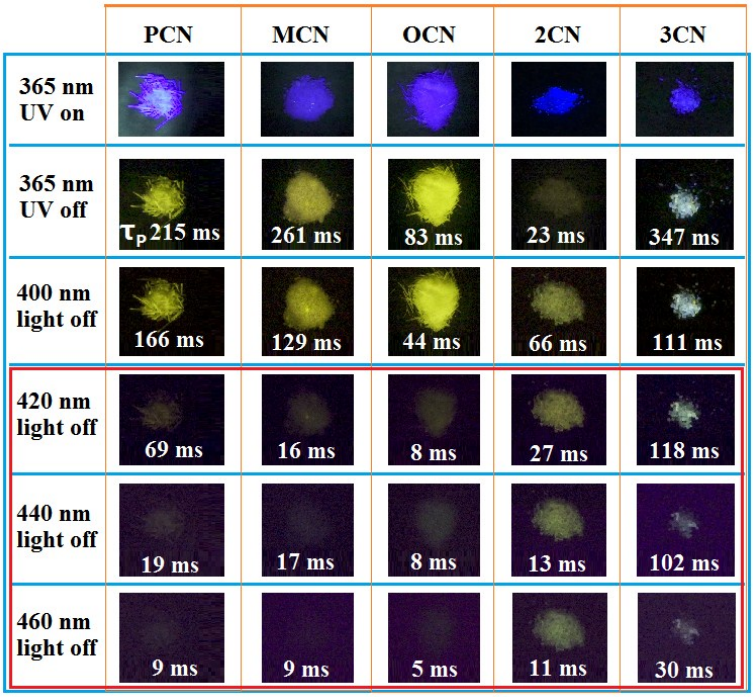


Figure S15 Photoluminescence photos of XCN crystalline powders upon exciting with 365 nm UV light and removing UV and visible excitation light. The labeled number is the RTP lifetimes (τ in ms) under the excitation of different UV and visible light.

3. Tables

Table S1a Single crystal structural parameters of PCN.

Compound reference	colorless PCN crystal
Chemical formula	$C_{38}H_{24}N_4$
Formula weight	536.61
Crystal system	Monoclinic
a/Å	15.265(8)
b/ Å	8.089(4)
c/ Å	22.642(12)
α/°	90.00
β/°	92.613(11)
γ/°	90
Unit cell volume/ Å^3	2793(3)
Temperature/K	100
Space group	P2(1)/c
Z	8
Density (calculated) /g cm^{-3}	1.276
F(000)	1120.0
Theta range for data collection	2.290 to 24.995 deg.
Index ranges	-15<=h<=18, -9<=k<=9, -26<=l<=25
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.984 and 0.988
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	0.993
Final R_1 values ($I > 2\sigma(I)$)	0.0457
Final $wR(F^2)$ values (all data)	0.1276
CCDC number	193260

Table S1b Single crystal structural parameters of MCN.

Compound reference	colorless MCN crystal
Chemical formula	$C_{19}H_{12}N_2$
Formula weight	268.31
Crystal system	Monoclinic
a/Å	10.2050(3)
b/ Å	15.8800(5)
c/ Å	8.5080(7)
α/°	90.00
β/°	92.80(4)

γ/°	90.00
Unit cell volume/ Å^3	1377.12(13)
Temperature/K	293
Space group	P21/c
Z	4
Density (calculated) /g cm^{-3}	1.294
F(000)	560.0
Theta range for data collection	2.00 to 25.09 deg.
Index ranges	-12<=h<=10, -15<=k<=18, -10<=l<=10
Reflections measured	6921
Independent reflections	2444
R_{int}	0.1004
Completeness to theta = 25.09°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9870 and 0.9780
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2444 / 0 / 190
Goodness-of-fit on F^2	0.964
Final R_1 values (I> 2σ(I))	0.0636
Final wR(F^2) values (I> 2σ(I))	0.1199
Final R_1values (all data)	0.2031
Final wR(F^2) values (all data)	0.1715
CCDC number	1918561

Table S1c Single crystal structural parameters of OCN.

Compound reference	colorless OCN crystal
Chemical formula	$C_{19}H_{12}N_2$
Formula weight	268.32
Crystal system	orthorhombic
a/Å	14.7314(14)
b/ Å	24.585(2)
c/ Å	8.0451(8)
α/°	90.00
β/°	90.00
γ/°	90.00
Unit cell volume/ Å^3	2913.7(5)
Temperature/K	296
Space group	I 2 -2c
Z	8
Density (calculated) /g cm^{-3}	1.223
F(000)	1120
Index ranges	-19<=h<=18, -32<=k<=24, -10<=l<=10

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.984 and 0.988
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3248 / 1 / 190
Goodness-of-fit on F^2	0.968
Final R_1 values ($I > 2\sigma(I)$)	0.0411
Final R_1 values (all data)	0.1137
CCDC number	1918562

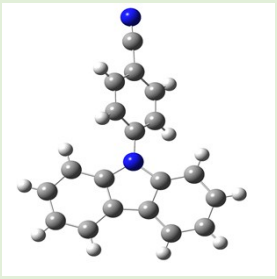
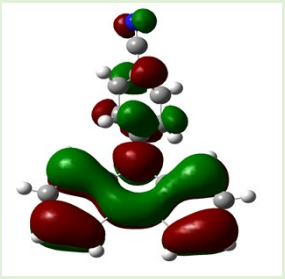
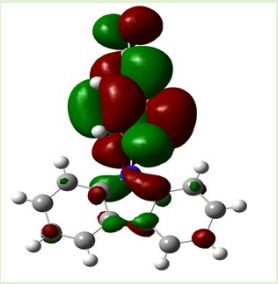
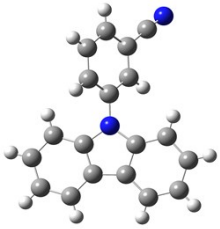
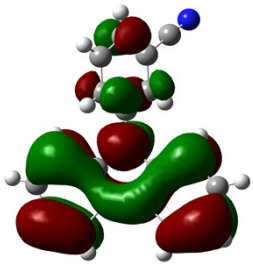
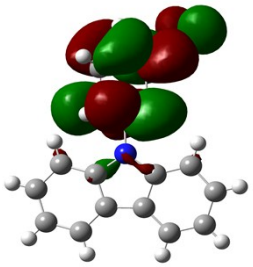
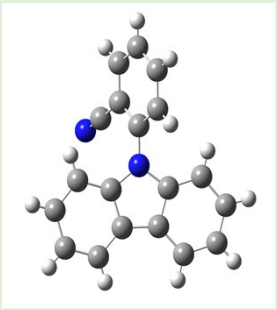
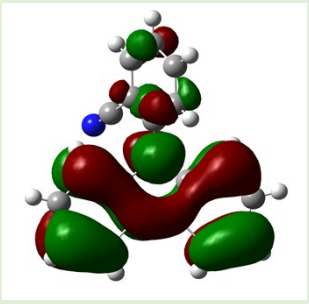
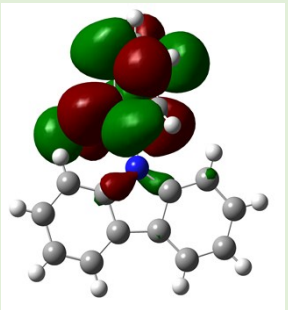
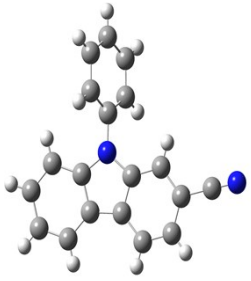
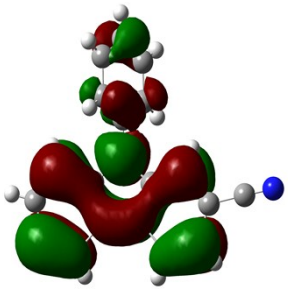
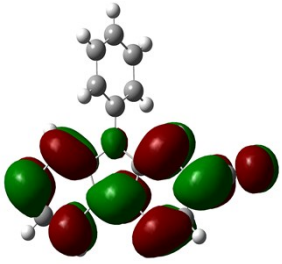
Table S1d Single crystal structural parameters of 2CN.

Compound reference	colorless 2CN crystal
Chemical formula	$C_{19}H_{12}N_2$
Formula weight	268.32
Crystal system	Monoclinic
a/Å	11.1664(15)
b/ Å	11.040(4)
c/ Å	11.208(4)
α/°	90.00
β/°	98.792(6)
γ/°	90.00
Unit cell volume/ Å^3	1365.4(7)
Temperature/K	100
Space group	P2(1)/c
Z	4
Density (calculated) /g cm^{-3}	1.305
F(000)	560.0
Theta range for data collection	1.85 to 24.99 deg.
Index ranges	-10<=h<=13, -13<=k<=11, -12<=l<=13
Reflections measured	6715
Independent reflections	2400
R_{int}	0.0451
Completeness to theta = 24.99°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9869 and 0.9786
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2400 / 0 / 191
Goodness-of-fit on F^2	1.004
Final R_1 values ($I > 2\sigma(I)$)	0.0424
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0843
Final R_1 values (all data)	0.0723
Final $wR(F^2)$ values (all data)	0.0942
CCDC number	1917793

Table S1e Single crystal structural parameters of 3CN.

Compound reference	colorless 3CN crystal
Chemical formula	$C_{19}H_{12}N_2$
Formula weight	268.31
Crystal system	Monoclinic
a/Å	13.648(3)
b/ Å	10.5450(10)
c/ Å	18.9249(8)
α/°	90.00
β/°	92.28(3)
γ/°	90.00
Unit cell volume/ Å^3	2721.4(6)
Temperature/K	100
Space group	C2/c
Z	8
Density (calculated) /g cm^{-3}	1.310
F(000)	1120
Theta range for data collection	2.15 to 25.00 deg.
Index ranges	-16<=h<=15, -7<=k<=12, -21<=l<=22
Reflections measured	6431
Independent reflections	2387
R_{int}	0.0369
Completeness to theta = 25.00°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9838 and 0.9777
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2387 / 0 / 179
Goodness-of-fit on F^2	1.086
Final R_1 values (I> 2σ(I))	0.0499
Final $wR(F^2)$ values (I> 2σ(I))	0.1323
Final R_1values (all data)	0.0736
Final $wR(F^2)$ values (all data)	0.1476
CCDC number	1918555

Table S2 The NTOs of XCN.

NAME	MOLECULE	HOMO	LUMO
PCN			
MCN			
OCN			
2CN			

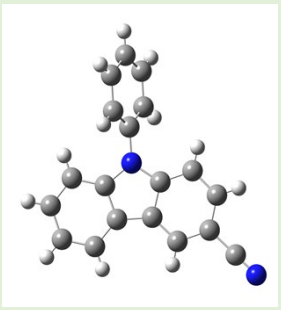
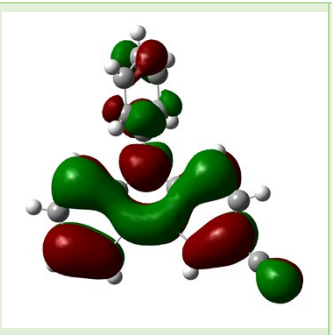
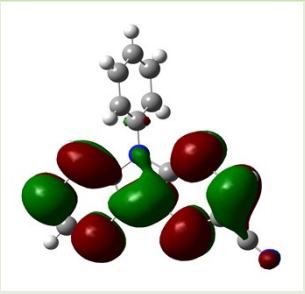
3CN			

Table S3a The singlet and triplet excited state transition configurations of the PCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1\text{-}T_n| < 0.3$ eV were highlighted in red. (for the upper interacted pair in Figure 5)

	n	Energy	Orbitals	Transition
S_n	S_1	3.6573 eV	HOMO -> LUMO+1	0.989908922
T_n	T_1	3.1875 eV	HOMO-13 -> LUMO+7	0.020624805
			HOMO-10 -> LUMO+1	0.111665928
			HOMO-1 -> LUMO+1	0.788366131
	T_2	3.2256 eV	HOMO-15 -> LUMO+4	0.024513408
			HOMO-11 -> LUMO	0.138211789
			HOMO-2 -> LUMO	0.76120525
	T_3	3.2404 eV	HOMO-12 -> LUMO+8	0.039564845
			HOMO-9 -> LUMO+2	0.123444867
			HOMO -> LUMO+2	0.721248541
			HOMO -> LUMO+5	0.03641221
	T_4	3.3204 eV	HOMO-14 -> LUMO+16	0.025669248
			HOMO-7 -> LUMO+6	0.027018826
			HOMO-7 -> LUMO+13	0.021565491
			HOMO-4 -> LUMO+4	0.274125697
			HOMO-4 -> LUMO+6	0.37672936
			HOMO-4 -> LUMO+7	0.022945104
			HOMO-1 -> LUMO+10	0.110873405
	T_5	3.3239 eV	HOMO-17 -> LUMO+15	0.030514381
			HOMO-8 -> LUMO+3	0.047765223
			HOMO-8 -> LUMO+12	0.024784285
			HOMO-5 -> LUMO+3	0.660721106
			HOMO-2 -> LUMO+3	0.037741034
			HOMO-2 -> LUMO+9	0.119394298
	T_6	3.3249 eV	HOMO-6 -> LUMO+5	0.0435125

			HOMO-6 -> LUMO+14	0.020168353
			HOMO-3 -> LUMO+5	0.597127776
			HOMO-3 -> LUMO+7	0.048105816
			HOMO -> LUMO+5	0.043418151
			HOMO -> LUMO+11	0.112461274
	T_7	3.4314 eV	HOMO-6 -> LUMO+11	0.029616912
			HOMO-3 -> LUMO+5	0.038536432
			HOMO -> LUMO+1	0.031330051
			HOMO -> LUMO+2	0.029758241
			HOMO -> LUMO+5	0.723027175
			HOMO -> LUMO+7	0.059781904
	T_8	3.4742 eV	HOMO-8 -> LUMO+9	0.032681018
			HOMO-5 -> LUMO+3	0.033493896
			HOMO-2 -> LUMO+3	0.843129037
	T_9	3.4952 eV	HOMO-7 -> LUMO+10	0.032543107
			HOMO-1 -> LUMO+4	0.365068035
			HOMO-1 -> LUMO+6	0.464995105
			HOMO-1 -> LUMO+7	0.023405825
	T_{10}	3.6638 eV	HOMO -> LUMO+1	0.942921514
			HOMO -> LUMO+5	0.039683079
	T_{11}	3.7330 eV	HOMO-1 -> LUMO	0.991598114
	T_{12}	3.8293 eV	HOMO -> LUMO	0.996872
	T_{13}	3.9764 eV	HOMO-10 -> LUMO+7	0.024650881
			HOMO-4 -> LUMO+1	0.148327258
			HOMO-1 -> LUMO+2	0.029660737
			HOMO-1 -> LUMO+5	0.102949069
			HOMO-1 -> LUMO+7	0.582573768
	T_{14}	3.9796 eV	HOMO-10 -> LUMO+1	0.029587714
			HOMO-4 -> LUMO+1	0.663505921
			HOMO-1 -> LUMO+5	0.026394829
			HOMO-1 -> LUMO+7	0.148556103
	T_{15}	4.0090 eV	HOMO-11 -> LUMO	0.020543645
			HOMO-11 -> LUMO+4	0.027626602
			HOMO-2 -> LUMO+4	0.587874931
			HOMO-2 -> LUMO+6	0.235902067
	T_{16}	4.0322 eV	HOMO-16 -> LUMO+7	0.02004002
			HOMO-13 -> LUMO+7	0.076745784
			HOMO-10 -> LUMO+1	0.222791475
			HOMO-4 -> LUMO+1	0.063810209
			HOMO-3 -> LUMO+1	0.273030941

			HOMO-3 -> LUMO+2	0.031415218
			HOMO-1 -> LUMO+1	0.067315143
			HOMO-1 -> LUMO+13	0.021611205
			HOMO -> LUMO+8	0.030277683
			HOMO -> LUMO+11	0.02738268
	T_{17}	4.0403 eV	HOMO-13 -> LUMO+7	0.04639058
			HOMO-10 -> LUMO+1	0.137592088
			HOMO-4 -> LUMO+1	0.026033056
			HOMO-3 -> LUMO+1	0.259473672
			HOMO-3 -> LUMO+2	0.043778405
			HOMO-3 -> LUMO+5	0.033862429
			HOMO-1 -> LUMO+1	0.043247405
			HOMO -> LUMO+8	0.176976802
			HOMO -> LUMO+11	0.069504833
	T_{18}	4.0451 eV	HOMO-15 -> LUMO+4	0.094569005
			HOMO-15 -> LUMO+6	0.052022477
			HOMO-11 -> LUMO	0.293868445
			HOMO-5 -> LUMO	0.219466375
			HOMO-2 -> LUMO	0.10765728
			HOMO-2 -> LUMO+4	0.04749362
			HOMO-2 -> LUMO+12	0.042649522
	T_{19}	4.0527 eV	HOMO-12 -> LUMO+8	0.061236001
			HOMO-9 -> LUMO+2	0.123773026
			HOMO-9 -> LUMO+8	0.035420573
			HOMO-3 -> LUMO+1	0.122690765
			HOMO-3 -> LUMO+2	0.055231585
			HOMO -> LUMO+2	0.05359538
			HOMO -> LUMO+8	0.430814749
	T_{20}	4.0658 eV	HOMO-12 -> LUMO+8	0.145767602
			HOMO-9 -> LUMO+2	0.224798535
			HOMO-6 -> LUMO+11	0.020044024
			HOMO-3 -> LUMO+1	0.140821245
			HOMO -> LUMO+2	0.095283586
			HOMO -> LUMO+8	0.199749922
			HOMO -> LUMO+14	0.036628418
	T_{21}	4.0738 eV	HOMO-15 -> LUMO+4	0.031330051
			HOMO-11 -> LUMO	0.08910109
			HOMO-5 -> LUMO	0.503767069
			HOMO-5 -> LUMO+3	0.059781904
			HOMO-4 -> LUMO	0.157966963

			HOMO-2 -> LUMO	0.024257234
			HOMO-2 -> LUMO+9	0.040237171
	T_{22}	4.0998 eV	HOMO-11 -> LUMO	0.023709709
			HOMO-5 -> LUMO	0.0852845
			HOMO-4 -> LUMO	0.833882808
	T_{23}	4.1142 eV	HOMO-6 -> LUMO+5	0.034974835
			HOMO-3 -> LUMO+1	0.179844034
			HOMO-3 -> LUMO+2	0.16097138
			HOMO-3 -> LUMO+5	0.17119441
			HOMO -> LUMO+8	0.062565994
			HOMO -> LUMO+11	0.268439299
	T_{24}	4.1199 eV	HOMO-2 -> LUMO+1	0.978740405
	T_{25}	4.1429 eV	HOMO-8 -> LUMO+3	0.108196216
			HOMO-8 -> LUMO+12	0.025896328
			HOMO-5 -> LUMO	0.10758305
			HOMO-5 -> LUMO+3	0.13718322
			HOMO-2 -> LUMO+9	0.450091744
			HOMO-1 -> LUMO+3	0.033405955
			HOMO-1 -> LUMO+10	0.027289152
	T_{26}	4.1439 eV	HOMO-7 -> LUMO+4	0.033883251
			HOMO-7 -> LUMO+6	0.047296577
			HOMO-7 -> LUMO+13	0.021441063
			HOMO-4 -> LUMO+4	0.06444768
			HOMO-4 -> LUMO+6	0.070703041
			HOMO-3 -> LUMO+2	0.053687091
			HOMO-2 -> LUMO+9	0.034432128
			HOMO-1 -> LUMO+2	0.06802885
			HOMO-1 -> LUMO+3	0.044988001
			HOMO-1 -> LUMO+9	0.025864477
			HOMO-1 -> LUMO+10	0.367893264

Table S3b The singlet and triplet excited state transition configurations of the MCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1-T_n| < 0.3$ eV were highlighted in red. (for the upper interacted pair in Figure 5)

	n	Energy	Orbitals	Transition
S_n	S_1	3.3343 eV	HOMO -> LUMO+1	0.990134
T_n	T_1	3.0751 eV	HOMO-10 -> LUMO+1	0.067602
			HOMO -> LUMO+1	0.860856

	T_2	3.1424 eV	HOMO-11 -> LUMO	0.0941
			HOMO-1 -> LUMO	0.824688
	T_3	3.2895 eV	HOMO-9 -> LUMO+2	0.157843
			HOMO-2 -> LUMO+2	0.673078
			HOMO-2 -> LUMO+7	0.022659
	T_4	3.3550 eV	HOMO-6 -> LUMO+8	0.026982
			HOMO-3 -> LUMO+2	0.031757
			HOMO-3 -> LUMO+6	0.02837
			HOMO-3 -> LUMO+7	0.148175
			HOMO-3 -> LUMO+8	0.430945
			HOMO -> LUMO+7	0.02749
			HOMO -> LUMO+8	0.080096
			HOMO -> LUMO+11	0.082004
	T_5	3.3615 eV	HOMO-5 -> LUMO+3	0.30948
			HOMO-5 -> LUMO+6	0.169875
			HOMO-5 -> LUMO+7	0.036943
			HOMO-2 -> LUMO	0.043784
			HOMO-2 -> LUMO+3	0.105809
			HOMO-2 -> LUMO+6	0.04984
			HOMO-2 -> LUMO+9	0.070861
	T_6	3.3653 eV	HOMO-7 -> LUMO+5	0.038464
			HOMO-4 -> LUMO+5	0.588678
			HOMO-4 -> LUMO+6	0.060998
			HOMO-1 -> LUMO+5	0.133541
			HOMO-1 -> LUMO+10	0.085864
	T_7	3.4734 eV	HOMO-5 -> LUMO+3	0.110102
			HOMO-5 -> LUMO+6	0.061299
			HOMO-2 -> LUMO	0.144625
			HOMO-2 -> LUMO+1	0.032748
			HOMO-2 -> LUMO+3	0.299244
			HOMO-2 -> LUMO+6	0.150755
	T_8	3.4902 eV	HOMO-3 -> LUMO+8	0.044934
			HOMO -> LUMO+2	0.549236
			HOMO -> LUMO+4	0.044176
			HOMO -> LUMO+7	0.067609
			HOMO -> LUMO+8	0.197871
	T_9	3.5257 eV	HOMO-7 -> LUMO+10	0.031495
			HOMO-4 -> LUMO+5	0.118011
			HOMO-1 -> LUMO+5	0.711911
	T_{10}	3.5619 eV	HOMO-15 -> LUMO+4	0.026524

			HOMO-13 -> LUMO+1	0.023806
			HOMO-12 -> LUMO+1	0.022016
			HOMO-10 -> LUMO+1	0.05074
			HOMO-2 -> LUMO+1	0.204723
			HOMO -> LUMO+1	0.059154
			HOMO -> LUMO+2	0.097629
			HOMO -> LUMO+4	0.313664
			HOMO -> LUMO+6	0.032855
			HOMO -> LUMO+8	0.030224
	T_{11}	3.5942 eV	HOMO-2 -> LUMO	0.121702
			HOMO-2 -> LUMO+1	0.407434
			HOMO -> LUMO+2	0.174711
			HOMO -> LUMO+4	0.045192
			HOMO -> LUMO+7	0.029695
			HOMO -> LUMO+8	0.12949
	T_{12}	3.6140 eV	HOMO-2 -> LUMO+1	0.05416
			HOMO -> LUMO	0.843752
			HOMO -> LUMO+8	0.028141
	T_{13}	3.6154 eV	HOMO-10 -> LUMO+1	0.020386
			HOMO-2 -> LUMO	0.396317
			HOMO-2 -> LUMO+3	0.060191
			HOMO-2 -> LUMO+6	0.038442
			HOMO -> LUMO	0.067624
			HOMO -> LUMO+2	0.106667
			HOMO -> LUMO+4	0.025142
			HOMO -> LUMO+6	0.024651
			HOMO -> LUMO+7	0.05391
			HOMO -> LUMO+8	0.097382
	T_{14}	3.6286 eV	HOMO-2 -> LUMO	0.204058
			HOMO-2 -> LUMO+1	0.240749
			HOMO-2 -> LUMO+3	0.051784
			HOMO-2 -> LUMO+6	0.03045
			HOMO -> LUMO	0.065479
			HOMO -> LUMO+2	0.049795
			HOMO -> LUMO+4	0.061769
			HOMO -> LUMO+6	0.033246
			HOMO -> LUMO+7	0.041035
			HOMO -> LUMO+8	0.051379
	T_{15}	3.6375 eV	HOMO-14 -> LUMO	0.086686
			HOMO-14 -> LUMO+3	0.025783

			HOMO-11 -> LUMO	0.106657
			HOMO-2 -> LUMO	0.042056
			HOMO-1 -> LUMO	0.078543
			HOMO-1 -> LUMO+3	0.223393
			HOMO-1 -> LUMO+4	0.052767
			HOMO-1 -> LUMO+6	0.191172
	T_{16}	3.7274 eV	HOMO-3 -> LUMO+1	0.930084
	T_{17}	3.7489 eV	HOMO-13 -> LUMO+2	0.024381
			HOMO-13 -> LUMO+7	0.02662
			HOMO-12 -> LUMO+7	0.043306
			HOMO-9 -> LUMO+2	0.18786
			HOMO-3 -> LUMO+1	0.040487
			HOMO-2 -> LUMO+2	0.208968
			HOMO-2 -> LUMO+4	0.035389
			HOMO-2 -> LUMO+7	0.229476
			HOMO-2 -> LUMO+8	0.04658
	T_{18}	3.8105 eV	HOMO-1 -> LUMO+1	0.979916
	T_{19}	3.8532 eV	HOMO-4 -> LUMO	0.960886
	T_{20}	3.9135 eV	HOMO-3 -> LUMO	0.02254
			HOMO-3 -> LUMO+2	0.899409
			HOMO-3 -> LUMO+8	0.021815
	T_{21}	3.9279 eV	HOMO-13 -> LUMO+1	0.097038
			HOMO-12 -> LUMO+1	0.118458
			HOMO-10 -> LUMO+1	0.314678
			HOMO -> LUMO+1	0.023779
			HOMO -> LUMO+4	0.19669
			HOMO -> LUMO+6	0.044545
			HOMO -> LUMO+7	0.02325
	T_{22}	3.9446 eV	HOMO-11 -> LUMO	0.046275
			HOMO-5 -> LUMO	0.350737
			HOMO-3 -> LUMO	0.475196
			HOMO-1 -> LUMO+3	0.030224
	T_{23}	3.9760 eV	HOMO-14 -> LUMO	0.103995
			HOMO-11 -> LUMO	0.176228
			HOMO-5 -> LUMO	0.059161
			HOMO-3 -> LUMO	0.3573
			HOMO-1 -> LUMO+3	0.10855
			HOMO-1 -> LUMO+6	0.068828
	T_{24}	3.9969 eV	HOMO-5 -> LUMO+2	0.047333
			HOMO-1 -> LUMO+2	0.897693

	T_{25}	4.0092 eV	HOMO-14 -> LUMO	0.078376
			HOMO-11 -> LUMO	0.074074
			HOMO-5 -> LUMO	0.53373
			HOMO-5 -> LUMO+1	0.021095
			HOMO-3 -> LUMO	0.134608
			HOMO-1 -> LUMO+3	0.044934
			HOMO-1 -> LUMO+6	0.029871
	T_{26}	4.0210 eV	HOMO-13 -> LUMO+2	0.020293
			HOMO-9 -> LUMO+2	0.254341
			HOMO-5 -> LUMO+1	0.130234
			HOMO-5 -> LUMO+2	0.02576
			HOMO-2 -> LUMO+4	0.057027
			HOMO-2 -> LUMO+7	0.25815
			HOMO-2 -> LUMO+8	0.04585
			HOMO-1 -> LUMO+2	0.049342

Table S3c The singlet and triplet excited state transition configurations of the OCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1\text{-}T_n| < 0.3$ eV were highlighted in red. (for the upper interacted pair in Figure 5)

	n	Energy	Orbitals	Transition
S_n	S_1	3.1569 eV	HOMO -> LUMO+2	0.990078
			HOMO -> LUMO+1	0.168954845
T_n	T_1	3.0065 eV	HOMO -> LUMO+2	0.915386
	T_2	3.1089 eV	HOMO-12 -> LUMO	0.03573
			HOMO-3 -> LUMO	0.810035
			HOMO-3 -> LUMO+3	0.033675
			HOMO-1 -> LUMO	0.055738
	T_3	3.1744 eV	HOMO-10 -> LUMO+1	0.059175
			HOMO-4 -> LUMO+7	0.020645
			HOMO-3 -> LUMO+1	0.027683
			HOMO-1 -> LUMO+1	0.784754
			HOMO-1 -> LUMO+4	0.030564
	T_4	3.2308 eV	HOMO-5 -> LUMO+2	0.022485
			HOMO-5 -> LUMO+4	0.158394
			HOMO-5 -> LUMO+5	0.135721
			HOMO-5 -> LUMO+6	0.39117
			HOMO-3 -> LUMO+9	0.084996
	T_5	3.2316 eV	HOMO-9 -> 231	0.022126

			HOMO-6 -> LUMO+8	0.038776
			HOMO-2 -> LUMO+2	0.024798
			HOMO-2 -> LUMO+8	0.710098
			HOMO -> LUMO+8	0.022748
			HOMO -> LUMO+11	0.098532
	T_6	3.2450 eV	HOMO-7 -> LUMO+7	0.03337
			HOMO-7 -> LUMO+13	0.020337
			HOMO-4 -> LUMO+7	0.689725
			HOMO-1 -> LUMO+1	0.032065
			HOMO-1 -> LUMO+7	0.029539
			HOMO-1 -> LUMO+10	0.092949
	T_7	3.2897 eV	HOMO -> LUMO	0.986394
	T_8	3.4456 eV	HOMO-14 -> LUMO+5	0.044665
			HOMO-14 -> LUMO+6	0.027303
			HOMO-11 -> LUMO+2	0.085913
			HOMO-9 -> LUMO+2	0.022817
			HOMO-3 -> LUMO+6	0.023766
			HOMO -> LUMO+2	0.046885
			HOMO -> LUMO+4	0.0621
			HOMO -> LUMO+5	0.243658
			HOMO -> LUMO+6	0.120816
			HOMO -> LUMO+8	0.172848
	T_9	3.4525 eV	HOMO-8 -> LUMO+9	0.027448
			HOMO-3 -> LUMO+2	0.06097
			HOMO-3 -> LUMO+3	0.104928
			HOMO-3 -> LUMO+4	0.13053
			HOMO-3 -> LUMO+5	0.110986
			HOMO-3 -> LUMO+6	0.313268
			HOMO -> LUMO+5	0.024642
	T_{10}	3.4607 eV	HOMO-7 -> LUMO+10	0.034406
			HOMO-4 -> LUMO+7	0.030022
			HOMO-3 -> LUMO+7	0.025124
			HOMO-1 -> LUMO+1	0.020845
			HOMO-1 -> LUMO+4	0.058742
			HOMO-1 -> LUMO+5	0.023091
			HOMO-1 -> LUMO+7	0.728376
	T_{11}	3.4741 eV	HOMO-2 -> LUMO+2	0.943718
			HOMO-2 -> LUMO+8	0.02395
	T_{12}	3.5135 eV	HOMO-14 -> LUMO+5	0.029132
			HOMO-11 -> LUMO+2	0.084905

			HOMO-9 -> LUMO+2	0.030199
			HOMO-6 -> LUMO+11	0.024847
			HOMO -> LUMO+5	0.025992
			HOMO -> LUMO+6	0.033941
			HOMO -> LUMO+8	0.641527
	T_{13}	3.5163 eV	HOMO-3 -> LUMO	0.023618
			HOMO-3 -> LUMO+3	0.0221
			HOMO-2 -> LUMO	0.85978
	T_{14}	3.5346 eV	HOMO-17 -> LUMO+3	0.103604
			HOMO-16 -> LUMO	0.100477
			HOMO-16 -> LUMO+3	0.021536
			HOMO-12 -> LUMO	0.13439
			HOMO-3 -> LUMO+3	0.213205
			HOMO-3 -> LUMO+4	0.022126
			HOMO-3 -> LUMO+6	0.043124
			HOMO-2 -> LUMO	0.099102
			HOMO-1 -> LUMO	0.151162
	T_{15}	3.5571 eV	HOMO-10 -> LUMO+1	0.039055
			HOMO-5 -> LUMO	0.026381
			HOMO-3 -> LUMO	0.078313
			HOMO-3 -> LUMO+3	0.030396
			HOMO-1 -> LUMO	0.651945
			HOMO-1 -> LUMO+4	0.027219
	T_{16}	3.5581 eV	HOMO-15 -> LUMO+4	0.069527
			HOMO-15 -> LUMO+5	0.029846
			HOMO-13 -> LUMO+1	0.087697
			HOMO-13 -> LUMO+4	0.033241
			HOMO-10 -> LUMO+1	0.229097
			HOMO-1 -> LUMO	0.105157
			HOMO-1 -> LUMO+1	0.091566
			HOMO-1 -> LUMO+4	0.132098
			HOMO-1 -> LUMO+5	0.057576
			HOMO-1 -> LUMO+7	0.05395
	T_{17}	3.5741 eV	HOMO -> LUMO+1	0.996928
	T_{18}	3.6201 eV	HOMO-5 -> LUMO	0.899623
			HOMO-4 -> LUMO	0.034706
			HOMO-1 -> LUMO	0.026986
	T_{19}	3.6905 eV	HOMO-3 -> LUMO+2	0.036213
			HOMO-1 -> LUMO+2	0.92597
	T_{20}	3.7231 eV	HOMO-4 -> LUMO+1	0.907312

			HOMO-3 -> LUMO+1	0.045705
	T_{21}	3.7333 eV	HOMO-11 -> LUMO+2	0.110647
			HOMO-9 -> LUMO+2	0.035288
			HOMO-5 -> LUMO+2	0.032579
			HOMO-3 -> LUMO+2	0.479455
			HOMO-1 -> LUMO+2	0.045258
			HOMO -> LUMO+4	0.022945
			HOMO -> LUMO+5	0.090032
			HOMO -> LUMO+6	0.0502
			HOMO -> LUMO+8	0.020523
	T_{22}	3.7402 eV	HOMO-4 -> LUMO+1	0.046433
			HOMO-3 -> LUMO+1	0.866665
			HOMO-2 -> LUMO+1	0.020451
			HOMO-1 -> LUMO+1	0.022206
	T_{23}	3.7591 eV	HOMO-11 -> LUMO+2	0.191296
			HOMO-9 -> LUMO+2	0.063453
			HOMO-5 -> LUMO+2	0.034144
			HOMO-3 -> LUMO+2	0.364078
			HOMO -> LUMO+4	0.031838
			HOMO -> LUMO+5	0.114232
			HOMO -> LUMO+6	0.050785
			HOMO -> LUMO+8	0.024735
	T_{24}	3.8114 eV	HOMO-16 -> LUMO	0.149102
			HOMO-12 -> LUMO	0.225389
			HOMO-3 -> LUMO+3	0.403705
			HOMO-3 -> LUMO+4	0.020084
			HOMO-3 -> LUMO+6	0.032375
			HOMO-1 -> LUMO+3	0.032994
	T_{25}	3.8168 eV	HOMO-3 -> LUMO+1	0.024465
			HOMO-2 -> LUMO+1	0.970865
	T_{26}	3.8519 eV	HOMO-5 -> LUMO	0.036218
			HOMO-4 -> LUMO	0.962661

Table S3d The singlet and triplet excited state transition configurations of the 2CN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1-T_n| < 0.3$ eV were highlighted in red. (for the upper interacted pair in Figure 5)

	n	Energy	Orbitals	Transition
S_n	S_1	3.5832 eV	HOMO -> LUMO	0.814981445

			HOMO -> LUMO+1	0.168954845
T_n	T_1	3.0024 eV	HOMO-4 -> LUMO+1	0.110816904
			HOMO-4 -> LUMO+2	0.225227873
			HOMO-3 -> LUMO+1	0.45907362
			HOMO-3 -> LUMO+2	0.025859928
			HOMO-2 -> LUMO+1	0.030489682
	T_2	3.0166 eV	HOMO-5 -> LUMO	0.725747424
			HOMO-2 -> LUMO	0.134722023
			HOMO-2 -> LUMO+9	0.027584307
	T_3	3.0353 eV	HOMO-4 -> LUMO+1	0.333401448
			HOMO-3 -> LUMO+2	0.4522005
			HOMO-2 -> LUMO+2	0.036148227
			HOMO -> LUMO+11	0.022607885
	T_4	3.0948 eV	HOMO-5 -> LUMO	0.129448896
			HOMO-3 -> LUMO	0.050867741
			HOMO-2 -> LUMO	0.698916645
			HOMO-1 -> LUMO	0.050759352
	T_5	3.1133 eV	HOMO-1 -> LUMO+1	0.240901287
			HOMO-1 -> LUMO+2	0.145627251
			HOMO -> LUMO+1	0.509504746
	T_6	3.1600 eV	HOMO-1 -> LUMO+1	0.26509393
			HOMO-1 -> LUMO+2	0.074783914
			HOMO -> LUMO+1	0.088831125
			HOMO -> LUMO+2	0.510757245
	T_7	3.5883 eV	HOMO -> LUMO	0.95579138
	T_8	3.6983 eV	HOMO-1 -> LUMO	0.095922
			HOMO-1 -> LUMO+1	0.258020545
			HOMO-1 -> LUMO+2	0.094499434
			HOMO -> LUMO	0.022459282
			HOMO -> LUMO+1	0.266829735
			HOMO -> LUMO+2	0.234297506
	T_9	3.7449 eV	HOMO-2 -> LUMO	0.049524339
			HOMO-1 -> LUMO	0.781900135
			HOMO-1 -> LUMO+1	0.089811696
			HOMO -> LUMO+2	0.048653282
	T_{10}	3.8053 eV	HOMO-12 -> LUMO+6	0.020072065
			HOMO-12 -> LUMO+8	0.035170824
			HOMO-10 -> LUMO+5	0.130877512
			HOMO-1 -> LUMO+1	0.023683585
			HOMO-1 -> LUMO+2	0.145616458

			HOMO-1 -> LUMO+5	0.02159042
			HOMO-1 -> LUMO+7	0.03847538
			HOMO-1 -> LUMO+8	0.041305128
			HOMO -> LUMO+2	0.032441139
			HOMO -> LUMO+7	0.020337411
			HOMO -> LUMO+8	0.169396922
	T_{11}	3.8173 eV	HOMO-13 -> LUMO+8	0.083378945
			HOMO-12 -> LUMO+8	0.041957251
			HOMO-10 -> LUMO+5	0.074127901
			HOMO-9 -> LUMO+6	0.027429504
			HOMO-8 -> LUMO+7	0.022620645
			HOMO-1 -> LUMO+2	0.037242663
			HOMO-1 -> LUMO+7	0.077846688
			HOMO-1 -> LUMO+8	0.055838136
			HOMO -> LUMO+2	0.134410755
			HOMO -> LUMO+5	0.026514439
			HOMO -> LUMO+6	0.126444147
			HOMO -> LUMO+7	0.05484672
	T_{12}	3.8338 eV	HOMO-11 -> LUMO+3	0.02603762
			HOMO-11 -> LUMO+4	0.071759873
			HOMO-9 -> LUMO+6	0.026823912
			HOMO-2 -> LUMO+3	0.114414145
			HOMO-1 -> LUMO+1	0.021669456
			HOMO-1 -> LUMO+2	0.21134101
			HOMO-1 -> LUMO+7	0.035687233
			HOMO -> LUMO+1	0.037823501
			HOMO -> LUMO+2	0.042177697
			HOMO -> LUMO+8	0.041685394
	T_{13}	3.8347 eV	HOMO-14 -> LUMO+3	0.025592269
			HOMO-14 -> LUMO+9	0.0226845
			HOMO-11 -> LUMO+3	0.043418151
			HOMO-11 -> LUMO+4	0.122255235
			HOMO-7 -> LUMO+4	0.02008008
			HOMO-2 -> LUMO+3	0.192014045
			HOMO-1 -> LUMO+2	0.135949837
			HOMO -> LUMO+1	0.021903245
			HOMO -> LUMO+2	0.031565794
			HOMO -> LUMO+8	0.023561863
	T_{14}	3.8717 eV	HOMO-4 -> LUMO	0.031340065
			HOMO-4 -> LUMO+1	0.020096115

			HOMO-3 -> LUMO	0.834967954
			HOMO-2 -> LUMO	0.05916112
	T_{15}	3.9359 eV	HOMO-6 -> LUMO+1	0.028222128
			HOMO-4 -> LUMO+1	0.098976903
			HOMO-4 -> LUMO+2	0.122690765
			HOMO-3 -> LUMO	0.067190448
			HOMO-3 -> LUMO+1	0.320144016
			HOMO-3 -> LUMO+2	0.062806768
			HOMO-2 -> LUMO+1	0.052689072
	T_{16}	4.0279 eV	HOMO-15 -> LUMO+2	0.026243405
			HOMO-6 -> LUMO+1	0.052786503
			HOMO-4 -> LUMO+1	0.22704365
			HOMO-4 -> LUMO+2	0.044712461
			HOMO-3 -> LUMO+2	0.174262465
			HOMO-2 -> LUMO+1	0.08522669
			HOMO -> LUMO+10	0.036137473
			HOMO -> LUMO+13	0.027088609
	T_{17}	4.0418 eV	HOMO-7 -> LUMO	0.035139005
			HOMO-5 -> LUMO	0.033846816
			HOMO-4 -> LUMO	0.028824005
			HOMO-4 -> LUMO+1	0.055464482
			HOMO-3 -> LUMO+1	0.045614081
			HOMO-2 -> LUMO+1	0.394662817
			HOMO-2 -> LUMO+9	0.124460583
			HOMO-2 -> LUMO+12	0.03864756
	T_{18}	4.0580 eV	HOMO-6 -> LUMO+1	0.020495026
			HOMO-4 -> LUMO	0.694501837
			HOMO-2 -> LUMO+1	0.06617522
			HOMO-1 -> LUMO+10	0.022966531
			HOMO -> LUMO+10	0.024296897
	T_{19}	4.0750 eV	HOMO-17 -> LUMO	0.050365032
			HOMO-14 -> LUMO	0.026065011
			HOMO-11 -> LUMO+4	0.022505933
			HOMO-8 -> LUMO	0.028293447
			HOMO-7 -> LUMO	0.08686112
			HOMO-5 -> LUMO+12	0.045264387
			HOMO-2 -> LUMO+1	0.133861728
			HOMO-2 -> LUMO+9	0.046500301
			HOMO-2 -> LUMO+12	0.133158962
			HOMO-1 -> LUMO+10	0.029432232

	T_{20}	4.0876 eV	HOMO-15 -> LUMO+1	0.02977288
			HOMO-6 -> LUMO+2	0.07881244
			HOMO-4 -> LUMO	0.165577106
			HOMO-4 -> LUMO+1	0.038887027
			HOMO-3 -> LUMO+13	0.025610371
			HOMO-2 -> LUMO+1	0.045952993
			HOMO-1 -> LUMO+10	0.068842762
			HOMO-1 -> LUMO+13	0.035229197
			HOMO -> LUMO+10	0.02981682
			HOMO -> LUMO+11	0.040509965
			HOMO -> LUMO+14	0.074389959
	T_{21}	4.1137 eV	HOMO-17 -> LUMO	0.020499075
			HOMO-16 -> LUMO+1	0.02690736
			HOMO-9 -> LUMO+6	0.022936536
			HOMO-4 -> LUMO	0.035064816
			HOMO-4 -> LUMO+2	0.126253125
			HOMO-2 -> LUMO+1	0.030100765
			HOMO-2 -> LUMO+3	0.022155125
			HOMO-2 -> LUMO+9	0.036352865
			HOMO-1 -> LUMO+10	0.022336525
			HOMO-1 -> LUMO+11	0.054568865
			HOMO -> LUMO+10	0.050695648
			HOMO -> LUMO+11	0.07242818
	T_{22}	4.1173 eV	HOMO-17 -> LUMO	0.048778138
			HOMO-14 -> LUMO+3	0.038270378
			HOMO-11 -> LUMO+4	0.05184844
			HOMO-5 -> LUMO	0.023181351
			HOMO-4 -> LUMO+2	0.077499845
			HOMO-2 -> LUMO+1	0.099591845
			HOMO-2 -> LUMO+3	0.071706845
			HOMO-2 -> LUMO+9	0.142524605
			HOMO-1 -> LUMO+11	0.032890995
			HOMO -> LUMO+11	0.06741792
	T_{23}	4.1240 eV	HOMO-13 -> LUMO+7	0.024129651
			HOMO-9 -> LUMO+6	0.027928298
			HOMO-8 -> LUMO+6	0.022071005
			HOMO-6 -> LUMO+1	0.02438957
			HOMO-6 -> LUMO+10	0.023897352
			HOMO-4 -> LUMO+2	0.036834408
			HOMO-3 -> LUMO+1	0.049757506

			HOMO-3 -> LUMO+2	0.031948864
			HOMO-1 -> LUMO+10	0.0840582
			HOMO -> LUMO+11	0.091746145
	T_{24}	4.1611 eV	HOMO-10 -> LUMO+5	0.052994657
			HOMO-6 -> LUMO+1	0.032217373
			HOMO-6 -> LUMO+11	0.026902721
			HOMO-4 -> LUMO+1	0.029069427
			HOMO-4 -> LUMO+2	0.231662631
			HOMO-3 -> LUMO+1	0.033302643
			HOMO-3 -> LUMO+2	0.079816106
			HOMO-1 -> LUMO+11	0.020592322
			HOMO-1 -> LUMO+14	0.02024072
			HOMO -> LUMO+5	0.056052216
			HOMO -> LUMO+11	0.028809601
			HOMO -> LUMO+13	0.045156135
	T_{25}	4.2307 eV	HOMO-10 -> LUMO+5	0.032126055
			HOMO-1 -> LUMO+5	0.163901026
			HOMO-1 -> LUMO+6	0.050403125
			HOMO -> LUMO+5	0.396601992
			HOMO -> LUMO+6	0.156195783
			HOMO -> LUMO+7	0.042649522
	T_{26}	4.2449 eV	HOMO-3 -> LUMO+2	0.087855936
			HOMO-2 -> LUMO+2	0.866559795
			HOMO-1 -> LUMO+2	0.022408445

Table S3e The singlet and triplet excited state transition configurations of the 3CN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1-T_n| < 0.3$ eV were highlighted in red. (for the upper interacted pair in Figure 5)

	n	Energy	Orbitals	Transition
S_n	S_1	3.9085 eV	HOMO-2 -> LUMO+1	0.0534449
			HOMO-1 -> LUMO	0.0784476
			HOMO -> LUMO	0.6266625
			HOMO -> LUMO+1	0.144002
T_n	T_1	3.2314 eV	HOMO-5 -> LUMO	0.02686562
			HOMO-5 -> LUMO+1	0.036132096
			HOMO-4 -> LUMO	0.09122429
			HOMO-4 -> LUMO+1	0.065225496
			HOMO-4 -> LUMO+3	0.028771207

			HOMO-3 -> LUMO	0.021197405
			HOMO-3 -> LUMO+2	0.125690952
			HOMO-1 -> LUMO+5	0.060795845
			HOMO -> LUMO	0.052962106
			HOMO -> LUMO+1	0.076073402
			HOMO -> LUMO+3	0.061523304
	T_2	3.2514 eV	HOMO-7 -> LUMO+2	0.030563809
			HOMO-5 -> LUMO+2	0.022675981
			HOMO-4 -> LUMO	0.022774048
			HOMO-4 -> LUMO+2	0.059229936
			HOMO-3 -> LUMO	0.038414376
			HOMO-3 -> LUMO+1	0.082946645
			HOMO-3 -> LUMO+2	0.181864805
			HOMO-1 -> LUMO+3	0.08176968
			HOMO-1 -> LUMO+4	0.022493205
			HOMO-1 -> LUMO+5	0.045989379
			HOMO-1 -> LUMO+9	0.033122232
			HOMO -> LUMO+2	0.063553255
			HOMO -> LUMO+5	0.034463626
	T_3	3.2651 eV	HOMO-5 -> LUMO	0.170598087
			HOMO-5 -> LUMO+1	0.122472903
			HOMO-5 -> LUMO+4	0.02856528
			HOMO-4 -> LUMO	0.067285793
			HOMO-4 -> LUMO+1	0.074482561
			HOMO-2 -> LUMO	0.038875873
			HOMO-2 -> LUMO+1	0.030662785
			HOMO-2 -> LUMO+3	0.042305587
			HOMO-2 -> LUMO+4	0.092975344
			HOMO-2 -> LUMO+8	0.029548805
			HOMO -> LUMO+4	0.02827442
	T_4	3.3448 eV	HOMO-4 -> LUMO	0.026367265
			HOMO-2 -> LUMO+1	0.124340871
			HOMO-2 -> LUMO+2	0.02401117
			HOMO-1 -> LUMO	0.135241603
			HOMO-1 -> LUMO+1	0.04274888
			HOMO -> LUMO	0.325156608
			HOMO -> LUMO+1	0.097726205
			HOMO -> LUMO+2	0.050333299
	T_5	3.3770 eV	HOMO-5 -> LUMO	0.038953987
			HOMO-2 -> LUMO	0.37134962

			HOMO-2 -> LUMO+1	0.142994824
			HOMO-1 -> LUMO+1	0.07434368
			HOMO -> LUMO	0.03538332
			HOMO -> LUMO+1	0.149462314
	T_6	3.3962 eV	HOMO-1 -> LUMO	0.024279265
			HOMO-1 -> LUMO+1	0.096553757
			HOMO-1 -> LUMO+2	0.532140545
			HOMO -> LUMO+1	0.03256352
			HOMO -> LUMO+2	0.151184007
	T_7	3.6386 eV	HOMO-10 -> LUMO+10	0.02290228
			HOMO-9 -> LUMO+10	0.038614205
			HOMO-8 -> LUMO+11	0.039920077
			HOMO-5 -> LUMO	0.028973059
			HOMO-4 -> LUMO+1	0.032696359
			HOMO-2 -> LUMO+3	0.0718205
			HOMO-1 -> LUMO+3	0.070936378
			HOMO-1 -> LUMO+4	0.04122469
			HOMO -> LUMO+2	0.040299605
			HOMO -> LUMO+3	0.079488819
			HOMO -> LUMO+4	0.047604637
			HOMO -> LUMO+5	0.098319517
	T_8	3.6521 eV	HOMO-13 -> LUMO+6	0.071881153
			HOMO-12 -> LUMO+6	0.021250973
			HOMO-11 -> LUMO+5	0.029344954
			HOMO-11 -> LUMO+9	0.079904029
			HOMO-3 -> LUMO+2	0.071162554
			HOMO-1 -> LUMO+3	0.061362051
			HOMO-1 -> LUMO+5	0.224932659
			HOMO -> LUMO+2	0.023535821
			HOMO -> LUMO+3	0.041639208
			HOMO -> LUMO+4	0.047228938
			HOMO -> LUMO+5	0.037177191
	T_9	3.6580 eV	HOMO-14 -> LUMO+7	0.022455043
			HOMO-14 -> LUMO+11	0.024354245
			HOMO-12 -> LUMO+7	0.028498394
			HOMO-12 -> LUMO+8	0.048186497
			HOMO-10 -> LUMO+7	0.03301936
			HOMO-9 -> LUMO+7	0.036747605
			HOMO-5 -> LUMO+1	0.040401874
			HOMO-4 -> LUMO	0.03661218

			HOMO-2 -> LUMO+4	0.194475898
			HOMO-2 -> LUMO+8	0.023427466
			HOMO-1 -> LUMO+4	0.02876641
			HOMO -> LUMO+3	0.076143629
			HOMO -> LUMO+4	0.024477994
	T_{10}	3.7399 eV	HOMO-14 -> LUMO+11	0.026583568
			HOMO-10 -> LUMO+10	0.026791495
			HOMO-9 -> LUMO+10	0.07886009
			HOMO-8 -> LUMO+11	0.052526887
			HOMO-6 -> LUMO+10	0.039553594
			HOMO-4 -> LUMO	0.031130115
			HOMO-1 -> LUMO+1	0.03053909
			HOMO-1 -> LUMO+3	0.03125
			HOMO -> LUMO+3	0.028689706
			HOMO -> LUMO+10	0.028886465
			HOMO -> LUMO+11	0.073076645
	T_{11}	3.7647 eV	HOMO-13 -> LUMO+6	0.083378945
			HOMO-11 -> LUMO+5	0.041957251
			HOMO-11 -> LUMO+9	0.074127901
			HOMO-7 -> LUMO+6	0.020466691
			HOMO-3 -> LUMO+2	0.092863261
			HOMO-1 -> LUMO+5	0.049467706
			HOMO-1 -> LUMO+9	0.156341136
			HOMO -> LUMO+2	0.022361895
			HOMO -> LUMO+3	0.034948392
			HOMO -> LUMO+9	0.046305331
	T_{12}	3.7746 eV	HOMO-14 -> LUMO+7	0.021652805
			HOMO-14 -> LUMO+8	0.026206762
			HOMO-12 -> LUMO+4	0.033111938
			HOMO-12 -> LUMO+7	0.022024807
			HOMO-9 -> LUMO+7	0.027233112
			HOMO-5 -> LUMO	0.09895021
			HOMO-5 -> LUMO+1	0.053451421
			HOMO-4 -> LUMO	0.025646595
			HOMO-4 -> LUMO+1	0.045638247
			HOMO-2 -> LUMO+3	0.052475041
			HOMO-2 -> LUMO+4	0.087554386
			HOMO-2 -> LUMO+8	0.08862892
			HOMO-2 -> LUMO+11	0.024129651
			HOMO -> LUMO+4	0.029782642

			HOMO -> LUMO+8	0.047876557
	T_{13}	4.0154 eV	HOMO-5 -> LUMO+3	0.04003884
			HOMO-4 -> LUMO+3	0.09996709
			HOMO-3 -> LUMO+5	0.125921693
			HOMO-3 -> LUMO+9	0.022603632
			HOMO-1 -> LUMO	0.074389959
			HOMO-1 -> LUMO+1	0.037642192
			HOMO-1 -> LUMO+3	0.034050061
			HOMO-1 -> LUMO+5	0.061712871
			HOMO -> LUMO	0.027028125
			HOMO -> LUMO+1	0.064706434
			HOMO -> LUMO+3	0.138306442
			HOMO -> LUMO+4	0.024142834
	T_{14}	4.0377 eV	HOMO-4 -> LUMO	0.028929746
			HOMO-4 -> LUMO+1	0.031385146
			HOMO-4 -> LUMO+3	0.023613991
			HOMO-1 -> LUMO	0.253244211
			HOMO-1 -> LUMO+1	0.12393229
			HOMO-1 -> LUMO+2	0.079648387
			HOMO-1 -> LUMO+3	0.023535821
			HOMO -> LUMO	0.07872512
			HOMO -> LUMO+2	0.022087816
	T_{15}	4.0645 eV	HOMO-5 -> LUMO+5	0.024116472
			HOMO-4 -> LUMO+3	0.021337648
			HOMO-4 -> LUMO+5	0.064756807
			HOMO-3 -> LUMO+3	0.178431432
			HOMO-3 -> LUMO+4	0.053719864
			HOMO-3 -> LUMO+5	0.090874371
			HOMO-3 -> LUMO+9	0.05766408
			HOMO-2 -> LUMO+5	0.032742405
			HOMO-1 -> LUMO+3	0.023315042
			HOMO -> LUMO+5	0.196526882
			HOMO -> LUMO+9	0.04529448
	T_{16}	4.1150 eV	HOMO-5 -> LUMO+3	0.025249539
			HOMO-5 -> LUMO+4	0.051174403
			HOMO-4 -> LUMO+4	0.028393445
			HOMO-2 -> LUMO	0.065413445
			HOMO-2 -> LUMO+1	0.091412328
			HOMO-1 -> LUMO+1	0.0335405
			HOMO-1 -> LUMO+2	0.074498

			HOMO -> LUMO	0.04831697
			HOMO -> LUMO+1	0.205748295
			HOMO -> LUMO+2	0.072923805
	T_{17}	4.1195 eV	HOMO-5 -> LUMO+3	0.059740418
			HOMO-5 -> LUMO+4	0.159104405
			HOMO-5 -> LUMO+8	0.033282
			HOMO-4 -> LUMO+4	0.071245575
			HOMO-3 -> LUMO+2	0.024191201
			HOMO-2 -> LUMO+2	0.05285801
			HOMO-2 -> LUMO+8	0.030395917
			HOMO-2 -> LUMO+12	0.024579879
			HOMO-1 -> LUMO+1	0.02271433
			HOMO-1 -> LUMO+2	0.054906352
			HOMO -> LUMO+1	0.042824938
			HOMO -> LUMO+2	0.104662275
	T_{18}	4.1264 eV	HOMO-5 -> LUMO+4	0.040254194
			HOMO-3 -> LUMO+2	0.022319619
			HOMO-2 -> LUMO	0.124031882
			HOMO-2 -> LUMO+2	0.020495026
			HOMO-1 -> LUMO	0.03484272
			HOMO-1 -> LUMO+2	0.070050245
			HOMO -> LUMO	0.164795405
			HOMO -> LUMO+1	0.107379048
			HOMO -> LUMO+2	0.198903859
	T_{19}	4.1861 eV	HOMO-5 -> LUMO+4	0.027378
			HOMO-2 -> LUMO	0.23875432
			HOMO-2 -> LUMO+1	0.304106407
			HOMO-2 -> LUMO+2	0.046952737
			HOMO-2 -> LUMO+7	0.030910925
			HOMO-1 -> LUMO	0.040418931
			HOMO-1 -> LUMO+1	0.023078113
			HOMO -> LUMO	0.043559713
			HOMO -> LUMO+1	0.026101555
			HOMO -> LUMO+7	0.032589045
	T_{20}	4.2249 eV	HOMO-6 -> LUMO+10	0.024059405
			HOMO-3 -> LUMO	0.022277383
			HOMO-3 -> LUMO+1	0.027223778
			HOMO-2 -> LUMO+12	0.032430951
			HOMO-1 -> LUMO+3	0.022842394
			HOMO -> LUMO	0.050995405

			HOMO -> LUMO+2	0.025750882
			HOMO -> LUMO+4	0.040470125
			HOMO -> LUMO+5	0.039121639
			HOMO -> LUMO+7	0.062636762
			HOMO -> LUMO+8	0.025814464
			HOMO -> LUMO+11	0.03563916
			HOMO -> LUMO+12	0.041287885
			HOMO -> LUMO+14	0.0647928
	T_{21}	4.2534 eV	HOMO-13 -> LUMO+6	0.051315265
			HOMO-7 -> LUMO+6	0.020535538
			HOMO-3 -> LUMO+2	0.074004739
			HOMO-3 -> LUMO+5	0.020208541
			HOMO-1 -> LUMO+5	0.021123346
			HOMO-1 -> LUMO+9	0.133086723
			HOMO-1 -> LUMO+13	0.103021683
			HOMO -> LUMO+2	0.052650125
			HOMO -> LUMO+4	0.02635808
			HOMO -> LUMO+5	0.027107233
			HOMO -> LUMO+9	0.040112449
			HOMO -> LUMO+13	0.047315032
	T_{22}	4.2592 eV	HOMO-12 -> LUMO+7	0.020438376
			HOMO-5 -> LUMO+1	0.0220542
			HOMO-5 -> LUMO+4	0.090951125
			HOMO-4 -> LUMO+3	0.025483789
			HOMO-4 -> LUMO+4	0.035128402
			HOMO-2 -> LUMO+4	0.057684458
			HOMO-2 -> LUMO+8	0.075567169
			HOMO-2 -> LUMO+12	0.040949496
			HOMO-2 -> LUMO+14	0.044515312
			HOMO -> LUMO	0.039155213
			HOMO -> LUMO+8	0.031135106
			HOMO -> LUMO+12	0.047179776
	T_{23}	4.2777	HOMO-11 -> LUMO+6	0.03942432
			HOMO-11 -> LUMO+9	0.028651392
			HOMO-1 -> LUMO	0.092209357
			HOMO-1 -> LUMO+1	0.104205255
			HOMO-1 -> LUMO+6	0.365238951
			HOMO-1 -> LUMO+7	0.026348897
			HOMO -> LUMO+1	0.026625089
			HOMO -> LUMO+6	0.161414256

	T_{24}	4.2832 eV	HOMO-1 -> LUMO	0.226895425
			HOMO-1 -> LUMO+1	0.322195754
			HOMO-1 -> LUMO+2	0.023622685
			HOMO-1 -> LUMO+6	0.124880029
			HOMO -> LUMO	0.033846816
			HOMO -> LUMO+1	0.069407928
			HOMO -> LUMO+6	0.048180288
	T_{25}	4.3432 eV	HOMO-12 -> LUMO+7	0.032865352
			HOMO-2 -> LUMO	0.031741921
			HOMO-2 -> LUMO+1	0.060246147
			HOMO-2 -> LUMO+7	0.245112013
			HOMO-1 -> LUMO+7	0.061012231
			HOMO-1 -> LUMO+11	0.020592322
			HOMO -> LUMO+7	0.153004056
			HOMO -> LUMO+8	0.020490977
			HOMO -> LUMO+10	0.023449117
			HOMO -> LUMO+11	0.061755037
	T_{26}	4.3589 eV	HOMO-3 -> LUMO	0.05707469
			HOMO-3 -> LUMO+1	0.02594642
			HOMO-2 -> LUMO	0.045138106
			HOMO-2 -> LUMO+7	0.048959463
			HOMO-2 -> LUMO+8	0.020856989
			HOMO-2 -> LUMO+10	0.027321869
			HOMO-1 -> LUMO+10	0.061586461
			HOMO -> LUMO+10	0.265997592
			HOMO -> LUMO+11	0.038547538

Table S4a The singlet and triplet excited state transition configurations of the PCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1\text{-}T_n| < 0.3$ eV were highlighted in red. (for the bottom interacted pair in Figure 5)

	n	Energy	Orbitals	Transition
S_n	S_1	3.4639 eV	HOMO-1 ->LUMO	0.596429
			HOMO ->LUMO+1	0.395196
T_n	T_1	3.0335 eV	HOMO-7 ->LUMO	0.029272321
			HOMO-6 ->LUMO+1	0.031440289
			HOMO-1 ->LUMO+1	0.392232245
			HOMO ->LUMO	0.477420833
	T_2	3.0344 eV	HOMO-7 ->LUMO+1	0.028070282

			HOMO-6 ->LUMO	0.032538005
			HOMO-1 ->LUMO	0.462298817
			HOMO ->LUMO+1	0.407198977
	T_3	3.3077 eV	HOMO-5 ->LUMO+4	0.022075207
			HOMO-3 ->LUMO+4	0.256270723
			HOMO-3 ->LUMO+5	0.046689568
			HOMO-2 ->LUMO+4	0.314614849
			HOMO-2 ->LUMO+5	0.037625731
			HOMO-1 ->LUMO+6	0.022561128
			HOMO-1 ->LUMO+7	0.036272018
			HOMO ->LUMO+7	0.040623901
	T_4	3.3079 eV	HOMO-4 ->LUMO+5	0.023099602
			HOMO-3 ->LUMO+4	0.05379856
			HOMO-3 ->LUMO+5	0.296850535
			HOMO-2 ->LUMO+4	0.032369857
			HOMO-2 ->LUMO+5	0.27242533
			HOMO-1 ->LUMO+6	0.036369045
			HOMO-1 ->LUMO+7	0.022586626
			HOMO ->LUMO+6	0.04066952
	T_5	3.5308 eV	HOMO-1 ->LUMO+4	0.315805834
			HOMO-1 ->LUMO+5	0.10448849
			HOMO ->LUMO+4	0.408517605
	T_6	3.5308 eV	HOMO-1 ->LUMO+4	0.106380394
			HOMO-1 ->LUMO+5	0.315583346
			HOMO ->LUMO+5	0.406639656
	T_7	3.6220 eV	HOMO-1 ->LUMO	0.470566407
			HOMO ->LUMO+1	0.512436385
	T_8	3.6225 eV	HOMO-1 ->LUMO+1	0.526851125
			HOMO ->LUMO	0.454409511
	T_9	3.7211 eV	HOMO-3 ->LUMO+1	0.364948418
			HOMO-3 ->LUMO+4	0.024336592
			HOMO-2 ->LUMO	0.541590689
			HOMO-2 ->LUMO+5	0.023151216
	T_{10}	3.7214 eV	HOMO-3 ->LUMO	0.536295818
			HOMO-3 ->LUMO+5	0.02608328
			HOMO-2 ->LUMO+1	0.370367818
			HOMO-2 ->LUMO+4	0.02441608
	T_{11}	3.7766 eV	HOMO-1 ->LUMO+3	0.360349562
			HOMO ->LUMO+2	0.560867587
	T_{12}	3.7789 eV	HOMO-1 ->LUMO+2	0.542381955

			HOMO ->LUMO+3	0.378380403
	T_{13}	3.9729 eV	HOMO-11 ->LUMO+3	0.026019367
			HOMO-10 ->LUMO+2	0.028627459
			HOMO-8 ->LUMO	0.023596609
			HOMO-7 ->LUMO	0.035960256
			HOMO-6 ->LUMO+1	0.049228944
			HOMO-3 ->LUMO	0.354246279
			HOMO-2 ->LUMO+1	0.42502356
	T_{14}	3.9750 eV	HOMO-6 ->LUMO	0.030184245
			HOMO-3 ->LUMO+1	0.537933409
			HOMO-2 ->LUMO	0.334087728
	T_{15}	3.9889 eV	HOMO-11 ->LUMO+2	0.11098645
			HOMO-10 ->LUMO+3	0.10719376
			HOMO-9 ->LUMO	0.071759873
			HOMO-8 ->LUMO+1	0.068679592
			HOMO-7 ->LUMO+1	0.154190151
			HOMO-6 ->LUMO	0.18363012
			HOMO-3 ->LUMO+1	0.050358685
			HOMO-2 ->LUMO	0.078677511
			HOMO-1 ->LUMO	0.032727053
			HOMO ->LUMO+1	0.044676583
	T_{16}	3.9896 eV	HOMO-11 ->LUMO+3	0.094769165
			HOMO-10 ->LUMO+2	0.104561645
			HOMO-9 ->LUMO+1	0.063424973
			HOMO-8 ->LUMO	0.064304152
			HOMO-7 ->LUMO	0.146470369
			HOMO-6 ->LUMO+1	0.154545761
			HOMO-3 ->LUMO	0.063988954
			HOMO-2 ->LUMO+1	0.1573605
			HOMO-1 ->LUMO+1	0.037444898
			HOMO ->LUMO	0.029846131
	T_{17}	4.1518 eV	HOMO-5 ->LUMO+5	0.040174786
			HOMO-4 ->LUMO+5	0.057895239
			HOMO-3 ->LUMO+5	0.098089063
			HOMO-2 ->LUMO+5	0.0820125
			HOMO-1 ->LUMO+6	0.187272
			HOMO-1 ->LUMO+7	0.091463645
			HOMO ->LUMO+6	0.177226765
			HOMO ->LUMO+7	0.104680577
	T_{18}	4.1520 eV	HOMO-5 ->LUMO+4	0.059747331

			HOMO-4 ->LUMO+4	0.038591976
			HOMO-3 ->LUMO+4	0.085168899
			HOMO-2 ->LUMO+4	0.095213752
			HOMO-1 ->LUMO+6	0.091301191
			HOMO-1 ->LUMO+7	0.187210805
			HOMO ->LUMO+6	0.104680577
			HOMO ->LUMO+7	0.177441159
	T_{19}	4.2973 eV	HOMO-1 ->LUMO+2	0.415306752
			HOMO ->LUMO+3	0.575986445
	T_{20}	4.2987 eV	HOMO-1 ->LUMO+3	0.591045409
			HOMO ->LUMO+2	0.394325282
	T_{21}	4.3855 eV	HOMO-3 ->LUMO+3	0.237677546
			HOMO-2 ->LUMO+2	0.52005721
			HOMO-1 ->LUMO+9	0.033050205
			HOMO ->LUMO+8	0.032060184
	T_{22}	4.3864 eV	HOMO-3 ->LUMO+2	0.521935445
			HOMO-2 ->LUMO+3	0.2429045
			HOMO-1 ->LUMO+8	0.02977288
			HOMO ->LUMO+9	0.031330051
	T_{23}	4.4192 eV	HOMO-11 ->LUMO+3	0.026110695
			HOMO-10 ->LUMO+2	0.029437085
			HOMO-9 ->LUMO+4	0.020689848
			HOMO-5 ->LUMO+7	0.066517634
			HOMO-4 ->LUMO+6	0.068405607
			HOMO-3 ->LUMO+3	0.06019756
			HOMO-3 ->LUMO+12	0.040983845
			HOMO-2 ->LUMO+2	0.146654448
			HOMO-2 ->LUMO+13	0.04158728
			HOMO-1 ->LUMO+9	0.143155303
			HOMO ->LUMO+8	0.138917205
	T_{24}	4.4196 eV	HOMO-11 ->LUMO+2	0.02807976
			HOMO-10 ->LUMO+3	0.027687751
			HOMO-9 ->LUMO+5	0.021164474
			HOMO-7 ->LUMO+4	0.020244744
			HOMO-5 ->LUMO+6	0.06386738
			HOMO-4 ->LUMO+7	0.064232448
			HOMO-3 ->LUMO+2	0.140736346
			HOMO-3 ->LUMO+13	0.042264874
			HOMO-2 ->LUMO+3	0.057081447
			HOMO-2 ->LUMO+12	0.043241523

			HOMO-1 ->LUMO+8	0.139043738
			HOMO ->LUMO+9	0.14558408
	T_{25}	4.6117 eV	HOMO-1 ->LUMO+4	0.423089607
			HOMO-1 ->LUMO+5	0.080737693
			HOMO ->LUMO+4	0.443757363
			HOMO ->LUMO+5	0.050155779
	T_{26}	4.6119 eV	HOMO-1 ->LUMO+4	0.080424562
			HOMO-1 ->LUMO+5	0.422960834
			HOMO ->LUMO+4	0.049940641
			HOMO ->LUMO+5	0.44443592

Table S4b The singlet and triplet excited state transition configurations of the MCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1\text{-}T_n| < 0.3$ eV were highlighted in red. **(**for the bottom interacted pair in Figure 5**)**

	n	Energy	Orbitals	Transition
S_n	S_1	3.4114 eV	HOMO -> LUMO+1	0.98470964
T_n	T_1	3.1322 eV	HOMO-10 -> LUMO+1	0.090806173
			HOMO -> LUMO+1	0.830683162
			HOMO -> LUMO+4	0.02556965
	T_2	3.1812 eV	HOMO-9 -> LUMO+2	0.1088671
			HOMO-1 -> LUMO	0.0360085
			HOMO-1 -> LUMO+2	0.7674862
	T_3	3.1951 eV	HOMO-11 -> LUMO	0.1065096
			HOMO-2 -> LUMO	0.7775294
			HOMO-2 -> LUMO+5	0.0254838
	T_4	3.3626 eV	HOMO-17 -> LUMO+16	0.0229537
			HOMO-8 -> LUMO+3	0.0361267
			HOMO-5 -> LUMO+3	0.5605287
			HOMO-5 -> LUMO+4	0.0423172
			HOMO-5 -> LUMO+5	0.0254657
			HOMO-2 -> LUMO+3	0.1595899
			HOMO-2 -> LUMO+9	0.0870363
	T_5	3.3653 eV	HOMO-15 -> LUMO+18	0.0227058
			HOMO-7 -> LUMO+6	0.0413626
			HOMO-4 -> LUMO+6	0.5744848
			HOMO-4 -> LUMO+7	0.0716538
			HOMO-1 -> LUMO+6	0.1435194
			HOMO-1 -> LUMO+10	0.0875711

	T_6	3.3668 eV	HOMO-6 -> LUMO+8	0.0376971
			HOMO-3 -> LUMO+8	0.6604682
			HOMO -> LUMO+8	0.1324683
			HOMO -> LUMO+11	0.085988
	T_7	3.5133 eV	HOMO-8 -> LUMO+9	0.0288048
			HOMO-5 -> LUMO+3	0.1429841
			HOMO-2 -> LUMO+3	0.6861593
			HOMO-2 -> LUMO+4	0.0559987
	T_8	3.5213 eV	HOMO-7 -> LUMO+10	0.0302285
			HOMO-4 -> LUMO+6	0.1291336
			HOMO-1 -> LUMO+6	0.7465198
	T_9	3.5294 eV	HOMO-6 -> LUMO+11	0.0300615
			HOMO-3 -> LUMO+8	0.111751
			HOMO -> LUMO	0.0451081
			HOMO -> LUMO+4	0.0492729
			HOMO -> LUMO+8	0.6953507
	T_{10}	3.6155 eV	HOMO-16 -> LUMO+4	0.054807
			HOMO-13 -> LUMO+1	0.0553846
			HOMO-13 -> LUMO+4	0.037549
			HOMO-10 -> LUMO+1	0.1131548
			HOMO-10 -> LUMO+4	0.0204182
			HOMO -> LUMO	0.0419978
			HOMO -> LUMO+1	0.0974611
			HOMO -> LUMO+3	0.0434182
			HOMO -> LUMO+4	0.4606464
			HOMO -> LUMO+8	0.024642
	T_{11}	3.6400 eV	HOMO -> LUMO	0.8647703
			HOMO -> LUMO+8	0.0526566
	T_{12}	3.6613 eV	HOMO-15 -> LUMO+7	0.0285653
			HOMO-12 -> LUMO+2	0.078511
			HOMO-12 -> LUMO+7	0.0679109
			HOMO-9 -> LUMO+2	0.1322522
			HOMO-9 -> LUMO+7	0.0270793
			HOMO-1 -> LUMO+2	0.1428451
			HOMO-1 -> LUMO+7	0.4303879
	T_{13}	3.6736 eV	HOMO-17 -> LUMO+5	0.0237402
			HOMO-14 -> LUMO	0.0823531
			HOMO-14 -> LUMO+5	0.0727788
			HOMO-11 -> LUMO	0.1216527
			HOMO-11 -> LUMO+5	0.029166

			HOMO-2 -> LUMO	0.106528
			HOMO-2 -> LUMO+2	0.0263719
			HOMO-2 -> LUMO+5	0.4214905
			HOMO -> LUMO	0.0383645
	T_{14}	3.7202 eV	HOMO -> LUMO+2	0.9894306
	T_{15}	3.7555 eV	HOMO-1 -> LUMO	0.9412743
	T_{16}	3.8283 eV	HOMO-3 -> LUMO+1	0.9555978
	T_{17}	3.8487 ev	HOMO-1 -> LUMO+1	0.9952912
	T_{18}	3.8703 eV	HOMO-2 -> LUMO	0.0427664
			HOMO-2 -> LUMO+2	0.918907
	T_{19}	3.8988 eV	HOMO-2 -> LUMO+1	0.9859169
	T_{20}	3.9126 eV	HOMO-4 -> LUMO	0.0468915
			HOMO-4 -> LUMO+2	0.8905252
			HOMO-1 -> LUMO+7	0.0250253
	T_{21}	3.9415 eV	HOMO-5 -> LUMO	0.8872985
			HOMO-5 -> LUMO+2	0.0205599
			HOMO-2 -> LUMO+5	0.0327066
	T_{22}	3.9472 eV	HOMO-13 -> LUMO+1	0.1403122
			HOMO-11 -> LUMO+1	0.0284173
			HOMO-10 -> LUMO+1	0.3662824
			HOMO-3 -> LUMO+1	0.0245178
			HOMO -> LUMO+1	0.0227783
			HOMO -> LUMO+3	0.0276736
			HOMO -> LUMO+4	0.2744664
	T_{23}	3.9809 eV	HOMO-3 -> LUMO	0.9581432
	T_{24}	4.0022 eV	HOMO-12 -> LUMO+2	0.1213964
	T_{25}	4.0189 eV	HOMO-9 -> LUMO+2	0.3012277
			HOMO-4 -> LUMO+2	0.0396549
			HOMO-1 -> LUMO+7	0.3846697
	T_{26}	4.0706 eV	HOMO-3 -> LUMO+2	0.9906689

Table S4c The singlet and triplet excited state transition configurations of the OCN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1\text{-}T_n| < 0.3$ eV were highlighted in red. **(**for the bottom interacted pair in Figure 5**)**

	n	Energy	Orbitals	Transition
S_n	S_1	2.7256 eV	HOMO -> LUMO	0.99913248
T_n	T_1	2.7255 eV	HOMO-22 -> LUMO	0.021057624
			HOMO-6 -> LUMO	0.903275523

			HOMO-6 -> LUMO+3	0.021736125
	T_2	2.9890 eV	HOMO-22 -> LUMO	0.021057624
			HOMO-6 -> LUMO	0.903275523
			HOMO-6 -> LUMO+3	0.021736125
	T_3	3.0225 eV	HOMO-1 -> LUMO	0.972928802
			HOMO-1 -> LUMO+2	0.023531482
	T_4	3.0574 eV	HOMO-16 -> LUMO+1	0.020697986
			HOMO-3 -> LUMO	0.055617795
			HOMO-3 -> LUMO+1	0.810162663
			HOMO-3 -> LUMO+5	0.022518664
	T_5	3.0797 eV	HOMO-2 -> LUMO	0.955266064
	T_6	3.1152 eV	HOMO-3 -> LUMO	0.89932825
			HOMO-3 -> LUMO+1	0.02700488
			HOMO-2 -> LUMO	0.030066424
	T_7	3.1295 eV	HOMO-15 -> LUMO+2	0.039812776
			HOMO-1 -> LUMO	0.024962717
			HOMO-1 -> LUMO+2	0.81971208
			HOMO-1 -> LUMO+6	0.041893546
	T_8	3.1302 eV	HOMO -> LUMO+1	0.967078874
	T_9	3.2260 eV	HOMO-13 -> LUMO+4	0.026325946
			HOMO-7 -> LUMO	0.025651125
			HOMO-7 -> LUMO+4	0.518263805
			HOMO-7 -> LUMO+5	0.060649479
			HOMO-6 -> LUMO+4	0.026491416
			HOMO-6 -> LUMO+11	0.024134045
			HOMO-6 -> LUMO+12	0.054100762
			HOMO-5 -> LUMO+8	0.107165981
	T_{10}	3.2281 eV	HOMO-11 -> LUMO+8	0.028910506
			HOMO-7 -> LUMO+4	0.099181672
			HOMO-5 -> LUMO+7	0.04404512
			HOMO-5 -> LUMO+8	0.5607405
			HOMO-3 -> LUMO+13	0.078614055
	T_{11}	3.2332 eV	HOMO-10 -> LUMO+9	0.038270378
			HOMO-10 -> LUMO+20	0.02259938
			HOMO-4 -> LUMO+9	0.729003975
			HOMO-1 -> LUMO+9	0.024584314
			HOMO-1 -> LUMO+15	0.098408225
	T_{12}	3.2373 eV	HOMO-14 -> 309	0.030960673
			HOMO-8 -> LUMO+10	0.043890919
			HOMO-2 -> LUMO+10	0.697687594

			HOMO -> LUMO+10	0.038820125
			HOMO -> LUMO+17	0.100486445
	T_{13}	3.3148 eV	HOMO-4 -> LUMO	0.996984963
	T_{14}	3.3617 eV	HOMO-9 -> LUMO+7	0.061719898
			HOMO -> LUMO+2	0.55398338
			HOMO -> LUMO+4	0.02687953
			HOMO -> LUMO+7	0.178407538
			HOMO -> LUMO+8	0.02324168
			HOMO -> LUMO+10	0.066117025
	T_{15}	3.3790 eV	HOMO-9 -> LUMO+7	0.067021927
			HOMO -> LUMO+2	0.422004845
			HOMO -> LUMO+4	0.025773581
			HOMO -> LUMO+7	0.14587561
			HOMO -> LUMO+8	0.02544768
			HOMO -> LUMO+10	0.176382362
	T_{16}	3.3911 eV	HOMO-7 -> LUMO	0.024296897
			HOMO-5 -> LUMO	0.95615089
	T_{17}	3.4190 eV	HOMO -> LUMO+3	0.965077245
			HOMO -> LUMO+10	0.022663205
	T_{18}	3.4319 eV	HOMO-9 -> LUMO+7	0.073827874
			HOMO -> LUMO+4	0.025633008
			HOMO -> LUMO+7	0.132313968
			HOMO -> LUMO+10	0.604758024
			HOMO -> LUMO+11	0.022979392
	T_{19}	3.4507 eV	HOMO-23 -> LUMO+3	0.077263805
			HOMO-22 -> LUMO	0.077917729
			HOMO-6 -> LUMO	0.043459416
			HOMO-6 -> LUMO+3	0.419015197
			HOMO-6 -> LUMO+4	0.220501123
	T_{20}	3.4522 eV	HOMO-18 -> LUMO+5	0.029568256
			HOMO-19 -> LUMO+1	0.028982689
			HOMO-11 -> LUMO+13	0.020454554
			HOMO-7 -> LUMO	0.232916775
			HOMO-3 -> LUMO+1	0.038703184
			HOMO-3 -> LUMO+4	0.051417831
			HOMO-3 -> LUMO+5	0.194401066
			HOMO-3 -> LUMO+8	0.273607634
	T_{21}	3.4576 eV	HOMO-7 -> LUMO	0.689513731
			HOMO-5 -> LUMO	0.020951045
			HOMO-3 -> LUMO+5	0.055364609

			HOMO-3 -> LUMO+8	0.106869891
	T_{22}	3.4672 eV	HOMO-10 -> LUMO+15	0.038558645
			HOMO-4 -> LUMO+9	0.021773671
			HOMO-1 -> LUMO+2	0.02976312
			HOMO-1 -> LUMO+6	0.130754752
			HOMO-1 -> LUMO+9	0.70465069
	T_{23}	3.4874 eV	HOMO-1 -> LUMO+1	0.996730805
	T_{24}	3.4942 eV	HOMO-5 -> LUMO+1	0.032364768
			HOMO-2 -> LUMO+1	0.947568845
	T_{25}	3.5123 eV	HOMO-18 -> LUMO+5	0.076863363
			HOMO-19 -> LUMO+1	0.107675842
			HOMO-16 -> LUMO+1	0.073130177
			HOMO-3 -> LUMO+1	0.031626125
			HOMO-3 -> LUMO+5	0.174605042
			HOMO-3 -> LUMO+7	0.032344418
			HOMO-3 -> LUMO+8	0.38206037
	T_{26}	3.5162 eV	HOMO-23 -> LUMO+3	0.066963361
			HOMO-22 -> LUMO	0.098674589
			HOMO-21 -> LUMO	0.023289136
			HOMO-6 -> LUMO+3	0.095205025
			HOMO-6 -> LUMO+4	0.511384071
			HOMO-6 -> LUMO+5	0.06485041

Table S4d The singlet and triplet excited state transition configurations of the 2CN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1-T_n| < 0.3$ eV were highlighted in red. **(**for the bottom interacted pair in Figure 5**)**

	n	Energy	Orbitals	Transition
S_n	S_1	3.5528 eV	HOMO -> LUMO	0.990584426
T_n	T_1	3.0425 eV	HOMO-4 -> LUMO+1	0.844662034
			HOMO-1 -> LUMO+10	0.045499378
	T_2	3.0435 eV	HOMO-5 -> LUMO	0.811614442
			HOMO-3 -> LUMO	0.03936818
			HOMO-3 -> LUMO+9	0.040186125
	T_3	3.0459 eV	HOMO-3 -> LUMO+2	0.034447875
			HOMO-2 -> LUMO+2	0.79776133
			HOMO -> LUMO+12	0.031385146
	T_4	3.1389 eV	HOMO-5 -> LUMO	0.032466616
			HOMO-3 -> LUMO	0.858416839

			HOMO-2 -> LUMO	0.05235848
	T_5	3.1634 eV	HOMO-1 -> LUMO+1	0.918988359
	T_6	3.1912 eV	HOMO -> LUMO+2	0.9248272
	T_7	3.5544 eV	HOMO -> LUMO	0.977202
	T_8	3.8116 eV	HOMO-2 -> LUMO	0.05852989
			HOMO-1 -> LUMO	0.892314405
	T_9	3.8172 eV	HOMO-10 -> LUMO+8	0.14527128
			HOMO-8 -> LUMO+6	0.141267386
			HOMO-8 -> LUMO+7	0.077122354
			HOMO-6 -> LUMO+8	0.031440289
			HOMO-1 -> LUMO	0.027626602
			HOMO -> LUMO+1	0.040829389
			HOMO -> LUMO+6	0.051559027
			HOMO -> LUMO+8	0.346644685
	T_{10}	3.8356 eV	HOMO-12 -> LUMO+6	0.028507944
			HOMO-12 -> LUMO+7	0.037823501
			HOMO-9 -> LUMO+5	0.14795712
			HOMO-9 -> LUMO+7	0.02576904
			HOMO-7 -> LUMO+6	0.022987968
			HOMO-7 -> LUMO+7	0.041922497
			HOMO-2 -> LUMO	0.266785906
			HOMO-1 -> LUMO+5	0.118867128
			HOMO-1 -> LUMO+6	0.081963907
			HOMO-1 -> LUMO+7	0.067955098
	T_{11}	3.8387 eV	HOMO-9 -> LUMO+5	0.057297895
			HOMO-3 -> LUMO	0.033742824
			HOMO-2 -> LUMO	0.59470418
			HOMO-1 -> LUMO	0.070921312
			HOMO-1 -> LUMO+5	0.046494202
			HOMO-1 -> LUMO+6	0.033055347
			HOMO-1 -> LUMO+7	0.025398072
	T_{12}	3.8480 eV	HOMO-15 -> LUMO+3	0.070447565
			HOMO-15 -> LUMO+9	0.024248424
			HOMO-13 -> LUMO+3	0.064785601
			HOMO-13 -> LUMO+4	0.160925991
			HOMO-11 -> LUMO+3	0.0441045
			HOMO-11 -> LUMO+4	0.113116705
			HOMO-3 -> LUMO+3	0.367018849
	T_{13}	3.9399 eV	HOMO -> LUMO+1	0.930357123
	T_{14}	4.0749 eV	HOMO-16 -> LUMO+1	0.052313186

			HOMO-12 -> LUMO+1	0.022163546
			HOMO-7 -> LUMO+1	0.151569168
			HOMO-7 -> LUMO+10	0.02068578
			HOMO-7 -> LUMO+13	0.037286343
			HOMO-4 -> LUMO+1	0.04917248
			HOMO-4 -> LUMO+13	0.040875123
			HOMO-4 -> LUMO+16	0.025159731
			HOMO-1 -> LUMO+10	0.252490392
			HOMO-1 -> LUMO+13	0.153701857
	T_{15}	4.0777 eV	HOMO-17 -> LUMO	0.042486125
			HOMO-15 -> LUMO	0.040823674
			HOMO-13 -> LUMO	0.03411272
			HOMO-11 -> LUMO	0.087713473
			HOMO-6 -> LUMO+2	0.02695842
			HOMO-5 -> LUMO	0.044622794
			HOMO-5 -> LUMO+11	0.02225628
			HOMO-3 -> LUMO+9	0.208903552
			HOMO-3 -> LUMO+11	0.089261575
			HOMO-3 -> LUMO+12	0.036736762
			HOMO -> LUMO+12	0.024398405
			HOMO -> LUMO+14	0.02281248
	T_{16}	4.0810 eV	HOMO-14 -> LUMO+2	0.04986482
			HOMO-6 -> LUMO+2	0.131779512
			HOMO-6 -> LUMO+14	0.025919091
			HOMO-3 -> LUMO+9	0.035762077
			HOMO-3 -> LUMO+11	0.026284659
			HOMO-2 -> LUMO+2	0.029141808
			HOMO-2 -> LUMO+14	0.04057261
			HOMO-2 -> LUMO+17	0.020861074
			HOMO -> LUMO+11	0.064175114
			HOMO -> LUMO+12	0.109999261
			HOMO -> LUMO+14	0.111836122
	T_{17}	4.1331 eV	HOMO-17 -> LUMO	0.10405922
			HOMO-15 -> LUMO+3	0.070928845
			HOMO-15 -> LUMO+9	0.028003978
			HOMO-13 -> LUMO+4	0.062594296
			HOMO-11 -> LUMO+4	0.0528125
			HOMO-11 -> LUMO+9	0.026316768
			HOMO-5 -> LUMO	0.042032602
			HOMO-5 -> LUMO+11	0.029904797

			HOMO-3 -> LUMO+3	0.092949473
			HOMO-3 -> LUMO+9	0.223325811
			HOMO-3 -> LUMO+15	0.045959056
	T_{18}	4.1339 eV	HOMO-16 -> LUMO+1	0.096307827
			HOMO-12 -> LUMO+6	0.029675352
			HOMO-12 -> LUMO+7	0.025556083
			HOMO-12 -> LUMO+10	0.022180392
			HOMO-9 -> LUMO+5	0.070245016
			HOMO-9 -> LUMO+7	0.020681712
			HOMO-7 -> LUMO+10	0.044676583
			HOMO-4 -> LUMO+1	0.044934024
			HOMO-4 -> LUMO+10	0.02522258
			HOMO-4 -> LUMO+13	0.047099943
			HOMO-1 -> LUMO+5	0.039925728
			HOMO-1 -> LUMO+6	0.034542433
			HOMO-1 -> LUMO+10	0.255069389
			HOMO-1 -> LUMO+13	0.02292797
			HOMO-1 -> LUMO+16	0.046848605
	T_{19}	4.1522 eV	HOMO-14 -> LUMO+2	0.070500125
			HOMO-10 -> LUMO+8	0.062934424
			HOMO-8 -> LUMO+6	0.05664978
			HOMO-8 -> LUMO+7	0.033602689
			HOMO-6 -> LUMO+12	0.031180039
			HOMO-2 -> LUMO+2	0.05539789
			HOMO-2 -> LUMO+14	0.037829002
			HOMO -> LUMO+8	0.052916551
			HOMO -> LUMO+11	0.106481895
			HOMO -> LUMO+12	0.207522589
			HOMO -> LUMO+17	0.049681824
	T_{20}	4.1563 eV	HOMO-4 -> LUMO	0.998030176
	T_{21}	4.1796 eV	HOMO-1 -> LUMO+2	0.944157853
	T_{22}	4.2450 eV	HOMO-2 -> LUMO+1	0.984934195
	T_{23}	4.2793 eV	HOMO-10 -> LUMO+6	0.027387361
			HOMO-10 -> LUMO+7	0.022155125
			HOMO -> LUMO+5	0.052449127
			HOMO -> LUMO+6	0.414268429
			HOMO -> LUMO+7	0.305934064
			HOMO -> LUMO+8	0.085267981
	T_{24}	4.3426 eV	HOMO-12 -> LUMO+5	0.021478354
			HOMO-12 -> LUMO+7	0.026912

			HOMO-9 -> LUMO+5	0.028108205
			HOMO-1 -> LUMO+2	0.02063293
			HOMO-1 -> LUMO+4	0.028184128
			HOMO-1 -> LUMO+5	0.393650645
			HOMO-1 -> LUMO+6	0.03869762
			HOMO-1 -> LUMO+7	0.306967466
	T_{25}	4.3616 eV	HOMO-3 -> LUMO+1	0.986029245
	T_{26}	4.3740 eV	HOMO-3 -> LUMO+2	0.887884728
			HOMO-3 -> LUMO+4	0.033815602
			HOMO-2 -> LUMO+2	0.040430305

Table S4e The singlet and triplet excited state transition configurations of the 3CN from single crystal revealed by TD-DFT calculations. The matched excited states that contain the same orbital transition components of S_1 and $|S_1-T_n| < 0.3$ eV were highlighted in red. **(**for the bottom interacted pair in Figure 5**)**

	n	Energy	Orbitals	Transition
S_n	S_1	3.9501 eV	HOMO-2 -> LUMO	0.064462042
			HOMO-2 -> LUMO+2	0.05081672
			HOMO -> LUMO	0.724928405
			HOMO -> LUMO+2	0.090363507
T_n	T_1	3.2651 eV	HOMO-5 -> LUMO	0.12060925
			HOMO-5 -> LUMO+2	0.039525473
			HOMO-3 -> LUMO	0.078479296
			HOMO-3 -> LUMO+2	0.21687698
			HOMO-3 -> LUMO+6	0.020539591
			HOMO-2 -> LUMO+2	0.03050944
			HOMO-2 -> LUMO+6	0.020148274
			HOMO -> LUMO+6	0.097682
			HOMO -> LUMO+11	0.021823783
	T_2	3.2690 eV	HOMO-11 -> LUMO	0.02160289
			HOMO-5 -> LUMO	0.25499797
			HOMO-5 -> LUMO+2	0.034311521
			HOMO-3 -> LUMO+2	0.145562497
			HOMO-2 -> LUMO	0.054926237
			HOMO-2 -> LUMO+4	0.053543009
			HOMO-2 -> LUMO+5	0.031948864
			HOMO-2 -> LUMO+6	0.020268898
			HOMO -> LUMO+2	0.034552947

			HOMO -> LUMO+6	0.042003613
	T_3	3.2719 eV	HOMO-7 -> LUMO+1	0.032578834
			HOMO-4 -> LUMO+1	0.48607828
			HOMO-4 -> LUMO+3	0.04798802
			HOMO-1 -> LUMO+1	0.02285522
			HOMO-1 -> LUMO+3	0.114003125
			HOMO-1 -> LUMO+7	0.093260167
			HOMO-1 -> LUMO+9	0.02677298
	T_4	3.3672 eV	HOMO-5 -> LUMO	0.025887226
			HOMO-3 -> LUMO+2	0.0210125
			HOMO-2 -> LUMO	0.141107969
			HOMO-2 -> LUMO+2	0.168850227
			HOMO -> LUMO	0.375393795
			HOMO -> LUMO+2	0.130744525
	T_5	3.3853 eV	HOMO-5 -> LUMO	0.035027751
			HOMO-3 -> LUMO+2	0.03409705
			HOMO-2 -> LUMO	0.373317123
			HOMO -> LUMO+2	0.417789405
	T_6	3.4184 eV	HOMO-4 -> LUMO+1	0.026735969
			HOMO-1 -> LUMO+1	0.843856387
			HOMO -> LUMO+1	0.02333232
	T_7	3.6463 eV	HOMO-14 -> LUMO+4	0.036132096
			HOMO-14 -> LUMO+5	0.066919453
			HOMO-14 -> LUMO+8	0.021765325
			HOMO-13 -> LUMO+3	0.109390354
			HOMO-13 -> LUMO+7	0.032212296
			HOMO-4 -> LUMO+1	0.067653133
			HOMO-1 -> LUMO+3	0.37549778
	T_8	3.6502 eV	HOMO-12 -> LUMO+4	0.033810401
			HOMO-12 -> LUMO+9	0.0400445
			HOMO-11 -> LUMO+8	0.032385125
			HOMO-10 -> LUMO+8	0.024628682
			HOMO-9 -> LUMO+8	0.025434146
			HOMO-5 -> LUMO	0.044904051
			HOMO-2 -> LUMO+4	0.116818445
			HOMO-2 -> LUMO+5	0.050682912
			HOMO-1 -> LUMO+3	0.0471245
			HOMO -> LUMO+4	0.055697869
			HOMO -> LUMO+5	0.021706945
			HOMO -> LUMO+6	0.070883655

	T_9	3.6648 eV	HOMO-12 -> LUMO+11	0.033966605
			HOMO-10 -> LUMO+10	0.02835533
			HOMO-9 -> LUMO+9	0.020515277
			HOMO-9 -> LUMO+10	0.053844493
			HOMO-8 -> LUMO+10	0.04780232
			HOMO-7 -> LUMO+6	0.021769498
			HOMO-7 -> LUMO+11	0.023099602
			HOMO-6 -> LUMO+10	0.022522909
			HOMO-6 -> LUMO+11	0.02645
			HOMO-3 -> LUMO+2	0.048261031
			HOMO-2 -> LUMO+4	0.029340109
			HOMO-2 -> LUMO+6	0.061719898
			HOMO -> LUMO+6	0.193230578
			HOMO -> LUMO+11	0.03516552
	T_{10}	3.7741 eV	HOMO-5 -> LUMO	0.110421802
			HOMO-5 -> LUMO+2	0.029403125
			HOMO-3 -> LUMO	0.03860309
			HOMO-3 -> LUMO+2	0.086869456
			HOMO-2 -> LUMO+4	0.035388641
			HOMO-2 -> LUMO+5	0.025705514
			HOMO-2 -> LUMO+7	0.050619256
			HOMO-2 -> LUMO+9	0.0496125
			HOMO -> LUMO+4	0.029403125
			HOMO -> LUMO+6	0.087320205
			HOMO -> LUMO+11	0.072215201
	T_{11}	3.7859 eV	HOMO-5 -> LUMO	0.10960562
			HOMO-3 -> LUMO+2	0.10266793
			HOMO-2 -> LUMO+4	0.049536929
			HOMO-2 -> LUMO+5	0.030474867
			HOMO-2 -> LUMO+6	0.03488497
			HOMO-2 -> LUMO+7	0.025651125
			HOMO-2 -> LUMO+11	0.03426962
			HOMO -> LUMO+6	0.057834005
			HOMO -> LUMO+7	0.028236385
			HOMO -> LUMO+9	0.046074337
			HOMO -> LUMO+10	0.032860225
			HOMO -> LUMO+11	0.037488696
	T_{12}	3.7902 eV	HOMO-14 -> LUMO+4	0.025416106
			HOMO-14 -> LUMO+5	0.044910045
			HOMO-13 -> LUMO+3	0.082109729

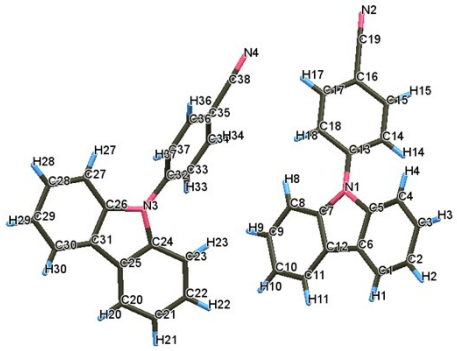
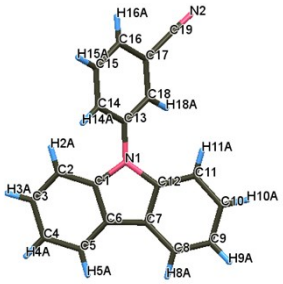
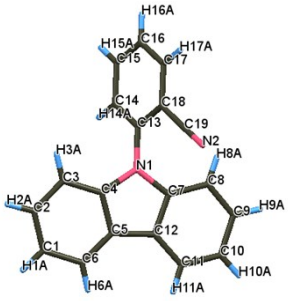
			HOMO-4 -> LUMO+1	0.245826696
			HOMO-1 -> LUMO+3	0.072359688
			HOMO-1 -> LUMO+5	0.037335514
			HOMO-1 -> LUMO+7	0.208658
			HOMO-1 -> LUMO+9	0.054087605
	T_{13}	4.0973 eV	HOMO-3 -> LUMO+6	0.064304152
			HOMO-2 -> LUMO	0.175480728
			HOMO-2 -> LUMO+2	0.060190621
			HOMO -> LUMO	0.347011143
			HOMO -> LUMO+2	0.121347085
			HOMO -> LUMO+10	0.022366125
	T_{14}	4.1320 eV	HOMO-5 -> LUMO+4	0.192063624
			HOMO-5 -> LUMO+5	0.100782541
			HOMO-5 -> LUMO+7	0.066999962
			HOMO-5 -> LUMO+9	0.040413245
			HOMO-2 -> LUMO+2	0.025950976
			HOMO-2 -> LUMO+7	0.027000232
			HOMO-2 -> LUMO+9	0.041564211
			HOMO-2 -> LUMO+12	0.062551845
			HOMO-2 -> LUMO+14	0.02251442
			HOMO -> LUMO	0.026087848
			HOMO -> LUMO+2	0.033266522
			HOMO -> LUMO+9	0.024504552
			HOMO -> LUMO+12	0.022391512
	T_{15}	4.1340 eV	HOMO-7 -> LUMO+1	0.022459282
			HOMO-4 -> LUMO+3	0.292643101
			HOMO-4 -> LUMO+5	0.03246152
			HOMO-4 -> LUMO+7	0.173048445
			HOMO-4 -> LUMO+9	0.043329792
			HOMO-1 -> LUMO+7	0.072649096
			HOMO-1 -> LUMO+9	0.023479445
			HOMO-1 -> LUMO+13	0.094734339
	T_{16}	4.1362 eV	HOMO-3 -> LUMO+6	0.269686368
			HOMO-3 -> LUMO+11	0.040163448
			HOMO-2 -> LUMO	0.069975405
			HOMO -> LUMO	0.100396805
			HOMO -> LUMO+4	0.039076897
			HOMO -> LUMO+8	0.036379834
			HOMO -> LUMO+9	0.027452931
			HOMO -> LUMO+11	0.03601928

			HOMO -> LUMO+12	0.026459201
			HOMO -> LUMO+14	0.04158728
	T_{17}	4.1699 eV	HOMO-13 -> LUMO+4	0.023449117
			HOMO-13 -> LUMO+5	0.041824104
			HOMO-1 -> LUMO+4	0.300684615
			HOMO-1 -> LUMO+5	0.428886173
			HOMO-1 -> LUMO+7	0.023488114
			HOMO-1 -> LUMO+8	0.028184128
			HOMO-1 -> LUMO+9	0.022285827
			HOMO -> LUMO+5	0.026339715
	T_{18}	4.2055 eV	HOMO-3 -> LUMO+6	0.057582605
			HOMO-2 -> LUMO	0.027527965
			HOMO-2 -> LUMO+1	0.02063293
			HOMO-2 -> LUMO+2	0.261726125
			HOMO-2 -> LUMO+4	0.021936746
			HOMO-2 -> LUMO+5	0.034369176
			HOMO-2 -> LUMO+8	0.08206921
			HOMO -> LUMO	0.03020882
			HOMO -> LUMO+1	0.084444061
			HOMO -> LUMO+2	0.037035533
			HOMO -> LUMO+5	0.037873024
			HOMO -> LUMO+8	0.070530168
	T_{19}	4.2405 eV	HOMO-5 -> LUMO+4	0.10441536
			HOMO-5 -> LUMO+5	0.068161704
			HOMO-5 -> LUMO+7	0.02522258
			HOMO-4 -> LUMO+3	0.026270904
			HOMO-3 -> LUMO+6	0.029563393
			HOMO-2 -> LUMO+2	0.087119728
			HOMO-1 -> LUMO+3	0.022037402
			HOMO -> LUMO+1	0.11347848
			HOMO -> LUMO+2	0.039222403
			HOMO -> LUMO+4	0.066473872
			HOMO -> LUMO+9	0.025678312
	T_{20}	4.2472 eV	HOMO-14 -> LUMO+4	0.041207463
			HOMO-14 -> LUMO+5	0.070830952
			HOMO-5 -> LUMO+4	0.020325312
			HOMO-4 -> LUMO+1	0.041581512
			HOMO-4 -> LUMO+3	0.145228162
			HOMO-4 -> LUMO+7	0.054866594
			HOMO-1 -> LUMO+3	0.138148705

			HOMO-1 -> LUMO+7	0.04512008
			HOMO-1 -> LUMO+13	0.069908083
	T_{21}	4.2667 eV	HOMO-3 -> LUMO+6	0.153879329
			HOMO -> LUMO+1	0.450547274
			HOMO -> LUMO+6	0.039920077
			HOMO -> LUMO+11	0.033878045
			HOMO -> LUMO+12	0.021744466
			HOMO -> LUMO+14	0.027228445
	T_{22}	4.2750 eV	HOMO-5 -> LUMO+4	0.058632577
			HOMO-5 -> LUMO+5	0.036856125
			HOMO-3 -> LUMO+6	0.078123139
			HOMO-2 -> LUMO+1	0.03273217
			HOMO-2 -> LUMO+4	0.076863363
			HOMO-2 -> LUMO+9	0.034416385
			HOMO-2 -> LUMO+14	0.022315394
			HOMO -> LUMO+1	0.231662631
			HOMO -> LUMO+11	0.022829571
			HOMO -> LUMO+12	0.047759042
	T_{23}	4.3248 eV	HOMO-2 -> LUMO+2	0.14247122
			HOMO-2 -> LUMO+5	0.022761245
			HOMO-2 -> LUMO+8	0.049329405
			HOMO-1 -> LUMO	0.080769843
			HOMO-1 -> LUMO+2	0.020738698
			HOMO -> LUMO	0.03730273
			HOMO -> LUMO+1	0.023134005
			HOMO -> LUMO+3	0.038619763
			HOMO -> LUMO+4	0.021358311
			HOMO -> LUMO+5	0.036845266
			HOMO -> LUMO+6	0.020478832
			HOMO -> LUMO+8	0.054999178
			HOMO -> LUMO+9	0.029680225
			HOMO -> LUMO+10	0.121110733
			HOMO -> LUMO+11	0.053982408
	T_{24}	4.3373 eV	HOMO-2 -> LUMO+2	0.036888712
			HOMO-1 -> LUMO	0.686393578
			HOMO-1 -> LUMO+2	0.173684392
	T_{25}	4.3543 eV	HOMO-2 -> LUMO	0.051880647
			HOMO-2 -> LUMO+2	0.071124833
			HOMO-2 -> LUMO+8	0.056905885
			HOMO-2 -> LUMO+10	0.0340605

			HOMO -> LUMO+2	0.03074704
			HOMO -> LUMO+5	0.024033089
			HOMO -> LUMO+9	0.032237683
			HOMO -> LUMO+10	0.341881805
			HOMO -> LUMO+11	0.025592269
	T_{26}	4.4132 eV	HOMO-2 -> LUMO+4	0.026638936
			HOMO-2 -> LUMO+5	0.027116547
			HOMO -> LUMO+3	0.440804162
			HOMO -> LUMO+4	0.257374426
			HOMO -> LUMO+7	0.02477538

Table S5 The ellipsoid plot of XCN crystal.

	Ellipsoid Plot
PCN	
MCN	
OCN	

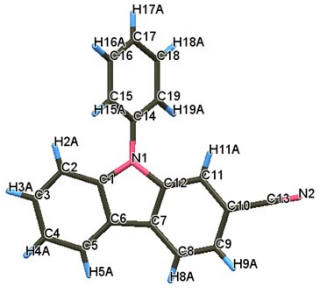
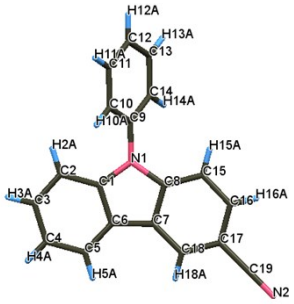
2CN	
3CN	

Table S6a The bond lengths of PCN in X-ray crystal structure.

Number	*Atom1*	*Atom2*	*Cyclicity*	*Length*
1	C1	H1	acyclic	0.95
2	C1	C2	cyclic	1.376(4)
3	C1	C6	cyclic	1.392(3)
4	C2	H2	acyclic	0.95
5	C2	C3	cyclic	1.379(4)
6	C3	H3	acyclic	0.95
7	C3	C4	cyclic	1.373(3)
8	C4	H4	acyclic	0.95
9	C4	C5	cyclic	1.382(3)
10	C5	C6	cyclic	1.391(3)
11	C5	N1	cyclic	1.396(3)
12	C6	C12	cyclic	1.443(3)
13	C7	C8	cyclic	1.393(3)
14	C7	C12	cyclic	1.394(3)
15	C7	N1	cyclic	1.391(3)
16	C8	H8	acyclic	0.95
17	C8	C9	cyclic	1.370(3)
18	C9	H9	acyclic	0.95
19	C9	C10	cyclic	1.385(4)
20	C10	H10	acyclic	0.95
21	C10	C11	cyclic	1.367(4)
22	C11	H11	acyclic	0.95
23	C11	C12	cyclic	1.387(3)
24	C13	C14	cyclic	1.375(3)
25	C13	C18	cyclic	1.381(3)

26	C13	N1	acyclic	1.414(2)
27	C14	H14	acyclic	0.95
28	C14	C15	cyclic	1.367(3)
29	C15	H15	acyclic	0.95
30	C15	C16	cyclic	1.378(3)
31	C16	C17	cyclic	1.367(3)
32	C16	C19	acyclic	1.435(3)
33	C17	H17	acyclic	0.95
34	C17	C18	cyclic	1.370(3)
35	C18	H18	acyclic	0.95
36	C19	N2	acyclic	1.137(3)
37	C20	H20	acyclic	0.95
38	C20	C21	cyclic	1.370(3)
39	C20	C25	cyclic	1.390(3)
40	C21	H21	acyclic	0.95
41	C21	C22	cyclic	1.386(3)
42	C22	H22	acyclic	0.95
43	C22	C23	cyclic	1.377(3)
44	C23	H23	acyclic	0.95
45	C23	C24	cyclic	1.378(3)
46	C24	C25	cyclic	1.402(3)
47	C24	N3	cyclic	1.392(2)
48	C25	C31	cyclic	1.433(3)
49	C26	C27	cyclic	1.384(3)
50	C26	C31	cyclic	1.397(3)
51	C26	N3	cyclic	1.393(2)
52	C27	H27	acyclic	0.95
53	C27	C28	cyclic	1.375(3)
54	C28	H28	acyclic	0.95
55	C28	C29	cyclic	1.389(3)
56	C29	H29	acyclic	0.95
57	C29	C30	cyclic	1.365(3)
58	C30	H30	acyclic	0.95
59	C30	C31	cyclic	1.380(3)
60	C32	C33	cyclic	1.380(3)
61	C32	C37	cyclic	1.379(3)
62	C32	N3	acyclic	1.410(2)
63	C33	H33	acyclic	0.95
64	C33	C34	cyclic	1.366(2)
65	C34	H34	acyclic	0.95
66	C34	C35	cyclic	1.382(3)
67	C35	C36	cyclic	1.381(3)
68	C35	C38	acyclic	1.435(2)
69	C36	H36	acyclic	0.95

70	C36	C37	cyclic	1.371(2)
71	C37	H37	acyclic	0.95
72	C38	N4	acyclic	1.141(2)

Table S6b The bond lengths of MCN in X-ray crystal structure.

Number	***Atom1***	***Atom2***	***Cyclicity***	***Length***
1	N1	C1	cyclic	1.383(6)
2	N1	C12	cyclic	1.375(5)
3	N1	C13	acyclic	1.403(5)
4	N2	C19	acyclic	1.130(7)
5	C1	C2	cyclic	1.366(6)
6	C1	C6	cyclic	1.362(6)
7	C2	H2A	acyclic	0.93
8	C2	C3	cyclic	1.368(8)
9	C3	H3A	acyclic	0.929
10	C3	C4	cyclic	1.362(8)
11	C4	H4A	acyclic	0.93
12	C4	C5	cyclic	1.365(8)
13	C5	H5A	acyclic	0.931
14	C5	C6	cyclic	1.367(7)
15	C6	C7	cyclic	1.415(6)
16	C7	C8	cyclic	1.374(6)
17	C7	C12	cyclic	1.386(6)
18	C8	H8A	acyclic	0.93
19	C8	C9	cyclic	1.347(8)
20	C9	H9A	acyclic	0.93
21	C9	C10	cyclic	1.375(8)
22	C10	H10A	acyclic	0.93
23	C10	C11	cyclic	1.373(7)
24	C11	H11A	acyclic	0.93
25	C11	C12	cyclic	1.366(7)
26	C13	C14	cyclic	1.386(6)
27	C13	C18	cyclic	1.367(7)
28	C14	H14A	acyclic	0.93
29	C14	C15	cyclic	1.362(6)
30	C15	H15A	acyclic	0.929
31	C15	C16	cyclic	1.361(7)
32	C16	H16A	acyclic	0.93
33	C16	C17	cyclic	1.381(6)
34	C17	C18	cyclic	1.366(6)
35	C17	C19	acyclic	1.408(6)
36	C18	H18A	acyclic	0.93

Table S6c The bond lengths of OCN in X-ray crystal structure.

Number	*Atom1*	*Atom2*	*Cyclicity*	*Length*
1	C1	H1A	acyclic	0.93
2	C1	C2	cyclic	1.368(6)
3	C1	C6	cyclic	1.376(5)
4	C2	H2A	acyclic	0.93
5	C2	C3	cyclic	1.387(4)
6	C3	H3A	acyclic	0.93
7	C3	C4	cyclic	1.381(4)
8	C4	C5	cyclic	1.403(4)
9	C4	N1	cyclic	1.401(3)
10	C5	C6	cyclic	1.393(4)
11	C5	C12	cyclic	1.447(4)
12	C6	H6A	acyclic	0.93
13	C7	C8	cyclic	1.386(3)
14	C7	C12	cyclic	1.404(3)
15	C7	N1	cyclic	1.399(3)
16	C8	H8A	acyclic	0.93
17	C8	C9	cyclic	1.381(3)
18	C9	H9A	acyclic	0.93
19	C9	C10	cyclic	1.391(4)
20	C10	H10A	acyclic	0.93
21	C10	C11	cyclic	1.375(5)
22	C11	H11A	acyclic	0.93
23	C11	C12	cyclic	1.399(3)
24	C13	C14	cyclic	1.388(3)
25	C13	C18	cyclic	1.397(3)
26	C13	N1	acyclic	1.415(3)
27	C14	H14A	acyclic	0.93
28	C14	C15	cyclic	1.380(4)
29	C15	H15A	acyclic	0.93
30	C15	C16	cyclic	1.373(4)
31	C16	H16A	acyclic	0.93
32	C16	C17	cyclic	1.372(5)
33	C17	H17A	acyclic	0.93
34	C17	C18	cyclic	1.394(4)
35	C18	C19	acyclic	1.434(4)
36	C19	N2	acyclic	1.143(4)

Table S6d The bond lengths of 2CN in X-ray crystal structure.

Number	*Atom1*	*Atom2*	*Cyclicity*	*Length*

1	N1	C1	cyclic	1.387(2)
2	N1	C12	cyclic	1.386(2)
3	N1	C14	acyclic	1.423(2)
4	N2	C13	acyclic	1.142(3)
5	C1	C2	cyclic	1.377(3)
6	C1	C6	cyclic	1.403(2)
7	C2	H2A	acyclic	0.93
8	C2	C3	cyclic	1.371(3)
9	C3	H3A	acyclic	0.929
10	C3	C4	cyclic	1.389(3)
11	C4	H4A	acyclic	0.93
12	C4	C5	cyclic	1.358(3)
13	C5	H5A	acyclic	0.93
14	C5	C6	cyclic	1.393(3)
15	C6	C7	cyclic	1.437(3)
16	C7	C8	cyclic	1.387(2)
17	C7	C12	cyclic	1.408(2)
18	C8	H8A	acyclic	0.93
19	C8	C9	cyclic	1.359(3)
20	C9	H9A	acyclic	0.93
21	C9	C10	cyclic	1.401(3)
22	C10	C11	cyclic	1.384(2)
23	C10	C13	acyclic	1.425(3)
24	C11	H11A	acyclic	0.93
25	C11	C12	cyclic	1.374(3)
26	C14	C15	cyclic	1.375(3)
27	C14	C19	cyclic	1.373(3)
28	C15	H15A	acyclic	0.93
29	C15	C16	cyclic	1.377(3)
30	C16	H16A	acyclic	0.93
31	C16	C17	cyclic	1.360(4)
32	C17	H17A	acyclic	0.93
33	C17	C18	cyclic	1.365(3)
34	C18	H18A	acyclic	0.93
35	C18	C19	cyclic	1.387(3)
36	C19	H19A	acyclic	0.93

Table S6e The bond lengths of 3CN in X-ray crystal structure.

Number	***Atom1***	***Atom2***	***Cyclicity***	***Length***
1	C9	C10	cyclic	1.390(2)
2	C9	C14	cyclic	1.390(2)
3	C9	N1	acyclic	1.399(2)
4	C10	H10A	acyclic	0.93

5	C10	C11	cyclic	1.390(2)
6	C11	H11A	acyclic	0.93
7	C11	C12	cyclic	1.390(3)
8	C12	H12A	acyclic	0.93
9	C12	C13	cyclic	1.390(3)
10	C13	H13A	acyclic	0.929
11	C13	C14	cyclic	1.390(2)
12	C14	H14A	acyclic	0.93
13	N1	C1	cyclic	1.388(3)
14	N1	C8	cyclic	1.375(3)
15	N2	C19	acyclic	1.138(4)
16	C1	C2	cyclic	1.373(4)
17	C1	C6	cyclic	1.397(3)
18	C2	H2A	acyclic	0.93
19	C2	C3	cyclic	1.370(4)
20	C3	H3A	acyclic	0.93
21	C3	C4	cyclic	1.379(4)
22	C4	H4A	acyclic	0.931
23	C4	C5	cyclic	1.365(4)
24	C5	H5A	acyclic	0.93
25	C5	C6	cyclic	1.382(4)
26	C6	C7	cyclic	1.434(3)
27	C7	C8	cyclic	1.407(3)
28	C7	C18	cyclic	1.379(3)
29	C8	C15	cyclic	1.380(3)
30	C15	H15A	acyclic	0.93
31	C15	C16	cyclic	1.366(3)
32	C16	H16A	acyclic	0.93
33	C16	C17	cyclic	1.391(3)
34	C17	C18	cyclic	1.382(3)
35	C17	C19	acyclic	1.429(4)
36	C18	H18A	acyclic	0.931

Table S7a The bond angles of PCN in X-ray crystal structure.

Number	*Atom1*	*Atom2*	*Atom3*	*Angle*
1	H1	C1	C2	120.8
2	H1	C1	C6	120.8
3	C2	C1	C6	118.3(2)
4	C1	C2	H2	119.4
5	C1	C2	C3	121.3(2)
6	H2	C2	C3	119.3
7	C2	C3	H3	119.3
8	C2	C3	C4	121.3(2)

9	H3	C3	C4	119.4
10	C3	C4	H4	121.2
11	C3	C4	C5	117.6(2)
12	H4	C4	C5	121.2
13	C4	C5	C6	121.9(2)
14	C4	C5	N1	129.1(2)
15	C6	C5	N1	108.9(2)
16	C1	C6	C5	119.5(2)
17	C1	C6	C12	133.5(2)
18	C5	C6	C12	107.0(2)
19	C8	C7	C12	121.7(2)
20	C8	C7	N1	129.4(2)
21	C12	C7	N1	108.9(2)
22	C7	C8	H8	121.3
23	C7	C8	C9	117.4(2)
24	H8	C8	C9	121.3
25	C8	C9	H9	119.2
26	C8	C9	C10	121.6(2)
27	H9	C9	C10	119.2
28	C9	C10	H10	119.6
29	C9	C10	C11	120.9(2)
30	H10	C10	C11	119.5
31	C10	C11	H11	120.4
32	C10	C11	C12	119.1(2)
33	H11	C11	C12	120.4
34	C6	C12	C7	107.0(2)
35	C6	C12	C11	133.7(2)
36	C7	C12	C11	119.3(2)
37	C14	C13	C18	119.5(2)
38	C14	C13	N1	120.5(2)
39	C18	C13	N1	120.0(2)
40	C13	C14	H14	119.8
41	C13	C14	C15	120.3(2)
42	H14	C14	C15	119.8
43	C14	C15	H15	119.9
44	C14	C15	C16	120.2(2)
45	H15	C15	C16	119.9
46	C15	C16	C17	119.4(2)
47	C15	C16	C19	120.5(2)
48	C17	C16	C19	120.0(2)
49	C16	C17	H17	119.7
50	C16	C17	C18	120.8(2)
51	H17	C17	C18	119.6
52	C13	C18	C17	119.8(2)

53	C13	C18	H18	120.1
54	C17	C18	H18	120.1
55	C16	C19	N2	179.2(3)
56	C5	N1	C7	108.2(2)
57	C5	N1	C13	125.4(2)
58	C7	N1	C13	126.0(2)
59	H20	C20	C21	120.6
60	H20	C20	C25	120.6
61	C21	C20	C25	118.8(2)
62	C20	C21	H21	119.6
63	C20	C21	C22	120.8(2)
64	H21	C21	C22	119.6
65	C21	C22	H22	119.2
66	C21	C22	C23	121.7(2)
67	H22	C22	C23	119.1
68	C22	C23	H23	121.3
69	C22	C23	C24	117.4(2)
70	H23	C23	C24	121.3
71	C23	C24	C25	121.8(2)
72	C23	C24	N3	129.6(2)
73	C25	C24	N3	108.5(2)
74	C20	C25	C24	119.4(2)
75	C20	C25	C31	133.3(2)
76	C24	C25	C31	107.3(2)
77	C27	C26	C31	121.5(2)
78	C27	C26	N3	129.5(2)
79	C31	C26	N3	109.0(2)
80	C26	C27	H27	121.4
81	C26	C27	C28	117.2(2)
82	H27	C27	C28	121.4
83	C27	C28	H28	119.1
84	C27	C28	C29	121.7(2)
85	H28	C28	C29	119.2
86	C28	C29	H29	119.7
87	C28	C29	C30	120.6(2)
88	H29	C29	C30	119.7
89	C29	C30	H30	120.4
90	C29	C30	C31	119.1(2)
91	H30	C30	C31	120.4
92	C25	C31	C26	106.9(2)
93	C25	C31	C30	133.3(2)
94	C26	C31	C30	119.8(2)
95	C33	C32	C37	119.8(2)
96	C33	C32	N3	120.3(2)

97	C37	C32	N3	119.9(2)
98	C32	C33	H33	120
99	C32	C33	C34	119.9(2)
100	H33	C33	C34	120.1
101	C33	C34	H34	119.9
102	C33	C34	C35	120.2(2)
103	H34	C34	C35	119.9
104	C34	C35	C36	120.0(2)
105	C34	C35	C38	120.0(2)
106	C36	C35	C38	120.0(2)
107	C35	C36	H36	120.2
108	C35	C36	C37	119.5(2)
109	H36	C36	C37	120.3
110	C32	C37	C36	120.4(2)
111	C32	C37	H37	119.8
112	C36	C37	H37	119.8
113	C35	C38	N4	178.5(2)
114	C24	N3	C26	108.2(1)
115	C24	N3	C32	126.0(1)
116	C26	N3	C32	125.4(1)

Table S7b The bond angles of MCN in X-ray crystal structure.

Number	*Atom1*	*Atom2*	*Atom3*	*Angle*
1	C1	N1	C12	107.4(3)
2	C1	N1	C13	124.9(3)
3	C12	N1	C13	127.6(3)
4	N1	C1	C2	127.7(4)
5	N1	C1	C6	109.8(4)
6	C2	C1	C6	122.3(4)
7	C1	C2	H2A	121.2
8	C1	C2	C3	117.8(4)
9	H2A	C2	C3	121
10	C2	C3	H3A	119.9
11	C2	C3	C4	120.2(5)
12	H3A	C3	C4	119.8
13	C3	C4	H4A	119.2
14	C3	C4	C5	121.5(5)
15	H4A	C4	C5	119.3
16	C4	C5	H5A	120.7
17	C4	C5	C6	118.7(5)
18	H5A	C5	C6	120.7
19	C1	C6	C5	119.4(4)
20	C1	C6	C7	107.0(4)

21	C5	C6	C7	133.6(4)
22	C6	C7	C8	134.1(4)
23	C6	C7	C12	107.2(4)
24	C8	C7	C12	118.7(4)
25	C7	C8	H8A	120.1
26	C7	C8	C9	119.7(5)
27	H8A	C8	C9	120.2
28	C8	C9	H9A	119.5
29	C8	C9	C10	120.9(5)
30	H9A	C9	C10	119.5
31	C9	C10	H10A	119.4
32	C9	C10	C11	121.3(5)
33	H10A	C10	C11	119.4
34	C10	C11	H11A	121.5
35	C10	C11	C12	117.0(4)
36	H11A	C11	C12	121.6
37	N1	C12	C7	108.6(4)
38	N1	C12	C11	128.9(4)
39	C7	C12	C11	122.4(4)
40	N1	C13	C14	119.8(4)
41	N1	C13	C18	119.9(4)
42	C14	C13	C18	120.4(4)
43	C13	C14	H14A	120.7
44	C13	C14	C15	118.5(4)
45	H14A	C14	C15	120.8
46	C14	C15	H15A	118.9
47	C14	C15	C16	122.3(4)
48	H15A	C15	C16	118.8
49	C15	C16	H16A	120.9
50	C15	C16	C17	118.2(4)
51	H16A	C16	C17	120.9
52	C16	C17	C18	121.0(4)
53	C16	C17	C19	118.8(4)
54	C18	C17	C19	120.2(4)
55	C13	C18	C17	119.6(4)
56	C13	C18	H18A	120.1
57	C17	C18	H18A	120.3
58	N2	C19	C17	178.1(5)

Table S7c The bond angles of OCN in X-ray crystal structure.

Number	***Atom1***	***Atom2***	***Atom3***	***Angle***
1	H1A	C1	C2	119.1
2	H1A	C1	C6	119.1

3	C2	C1	C6	121.9(3)
4	C1	C2	H2A	119.2
5	C1	C2	C3	121.6(4)
6	H2A	C2	C3	119.2
7	C2	C3	H3A	121.6
8	C2	C3	C4	116.8(3)
9	H3A	C3	C4	121.6
10	C3	C4	C5	122.4(3)
11	C3	C4	N1	129.1(2)
12	C5	C4	N1	108.4(2)
13	C4	C5	C6	119.1(3)
14	C4	C5	C12	107.3(2)
15	C6	C5	C12	133.6(3)
16	C1	C6	C5	118.3(3)
17	C1	C6	H6A	120.8
18	C5	C6	H6A	120.9
19	C8	C7	C12	122.2(2)
20	C8	C7	N1	129.0(2)
21	C12	C7	N1	108.7(2)
22	C7	C8	H8A	121.3
23	C7	C8	C9	117.4(2)
24	H8A	C8	C9	121.3
25	C8	C9	H9A	119.2
26	C8	C9	C10	121.7(2)
27	H9A	C9	C10	119.2
28	C9	C10	H10A	119.7
29	C9	C10	C11	120.6(3)
30	H10A	C10	C11	119.7
31	C10	C11	H11A	120.3
32	C10	C11	C12	119.4(3)
33	H11A	C11	C12	120.3
34	C5	C12	C7	106.9(2)
35	C5	C12	C11	134.3(2)
36	C7	C12	C11	118.7(2)
37	C14	C13	C18	119.3(2)
38	C14	C13	N1	120.7(2)
39	C18	C13	N1	120.0(2)
40	C13	C14	H14A	120
41	C13	C14	C15	119.9(2)
42	H14A	C14	C15	120.1
43	C14	C15	H15A	119.6
44	C14	C15	C16	120.8(3)
45	H15A	C15	C16	119.6
46	C15	C16	H16A	120

47	C15	C16	C17	120.0(3)
48	H16A	C16	C17	120
49	C16	C17	H17A	119.9
50	C16	C17	C18	120.1(3)
51	H17A	C17	C18	119.9
52	C13	C18	C17	119.8(2)
53	C13	C18	C19	120.2(2)
54	C17	C18	C19	120.0(2)
55	C18	C19	N2	178.3(3)
56	C4	N1	C7	108.6(2)
57	C4	N1	C13	125.4(2)
58	C7	N1	C13	125.2(2)

Table S7d The bond angles of 2CN in X-ray crystal structure.

Number	*Atom1*	*Atom2*	*Atom3*	*Angle*
1	C1	N1	C12	108.5(1)
2	C1	N1	C14	124.4(1)
3	C12	N1	C14	126.2(1)
4	N1	C1	C2	129.6(2)
5	N1	C1	C6	109.1(1)
6	C2	C1	C6	121.3(2)
7	C1	C2	H2A	120.8
8	C1	C2	C3	118.3(2)
9	H2A	C2	C3	120.8
10	C2	C3	H3A	119.4
11	C2	C3	C4	121.2(2)
12	H3A	C3	C4	119.4
13	C3	C4	H4A	119.7
14	C3	C4	C5	120.6(2)
15	H4A	C4	C5	119.7
16	C4	C5	H5A	120.1
17	C4	C5	C6	119.8(2)
18	H5A	C5	C6	120.1
19	C1	C6	C5	118.8(2)
20	C1	C6	C7	106.7(1)
21	C5	C6	C7	134.5(2)
22	C6	C7	C8	134.1(2)
23	C6	C7	C12	107.0(1)
24	C8	C7	C12	118.9(2)
25	C7	C8	H8A	120.1
26	C7	C8	C9	119.9(2)
27	H8A	C8	C9	120
28	C8	C9	H9A	119.7

29	C8	C9	C10	120.6(2)
30	H9A	C9	C10	119.7
31	C9	C10	C11	120.9(2)
32	C9	C10	C13	119.6(2)
33	C11	C10	C13	119.5(2)
34	C10	C11	H11A	121.1
35	C10	C11	C12	117.9(2)
36	H11A	C11	C12	121.1
37	N1	C12	C7	108.7(1)
38	N1	C12	C11	129.4(2)
39	C7	C12	C11	121.8(2)
40	N2	C13	C10	178.1(2)
41	N1	C14	C15	119.8(2)
42	N1	C14	C19	119.7(2)
43	C15	C14	C19	120.5(2)
44	C14	C15	H15A	120.2
45	C14	C15	C16	119.6(2)
46	H15A	C15	C16	120.2
47	C15	C16	H16A	119.9
48	C15	C16	C17	120.1(2)
49	H16A	C16	C17	119.9
50	C16	C17	H17A	119.8
51	C16	C17	C18	120.6(2)
52	H17A	C17	C18	119.6
53	C17	C18	H18A	120
54	C17	C18	C19	120.0(2)
55	H18A	C18	C19	120
56	C14	C19	C18	119.2(2)
57	C14	C19	H19A	120.4
58	C18	C19	H19A	120.5

Table S7e The bond angles of 3CN in X-ray crystal structure.

Number	***Atom1***	***Atom2***	***Atom3***	***Angle***
1	C10	C9	C14	120.0(1)
2	C10	C9	N1	120.3(2)
3	C14	C9	N1	119.7(2)
4	C9	C10	H10A	120
5	C9	C10	C11	120.0(2)
6	H10A	C10	C11	120
7	C10	C11	H11A	120
8	C10	C11	C12	120.0(2)
9	H11A	C11	C12	120
10	C11	C12	H12A	120
11	C11	C12	C13	120.0(2)

12	H12A	C12	C13	120
13	C12	C13	H13A	120
14	C12	C13	C14	120.0(2)
15	H13A	C13	C14	120
16	C9	C14	C13	120.0(2)
17	C9	C14	H14A	120
18	C13	C14	H14A	120
19	C9	N1	C1	125.5(2)
20	C9	N1	C8	125.6(2)
21	C1	N1	C8	108.8(2)
22	N1	C1	C2	128.9(2)
23	N1	C1	C6	108.9(2)
24	C2	C1	C6	122.2(2)
25	C1	C2	H2A	121.6
26	C1	C2	C3	117.0(3)
27	H2A	C2	C3	121.5
28	C2	C3	H3A	119
29	C2	C3	C4	121.8(3)
30	H3A	C3	C4	119.1
31	C3	C4	H4A	119.4
32	C3	C4	C5	121.0(3)
33	H4A	C4	C5	119.5
34	C4	C5	H5A	120.7
35	C4	C5	C6	118.6(3)
36	H5A	C5	C6	120.6
37	C1	C6	C5	119.3(2)
38	C1	C6	C7	106.7(2)
39	C5	C6	C7	134.0(2)
40	C6	C7	C8	107.0(2)
41	C6	C7	C18	134.0(2)
42	C8	C7	C18	118.9(2)
43	N1	C8	C7	108.5(2)
44	N1	C8	C15	129.5(2)
45	C7	C8	C15	122.0(2)
46	C8	C15	H15A	121
47	C8	C15	C16	118.1(2)
48	H15A	C15	C16	120.9
49	C15	C16	H16A	119.6
50	C15	C16	C17	120.9(2)
51	H16A	C16	C17	119.5
52	C16	C17	C18	121.0(2)
53	C16	C17	C19	119.7(2)
54	C18	C17	C19	119.3(2)
55	C7	C18	C17	119.1(2)

56	C7	C18	H18A	120.5
57	C17	C18	H18A	120.5
58	N2	C19	C17	178.8(3)