Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

N-Alkylcarbazoles: Homolog manipulating long-lived room-temperature phosphorescence

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Table S2c The singlet and triplet excited state transition configurations of the C4 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.

Table S2d The singlet and triplet excited state transition configurations of the C5 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.

1. Figures

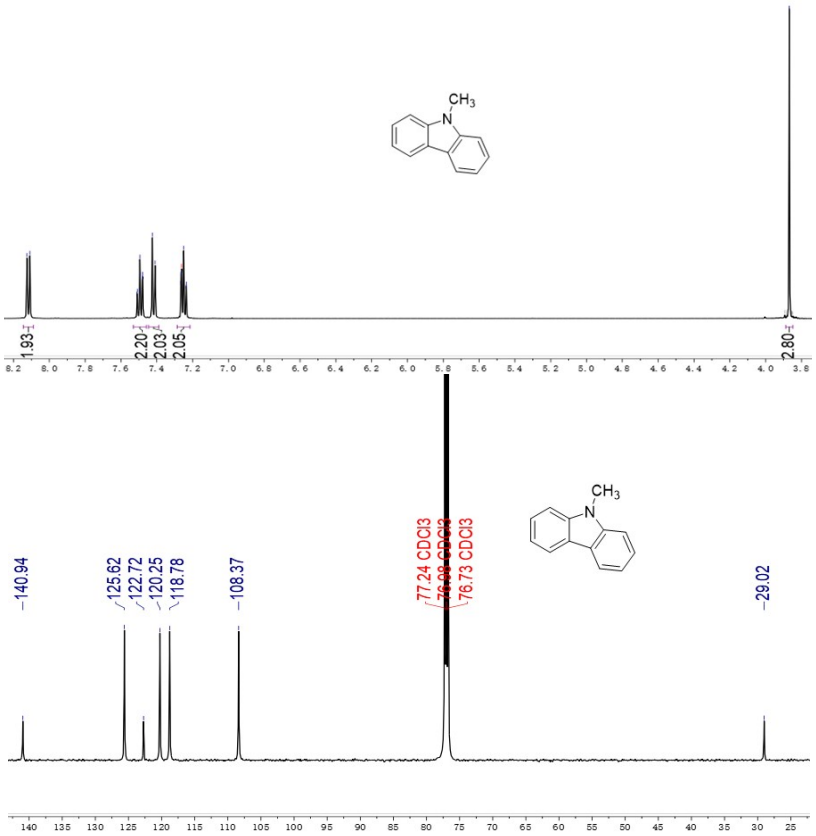


Figure S1a ^{1}H and ^{13}C NMR spectra of C1 in $CDCl_3$.

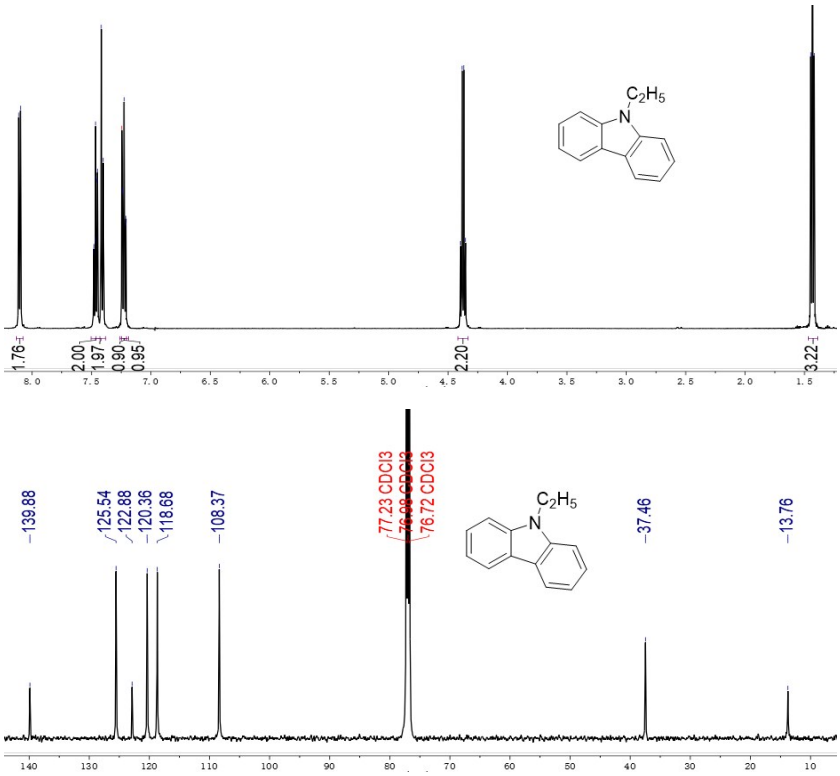


Figure S1b ^{1}H and ^{13}C NMR spectra of C2 in $CDCl_3$.

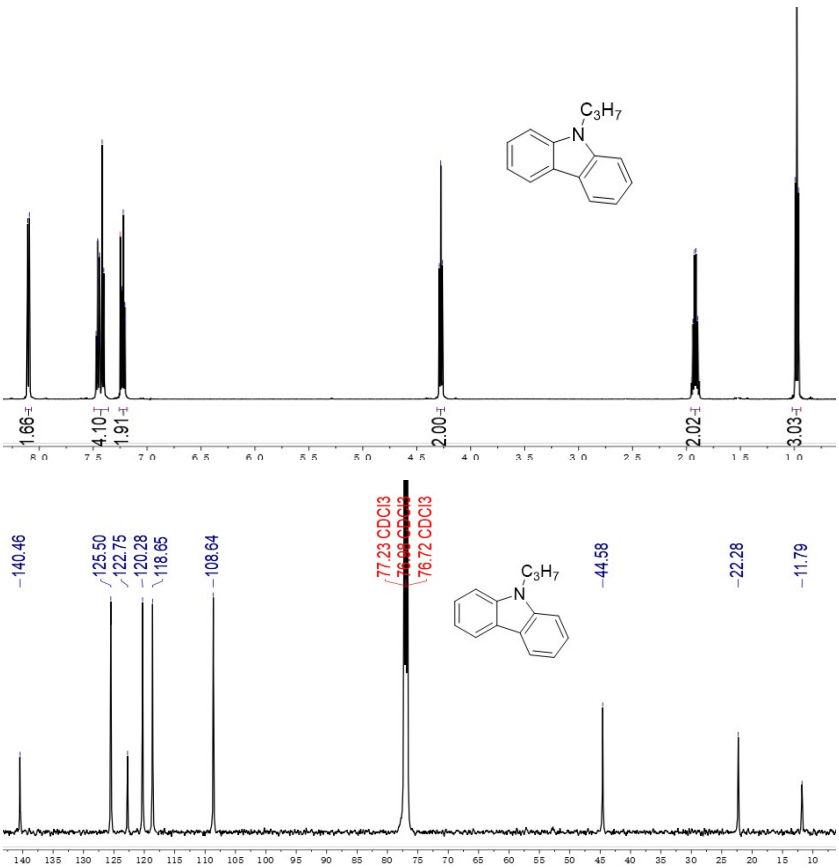


Figure S1c ^{1}H and ^{13}C NMR spectra of C3 in $CDCl_3$.

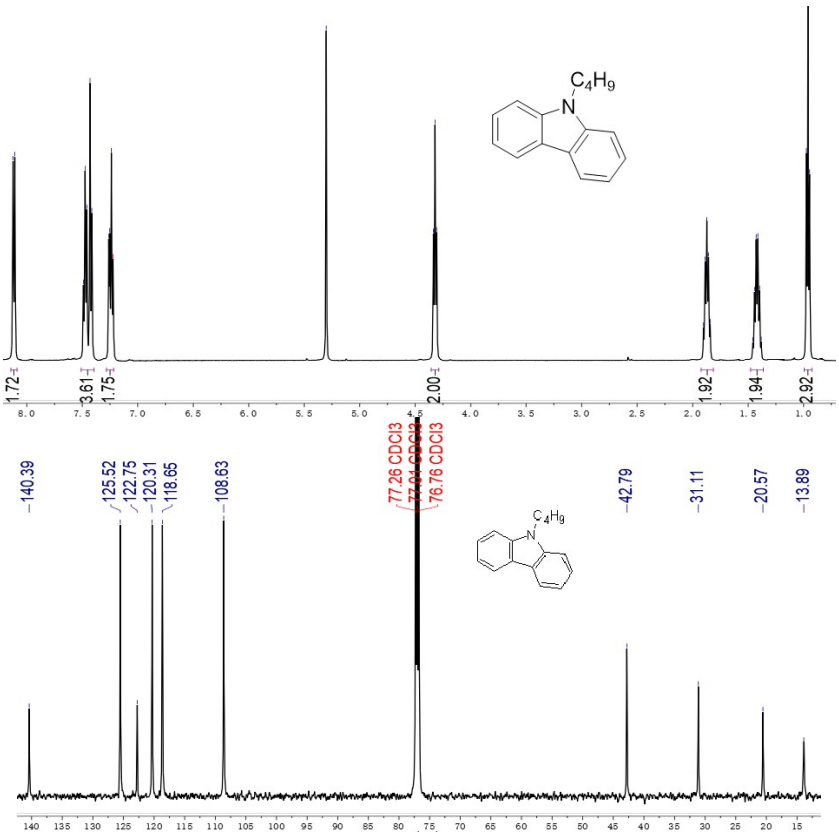


Figure S1d ^{1}H and ^{13}C NMR spectra of C4 in $CDCl_3$.

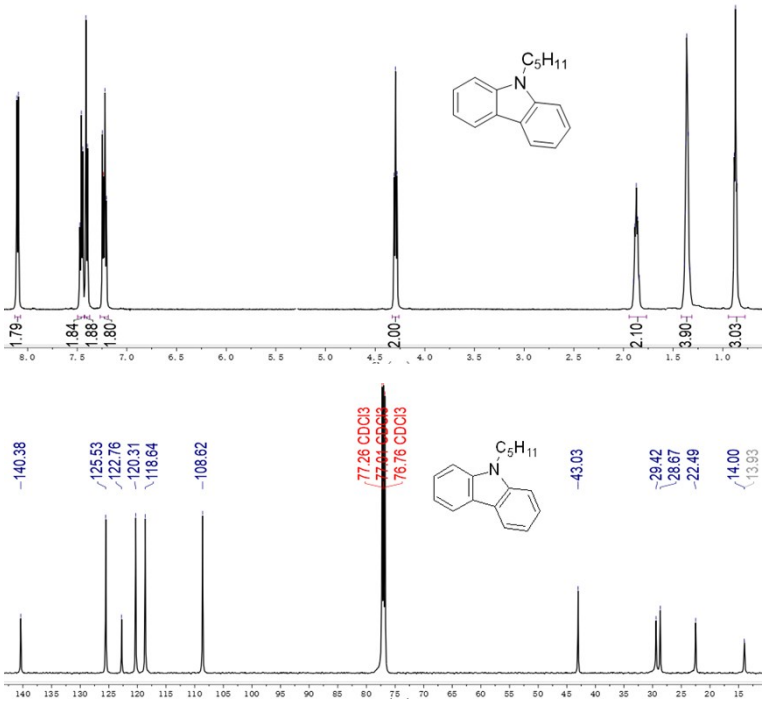


Figure S1e ^{1}H and ^{13}C NMR spectra of C5 in $CDCl_3$.

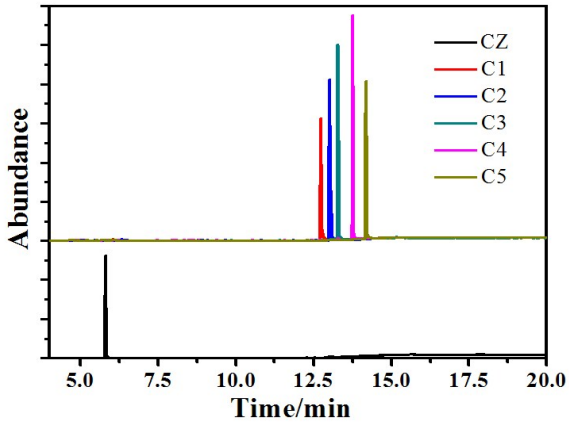
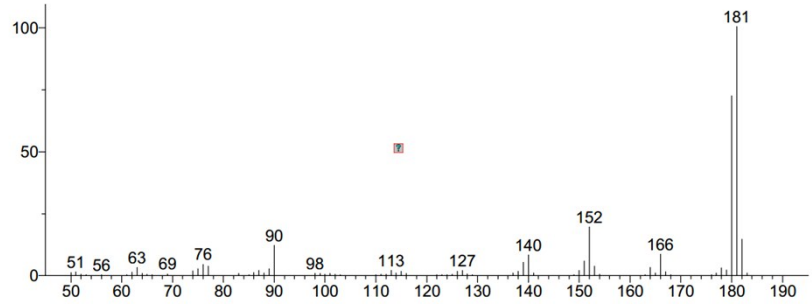
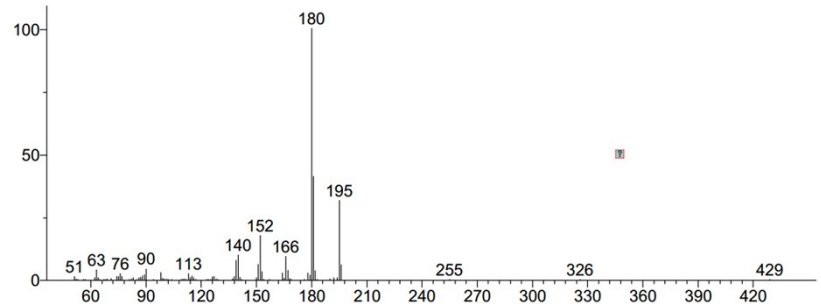


Figure S2 The gas chromatograms of carbazoles and Cn.



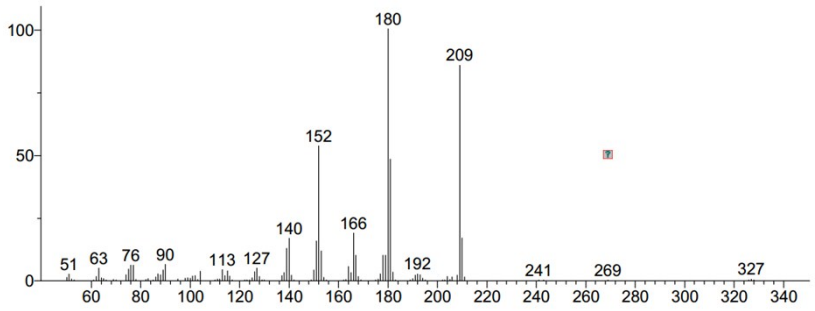
Hit 1 : 9H-Carbazole, 9-methyl-
C13H11N; MF: 930; RMF: 930; Prob 53.3%; CAS: 1484-12-4; Lib: replib; ID: 25051.

Figure S3a The mass spectra of C1.



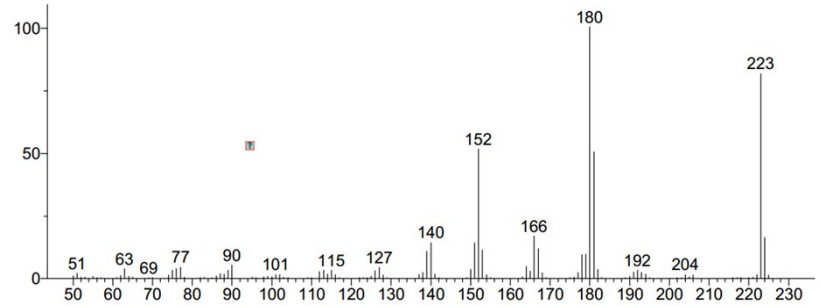
Hit 1 : 9H-Carbazole, 9-ethyl-
C14H13N; MF: 868; RMF: 869; Prob 75.4%; CAS: 86-28-2; Lib: mainlib; ID: 148111.

Figure S3b The mass spectra of C2.



Hit 1 : 9(10H)-Acridinone, 10-methyl-
C14H11NO; MF: 803; RMF: 807; Prob 33.1%; CAS: 719-54-0; Lib: mainlib; ID: 167394.

Figure S3c The mass spectra of C3.



Hit 1 : 9H-Carbazole, 9-butyl-
C16H17N; MF: 869; RMF: 883; Prob 69.0%; CAS: 1484-08-8; Lib: mainlib; ID: 148168.

Figure S3d The mass spectra of C4.

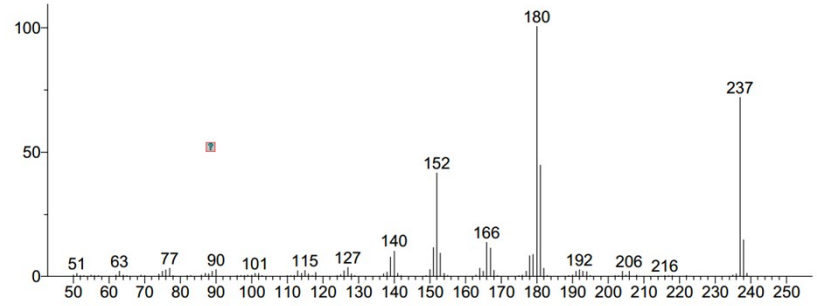


Figure S3e The mass spectra of C5.

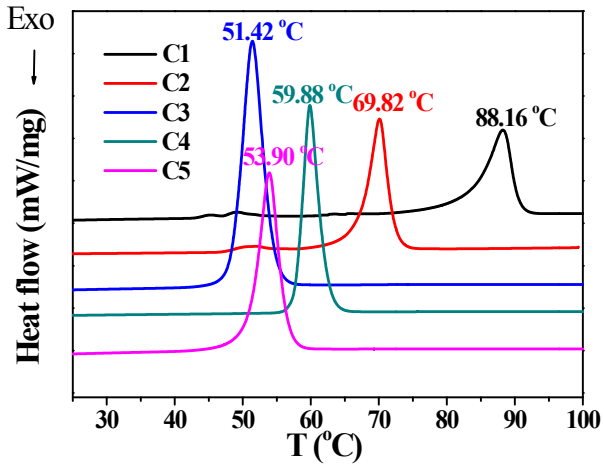


Figure S4 Differential scanning calorimetric (DSC) curves of Cn.

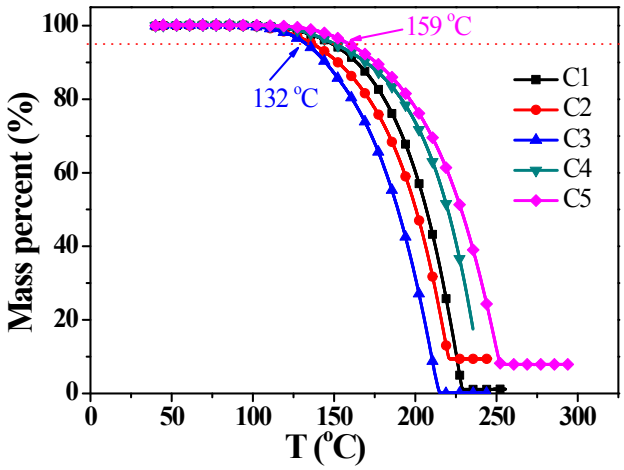


Figure S5 Thermogravimetric analysis (TGA) curves of Cn.

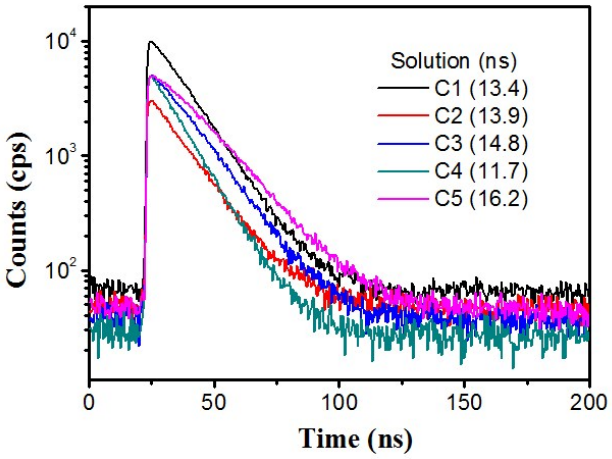


Figure S6 Time-resolved emission decay curves of Cn solution in THF at 298K.

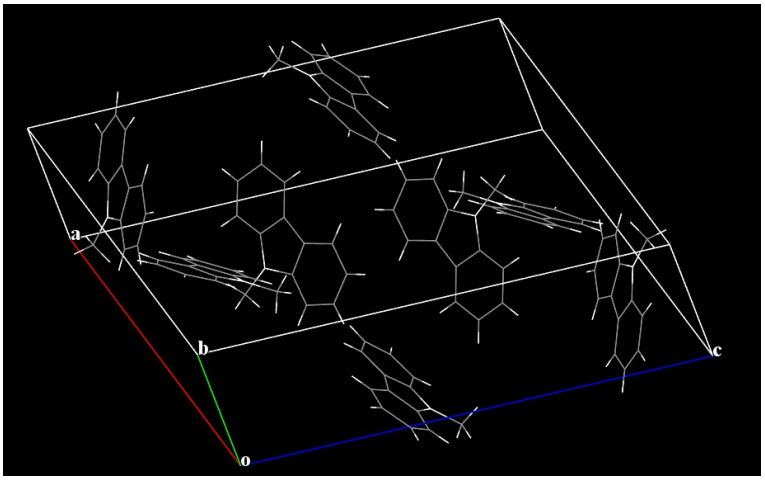


Figure S7a The unit cell of C1 single crystal.

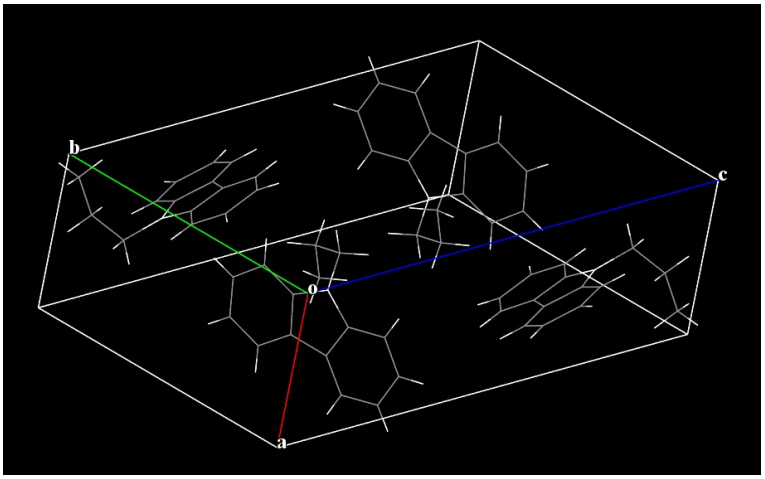


Figure S7b The unit cell of C3 single crystal.

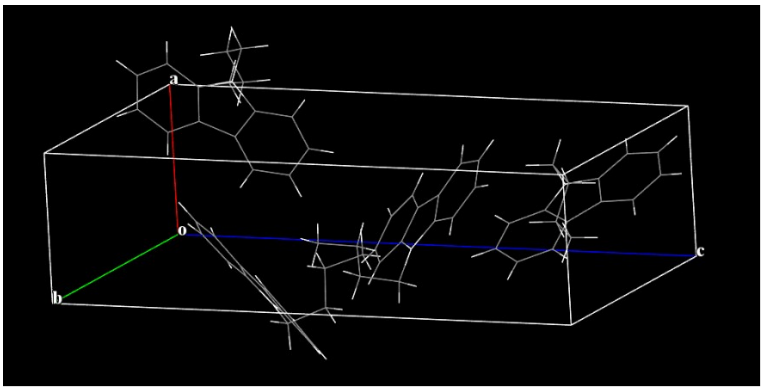


Figure S7c The unit cell of C4 single crystal.

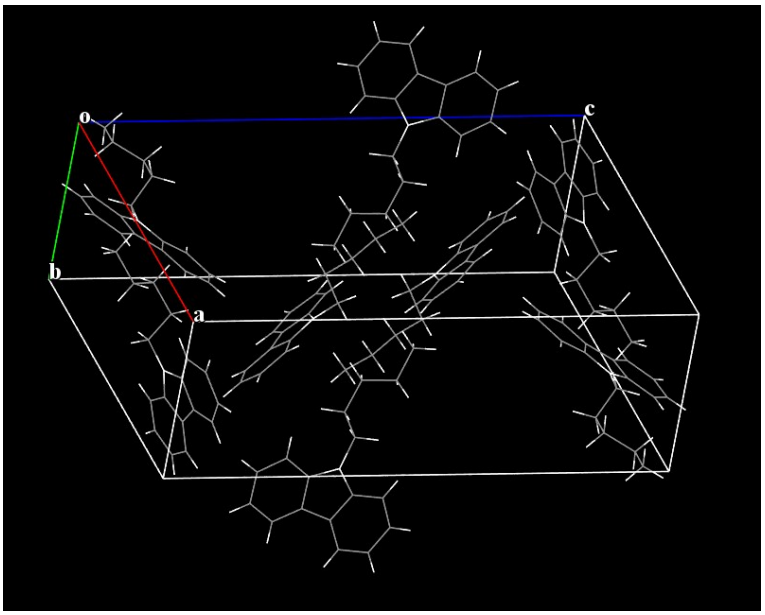


Figure S7d The unit cell of C5 single crystal.

2. Tables

Table S1a Single crystal structural parameters of C1.

Compound reference	colorless C1 crystal
Chemical formula	$C_{13}H_{11}N$
Formula weight	181.23
Crystal system	Monoclinic
a/Å	19.2078(18)
b/ Å	5.731(3)
c/ Å	19.5573(14)
α/°	90.00
β/°	113.257(9)
γ/°	90.00
Unit cell volume/ Å^3	1977.8(10)
Temperature/K	296
Space group	P2(1)/c
Z	8
Density (calculated) /g cm^{-3}	1.217
F(000)	768
Theta range for data collection	2.27 to 25.00 deg.
Index ranges	-22<=h<=22, -6<=k<=6, -23<=l<=18
Reflections measured	9397
Independent reflections	3470
R_{int}	0.0703
Completeness to theta = 25.00°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.986 and 0.980
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3470 / 0 / 253
Goodness-of-fit on F^2	0.967
Final R_1 values (I> 2σ(I))	0.0648
Final $wR(F^2)$ values (I> 2σ(I))	0.1303
Final R_1values (all data)	0.1685
Final $wR(F^2)$ values (all data)	0.1559
CCDC number	1845385

Table S1b Single crystal structural parameters of C3.

Compound reference	colorless C3 crystal
Chemical formula	C_{15} H_{15} N
Formula weight	209.29
Crystal system	Monoclinic
a/Å	5.455(4)
b/ Å	12.3116(19)
c/ Å	17.4777(13)
α/°	90.00
β/°	97.756(14)
γ/°	90.00
Unit cell volume/ Å^3	1163.1(9)
Temperature/K	296
Space group	P2(1)/c
Z	4
Density (calculated) /g cm^{-3}	1.195
F(000)	448.0
Theta range for data collection	2.03 to 25.00 deg.
Index ranges	-5<=h<=6, -14<=k<=14, -19<=l<=20
Reflections measured	5682
Independent reflections	2045
R_{int}	0.0403
Completeness to theta = 25.00°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9856 and 0.9775
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2045 / 0 / 146
Goodness-of-fit on F^2	1.095
Final R_1 values (I> 2σ(I))	0.0399
Final wR(F^2) values (I> 2σ(I))	0.0892
Final R_1values (all data)	0.0603
Final wR(F^2) values (all data)	0.0957
CCDC number	1845386

Table S1c Single crystal structural parameters of C4.

Compound reference	colorless C4 crystal
Chemical formula	$C_{16}H_{17}N$
Formula weight	223.31
Crystal system	Orthorhombic
a/Å	5.544(1)
b/ Å	11.276(2)
c/ Å	20.368(2)
α/°	90.00
β/°	90.00
γ/°	90.00
Unit cell volume/ Å^3	1273.4(4)
Temperature/K	298(2)
Space group	$P2_12_12_1(19)$
Z	4
Density (calculated) /g cm^{-3}	1.165
F(000)	480.0
Theta range for data collection	2.00 to 25.28 deg.
Reflections measured	2671
Independent reflections	1372
R_{int}	0.0616
Completeness to theta = 25.28°	99.9 %
Max. and min. transmission	0.9801 and 0.9933
Data / restraints / parameters	1372 / 0 / 154
Goodness-of-fit on F^2	1.000
Final R_1 values ($I > 2\sigma(I)$)	0.0589
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1290
Final R_1values (all data)	0.0836
Final $wR(F^2)$ values (all data)	0.1465
CCDC number	722961

Reference: L. Chen, W. Cheng, G. -L. Song and H, -J. Zhu, *Acta Crystallographica Section E,* 2009, **65**, o574.

Table S1d Single crystal structural parameters of C5.

Compound reference	colorless C5 crystal
Chemical formula	C_{17} H_{19} N
Formula weight	237.33
Crystal system	orthorhombic
a/Å	15.959(2)
b/ Å	7.5700(10)
c/ Å	22.1950(10)
α/°	90.00
β/°	90.00
γ/°	90.00
Unit cell volume/ Å^3	2681.4(5)
Temperature/K	100
Space group	P2(1)/c
Z	8
Density (calculated) /g cm^{-3}	1.176
F(000)	1024.0
Theta range for data collection	2.24 to 25.00 deg.
Index ranges	-14<=h<=18, -9<=k<=8, -26<=l<=26
Reflections measured	12465
Independent reflections	2342
R_{int}	0.1275
Completeness to theta = 25.00°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9859 and 0.9780
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2342 / 0 / 164
Goodness-of-fit on F^2	0.971
Final R_1 values ($I> 2\sigma(I)$)	0.0609
Final $wR(F^2)$ values ($I> 2\sigma(I)$)	0.1412
Final R_1values (all data)	0.1086
Final $wR(F^2)$ values (all data)	0.1649
CCDC number	1845387

Table S2a The singlet and triplet excited state transition configurations of the C1 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.

	n	Energy	Orbitals	Transition
S_n	S_1	4.0280 eV	HOMO-2 ->LUMO+1	0.022463521
			HOMO-1 ->LUMO+1	0.039373792
			HOMO ->LUMO	0.038942823
			HOMO ->LUMO+1	0.774390125
			HOMO ->LUMO+2	0.09732872
T_n	T_1	3.2893 eV	HOMO-7 ->LUMO	0.0392056
			HOMO-5 ->LUMO	0.136900514
			HOMO-4 ->LUMO	0.468182938
			HOMO-4 ->LUMO+1	0.02150738
			HOMO-2 ->LUMO	0.064526689
			HOMO-2 ->LUMO+4	0.062057645
			HOMO-1 ->LUMO	0.079050832
			HOMO-1 ->LUMO+4	0.042731338
	T_2	3.3159 eV	HOMO-8 ->LUMO+1	0.02459762
			HOMO-5 ->LUMO+1	0.250447954
			HOMO-4 ->LUMO+1	0.092063405
			HOMO-3 ->LUMO+2	0.159138253
			HOMO-2 ->LUMO+1	0.049978573
			HOMO-2 ->LUMO+3	0.024971655
			HOMO-1 ->LUMO+1	0.074675666
			HOMO-1 ->LUMO+3	0.037686106
			HOMO ->LUMO+1	0.0226845
			HOMO ->LUMO+2	0.105772402
			HOMO ->LUMO+5	0.03256352
	T_3	3.3184 eV	HOMO-6 ->LUMO+2	0.028613104
			HOMO-5 ->LUMO+1	0.134348545
			HOMO-4 ->LUMO+1	0.04936082
			HOMO-3 ->LUMO+2	0.30331145
			HOMO-2 ->LUMO+1	0.0285605
			HOMO-1 ->LUMO+1	0.042994849
			HOMO-1 ->LUMO+3	0.020402
			HOMO ->LUMO+2	0.196251125
			HOMO ->LUMO+5	0.06403189
	T_4	3.3882 eV	HOMO-7 ->LUMO+4	0.023384194

			HOMO-5 ->LUMO	0.025182168
			HOMO-4 ->LUMO	0.086037816
			HOMO-2 ->LUMO	0.464821536
			HOMO-2 ->LUMO+1	0.021561338
			HOMO-1 ->LUMO	0.29942965
	T_5	3.4093 eV	HOMO-6 ->LUMO+5	0.022370355
			HOMO-3 ->LUMO+2	0.241248472
			HOMO ->LUMO+2	0.602933767
			HOMO ->LUMO+5	0.050829473
	T_6	3.4307 eV	HOMO-5 ->LUMO+1	0.131533205
			HOMO-4 ->LUMO+1	0.03312738
			HOMO-2 ->LUMO+1	0.26570592
			HOMO-1 ->LUMO+1	0.409548701
			HOMO-1 ->LUMO+3	0.021690279
	T_7	4.0442 eV	HOMO-6 ->LUMO+2	0.027018826
			HOMO-3 ->LUMO+2	0.083419786
			HOMO ->LUMO	0.028963431
			HOMO ->LUMO+1	0.55953389
			HOMO ->LUMO+5	0.220328496
	T_8	4.0693 eV	HOMO-6 ->LUMO+2	0.046561313
			HOMO-3 ->LUMO+2	0.136482226
			HOMO ->LUMO+1	0.286494221
			HOMO ->LUMO+5	0.392568883
	T_9	4.0781 eV	HOMO-7 ->LUMO	0.091720445
			HOMO-5 ->LUMO	0.042860064
			HOMO-4 ->LUMO	0.154656973
			HOMO-2 ->LUMO+4	0.360621274
			HOMO-1 ->LUMO+4	0.249105053
	T_{10}	4.0879 eV	HOMO-8 ->LUMO+1	0.05930568
			HOMO-5 ->LUMO+1	0.14473276
			HOMO-4 ->LUMO+1	0.043088737
			HOMO-2 ->LUMO+3	0.226976269
			HOMO-1 ->LUMO+3	0.344234234
			HOMO ->LUMO+1	0.043808
	T_{11}	4.2144 eV	HOMO-2 ->LUMO	0.037609274
			HOMO-1 ->LUMO	0.047481293
			HOMO ->LUMO	0.864191751
			HOMO ->LUMO+1	0.04239872
	T_{12}	4.2753 eV	HOMO-2 ->LUMO	0.328422706
			HOMO-2 ->LUMO+1	0.03115008

			HOMO-1 ->LUMO	0.458786205
			HOMO ->LUMO	0.083485152
	T_{13}	4.2933 eV	HOMO-10 ->LUMO	0.021782019
			HOMO-7 ->LUMO+4	0.02986568
			HOMO-2 ->LUMO	0.0235445
			HOMO-2 ->LUMO+1	0.448745485
			HOMO-2 ->LUMO+7	0.047155205
			HOMO-1 ->LUMO+1	0.303451661
			HOMO-1 ->LUMO+6	0.031822599
	T_{14}	4.3154 eV	HOMO-9 ->LUMO+2	0.090278503
			HOMO-6 ->LUMO+2	0.037182645
			HOMO-6 ->LUMO+5	0.173884839
			HOMO-3 ->LUMO+5	0.081640323
			HOMO-3 ->LUMO+11	0.083828746
			HOMO ->LUMO+2	0.02416921
			HOMO ->LUMO+8	0.435599112
	T_{15}	4.3224 eV	HOMO-11 ->LUMO+1	0.088326045
			HOMO-8 ->LUMO+1	0.021865587
			HOMO-8 ->LUMO+3	0.140280451
			HOMO-7 ->LUMO+3	0.02329777
			HOMO-5 ->LUMO+3	0.052261445
			HOMO-5 ->LUMO+9	0.024266045
			HOMO-5 ->LUMO+10	0.03338528
			HOMO-2 ->LUMO	0.02640402
			HOMO-2 ->LUMO+6	0.105010279
			HOMO-2 ->LUMO+7	0.055591117
			HOMO-1 ->LUMO	0.027088609
			HOMO-1 ->LUMO+1	0.039233607
			HOMO-1 ->LUMO+6	0.150887218
			HOMO-1 ->LUMO+7	0.087554386
	T_{16}	4.3490 eV	HOMO-10 ->LUMO	0.096940851
			HOMO-7 ->LUMO+4	0.129357325
			HOMO-4 ->LUMO+4	0.028493619
			HOMO-4 ->LUMO+9	0.039925728
			HOMO-4 ->LUMO+10	0.0266805
			HOMO-2 ->LUMO+1	0.10717524
			HOMO-2 ->LUMO+6	0.074621571
			HOMO-2 ->LUMO+7	0.134141281
			HOMO-1 ->LUMO	0.04564429
			HOMO-1 ->LUMO+1	0.0574605

			HOMO-1 ->LUMO+6	0.046068266
			HOMO-1 ->LUMO+7	0.09686161

Table S2b The singlet and triplet excited state transition configurations of the C3 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.

	n	Energy	Orbitals	Transition
S_n	S_1	3.9781 eV	HOMO-2 ->LUMO	0.149243698
			HOMO-2 ->LUMO+1	0.030712333
			HOMO-1 ->LUMO	0.642887283
			HOMO ->LUMO	0.120010803
T_n	T_1	3.2997 eV	HOMO-5 ->LUMO	0.128666499
			HOMO-5 ->LUMO+1	0.06265092
			HOMO-4 ->LUMO	0.082938499
			HOMO-2 ->LUMO	0.260959777
			HOMO-2 ->LUMO+1	0.033462845
			HOMO-1 ->LUMO	0.230221837
			HOMO-1 ->LUMO+1	0.038248248
			HOMO-1 ->LUMO+3	0.028046593
	T_2	3.3130 eV	HOMO-7 ->LUMO+1	0.03688328
			HOMO-5 ->LUMO	0.063104834
			HOMO-5 ->LUMO+1	0.091994762
			HOMO-4 ->LUMO	0.07105696
			HOMO-4 ->LUMO+1	0.417168048
			HOMO-3 ->LUMO+2	0.029456499
			HOMO-2 ->LUMO+1	0.049574707
			HOMO-2 ->LUMO+3	0.02540258
			HOMO-2 ->LUMO+4	0.032543107
			HOMO-1 ->LUMO+4	0.049757506
	T_3	3.3134 eV	HOMO-9 ->LUMO+11	0.030450184
			HOMO-6 ->LUMO+2	0.049103512
			HOMO-6 ->LUMO+8	0.020714266
			HOMO-3 ->LUMO+2	0.64502082
			HOMO ->LUMO+2	0.062580144
			HOMO ->LUMO+5	0.119589842
	T_4	3.3289 eV	HOMO-8 ->LUMO	0.024593184
			HOMO-5 ->LUMO	0.279841767

			HOMO-5 ->LUMO+1	0.04422338
			HOMO-4 ->LUMO	0.11706025
			HOMO-4 ->LUMO+1	0.027730125
			HOMO-2 ->LUMO	0.102758578
			HOMO-2 ->LUMO+1	0.02438957
			HOMO-2 ->LUMO+3	0.037642192
			HOMO-1 ->LUMO	0.192758405
			HOMO-1 ->LUMO+3	0.031445304
	T_5	3.3722 eV	HOMO-6 ->LUMO+5	0.028780803
			HOMO-3 ->LUMO+2	0.048391605
			HOMO ->LUMO+2	0.865112272
	T_6	3.3778 eV	HOMO-2 ->LUMO	0.101862925
			HOMO-2 ->LUMO+1	0.289149706
			HOMO-1 ->LUMO	0.084937933
			HOMO-1 ->LUMO+1	0.432208234
	T_7	4.0218 eV	HOMO-8 ->LUMO	0.055085443
			HOMO-5 ->LUMO	0.09201192
			HOMO-4 ->LUMO	0.062036509
			HOMO-2 ->LUMO+3	0.177119616
			HOMO-2 ->LUMO+4	0.08096288
			HOMO-1 ->LUMO+3	0.235078531
			HOMO-1 ->LUMO+4	0.048472525
			HOMO ->LUMO	0.106048546
	T_8	4.0320 eV	HOMO-1 ->LUMO+3	0.033779203
			HOMO ->LUMO	0.86201076
	T_9	4.0624 eV	HOMO-6 ->LUMO+2	0.091549205
			HOMO-6 ->LUMO+8	0.03050944
			HOMO-3 ->LUMO+2	0.221937869
			HOMO ->LUMO+5	0.60607848
	T_{10}	4.0672 eV	HOMO-7 ->LUMO+1	0.070642887
			HOMO-5 ->LUMO	0.02603762
			HOMO-5 ->LUMO+1	0.03537268
			HOMO-4 ->LUMO	0.022383048
			HOMO-4 ->LUMO+1	0.144388632
			HOMO-2 ->LUMO+3	0.126635314
			HOMO-2 ->LUMO+4	0.143519389
			HOMO-1 ->LUMO+3	0.072496704
			HOMO-1 ->LUMO+4	0.24248648
	T_{11}	4.1438 eV	HOMO-2 ->LUMO+1	0.027219111
			HOMO ->LUMO+1	0.90882162

	T_{12}	4.1795 eV	HOMO-2 ->LUMO	0.19356642
			HOMO-2 ->LUMO+1	0.258782568
			HOMO-1 ->LUMO	0.428812083
	T_{13}	4.1867 eV	HOMO-2 ->LUMO	0.253785377
			HOMO-2 ->LUMO+1	0.181238122
			HOMO-1 ->LUMO+1	0.460857602
			HOMO ->LUMO+1	0.054542439
	T_{14}	4.3067 eV	HOMO-11 ->LUMO+1	0.039284045
			HOMO-10 ->LUMO	0.050174784
			HOMO-8 ->LUMO+3	0.096149895
			HOMO-7 ->LUMO+4	0.07388168
			HOMO-5 ->LUMO+3	0.03976764
			HOMO-5 ->LUMO+9	0.039609866
			HOMO-4 ->LUMO+10	0.0340605
			HOMO-2 ->LUMO+6	0.02308241
			HOMO-2 ->LUMO+7	0.17581264
			HOMO-1 ->LUMO+6	0.253272679
	T_{15}	4.3137 eV	HOMO-9 ->LUMO+2	0.111024144
			HOMO-6 ->LUMO+5	0.17769145
			HOMO-3 ->LUMO+5	0.056710384
			HOMO-3 ->LUMO+11	0.098585761
			HOMO ->LUMO+2	0.024125258
			HOMO ->LUMO+8	0.434554354
	T_{16}	4.3184 eV	HOMO-11 ->LUMO	0.036801845
			HOMO-10 ->LUMO+1	0.047265826
			HOMO-8 ->LUMO+4	0.041391399
			HOMO-7 ->LUMO+3	0.057874824
			HOMO-7 ->LUMO+4	0.037823501
			HOMO-4 ->LUMO+3	0.030381125
			HOMO-4 ->LUMO+10	0.03596562
			HOMO-2 ->LUMO+1	0.098071347
			HOMO-2 ->LUMO+6	0.189174005
			HOMO-1 ->LUMO+7	0.202744384

Table S2c The singlet and triplet excited state transition configurations of the C4 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.

	n	Energy	Orbitals	Transition
S_n	S_1	3.7401 eV	HOMO -> LUMO	0.98962753
T_n	T_1	3.2344 eV	HOMO-6 -> LUMO+2	0.035160216
			HOMO-3 -> LUMO+2	0.280980065
			HOMO-2 -> LUMO+2	0.144496128
			HOMO -> LUMO+2	0.318274333
			HOMO -> LUMO+5	0.08388608
	T_2	3.2411 eV	HOMO-10 -> LUMO+10	0.023858017
			HOMO-7 -> LUMO+1	0.044802218
			HOMO-4 -> LUMO+1	0.570141133
			HOMO-1 -> LUMO+1	0.174215239
			HOMO-1 -> LUMO+4	0.104050096
	T_3	3.2487 eV	HOMO-11 -> LUMO+8	0.023336641
			HOMO-8 -> LUMO	0.045354696
			HOMO-5 -> LUMO	0.600936845
			HOMO-3 -> LUMO+3	0.02784328
			HOMO-2 -> LUMO	0.113164274
			HOMO-2 -> LUMO+3	0.079186081
	T_4	3.3157 eV	HOMO-6 -> LUMO+5	0.020979713
			HOMO-3 -> LUMO+2	0.236383128
			HOMO-2 -> LUMO	0.021230362
			HOMO-2 -> LUMO+2	0.045819699
			HOMO -> LUMO	0.026981645
			HOMO -> LUMO+2	0.539033445
			HOMO -> LUMO+5	0.03585842
	T_5	3.3312 eV	HOMO-7 -> LUMO+4	0.024762026
			HOMO-4 -> LUMO+1	0.144969586
			HOMO-1 -> LUMO	0.020084088
			HOMO-1 -> LUMO+1	0.701449057
	T_6	3.3329 eV	HOMO-8 -> LUMO+3	0.024182403
			HOMO-5 -> LUMO	0.075233205
			HOMO-3 -> LUMO	0.231077616
			HOMO-2 -> LUMO	0.506460737
			HOMO-1 -> LUMO+1	0.032034867
			HOMO -> LUMO	0.032070314
			HOMO -> LUMO+2	0.025869026
	T_7	3.7541 eV	HOMO-2 -> LUMO	0.024757575
			HOMO -> LUMO	0.91392496
			HOMO -> LUMO+2	0.027457618
	T_8	4.0122 eV	HOMO-6 -> LUMO+2	0.088603661

			HOMO-6 -> LUMO+9	0.021999629
			HOMO-3 -> LUMO+2	0.112129537
			HOMO-2 -> LUMO+2	0.051867763
			HOMO -> LUMO+1	0.166718477
			HOMO -> LUMO+3	0.027824405
			HOMO -> LUMO+5	0.462818205
	T_9	4.0202 eV	HOMO-3 -> LUMO+2	0.022658947
			HOMO -> LUMO+1	0.805662792
			HOMO -> LUMO+5	0.088384897
	T_{10}	4.0339 eV	HOMO-7 -> LUMO+1	0.109830471
			HOMO-7 -> LUMO+7	0.030174418
			HOMO-4 -> LUMO+1	0.190381522
			HOMO-1 -> LUMO+4	0.598505523
	T_{11}	4.0422 eV	HOMO-8 -> LUMO	0.105818401
			HOMO-8 -> LUMO+6	0.030990541
			HOMO-5 -> LUMO	0.185574504
			HOMO-3 -> LUMO+3	0.1529045
			HOMO-2 -> LUMO+3	0.431836418
	T_{12}	4.0658 eV	HOMO-1 -> LUMO	0.956233863
			HOMO-1 -> LUMO+1	0.021333517
	T_{13}	4.2047 eV	HOMO-5 -> LUMO	0.028963431
			HOMO-3 -> LUMO	0.700999042
			HOMO-2 -> LUMO	0.233080609
	T_{14}	4.3152 eV	HOMO-11 -> LUMO	0.06160752
			HOMO-9 -> LUMO+2	0.055038984
			HOMO-8 -> LUMO+3	0.096307827
			HOMO-6 -> LUMO+5	0.08695284
			HOMO-5 -> LUMO+8	0.046183683
			HOMO-3 -> LUMO+6	0.046238405
			HOMO-3 -> LUMO+11	0.037160832
			HOMO-2 -> LUMO+6	0.178503125
			HOMO -> LUMO+9	0.201460129
	T_{15}	4.3211 eV	HOMO-11 -> LUMO	0.058297466
			HOMO-9 -> LUMO+2	0.054820227
			HOMO-8 -> LUMO+3	0.093018471
			HOMO-6 -> LUMO+5	0.09005768
			HOMO-5 -> LUMO+8	0.046536903
			HOMO-3 -> LUMO+6	0.075078125
			HOMO-3 -> LUMO+11	0.027485746
			HOMO-2 -> LUMO+6	0.140810631

			HOMO-2 -> LUMO+11	0.020897857
			HOMO -> LUMO+9	0.211068039
	T_{16}	4.3252 eV	HOMO-10 -> LUMO+1	0.119325895
			HOMO-7 -> LUMO+4	0.187553626
			HOMO-4 -> LUMO+4	0.04428288
			HOMO-4 -> LUMO+10	0.092063405
			HOMO-1 -> LUMO+1	0.028732839
			HOMO-1 -> LUMO+7	0.439997043

Table S2d The singlet and triplet excited state transition configurations of the C5 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.

	n	Energy	Orbitals	Transition
S_n	S_1	4.0190 eV	HOMO-1 -> LUMO	0.086661171
			HOMO-1 -> LUMO+1	0.174179824
			HOMO -> LUMO	0.286600205
			HOMO -> LUMO+1	0.26035328
			HOMO -> LUMO+2	0.13357213
T_n	T_1	3.3003 eV	HOMO-9 -> LUMO+11	0.0264546
			HOMO-6 -> LUMO+2	0.036894145
			HOMO-3 -> LUMO	0.032757761
			HOMO-3 -> LUMO+1	0.034558205
			HOMO-3 -> LUMO+2	0.5692445
			HOMO -> LUMO+2	0.100477479
			HOMO -> LUMO+5	0.097708522
	T_2	3.3024 eV	HOMO-11 -> LUMO+9	0.020192461
			HOMO-8 -> LUMO	0.035239815
			HOMO-8 -> LUMO+6	0.021974465
			HOMO-5 -> LUMO	0.4232184
			HOMO-5 -> LUMO+1	0.127674151
			HOMO-4 -> LUMO	0.089337645
			HOMO-2 -> LUMO	0.092338234
			HOMO-2 -> LUMO+3	0.107917288
	T_3	3.3103 eV	HOMO-7 -> LUMO+1	0.026860984
			HOMO-5 -> LUMO	0.032768
			HOMO-5 -> LUMO+1	0.026786866
			HOMO-4 -> LUMO	0.080970928

			HOMO-4 -> LUMO+1	0.393792626
			HOMO-4 -> LUMO+2	0.031270003
			HOMO-1 -> LUMO	0.03022357
			HOMO-1 -> LUMO+1	0.14279168
			HOMO-1 -> LUMO+2	0.020515277
			HOMO-1 -> LUMO+4	0.088502659
	T_4	3.3582 eV	HOMO-4 -> LUMO	0.025846285
			HOMO-4 -> LUMO+1	0.107527394
			HOMO-1 -> LUMO	0.150997106
			HOMO-1 -> LUMO+1	0.493461517
			HOMO-1 -> LUMO+2	0.039807133
			HOMO-1 -> LUMO+4	0.026509834
			HOMO -> LUMO+1	0.025891777
	T_5	3.3864 eV	HOMO-8 -> LUMO+3	0.026560515
			HOMO-5 -> LUMO	0.063981799
			HOMO-2 -> LUMO	0.646953125
			HOMO-2 -> LUMO+1	0.156755203
	T_6	3.3873 eV	HOMO-6 -> LUMO+5	0.022138288
			HOMO-3 -> LUMO+2	0.082914064
			HOMO-1 -> LUMO+2	0.029011587
			HOMO -> LUMO	0.050893261
			HOMO -> LUMO+1	0.046787405
			HOMO -> LUMO+2	0.676633445
	T_7	4.0654 eV	HOMO-7 -> LUMO+1	0.04675682
			HOMO-4 -> LUMO	0.025128336
			HOMO-4 -> LUMO+1	0.1057908
			HOMO-1 -> LUMO	0.09409122
			HOMO-1 -> LUMO+2	0.023224435
			HOMO-1 -> LUMO+4	0.392108257
			HOMO -> LUMO	0.025497336
			HOMO -> LUMO+1	0.059622951
			HOMO -> LUMO+2	0.02416921
			HOMO -> LUMO+5	0.040972394
	T_8	4.0746 eV	HOMO-6 -> LUMO+2	0.030896008
			HOMO-5 -> LUMO	0.032594151
			HOMO-3 -> LUMO+2	0.06793298
			HOMO-2 -> LUMO+3	0.149232771
			HOMO-1 -> LUMO+4	0.02788105
			HOMO -> LUMO	0.229205122
			HOMO -> LUMO+1	0.035091303

			HOMO -> LUMO+2	0.039835354
			HOMO -> LUMO+5	0.222924999
	T_9	4.0820 eV	HOMO-8 -> LUMO	0.05691938
			HOMO-8 -> LUMO+6	0.02289372
			HOMO-5 -> LUMO	0.087052954
			HOMO-5 -> LUMO+1	0.039773281
			HOMO-4 -> LUMO	0.041893546
			HOMO-3 -> LUMO+2	0.022650433
			HOMO-2 -> LUMO+3	0.463800067
			HOMO-1 -> LUMO+4	0.058707938
			HOMO -> LUMO	0.034558205
			HOMO -> LUMO+5	0.062580144
	T_{10}	4.1153 eV	HOMO-6 -> LUMO+2	0.036921314
			HOMO-3 -> LUMO+2	0.050345991
			HOMO-1 -> LUMO+1	0.027321869
			HOMO -> LUMO	0.128899954
			HOMO -> LUMO+1	0.371556481
			HOMO -> LUMO+2	0.060301699
			HOMO -> LUMO+5	0.230316845
	T_{11}	4.1899 eV	HOMO -> LUMO	0.482672775
			HOMO -> LUMO+1	0.412686125
			HOMO -> LUMO+5	0.039429936
	T_{12}	4.2545 eV	HOMO-1 -> LUMO	0.664105075
			HOMO-1 -> LUMO+1	0.18848572
			HOMO-1 -> LUMO+4	0.0561058
	T_{13}	4.2971 eV	HOMO-10 -> LUMO+1	0.028108205
			HOMO-7 -> LUMO+4	0.054370829
			HOMO-4 -> LUMO+10	0.022936536
			HOMO-1 -> LUMO+1	0.06629897
			HOMO-1 -> LUMO+2	0.520669306
			HOMO-1 -> LUMO+7	0.162655265
	T_{14}	4.3158 eV	HOMO-11 -> LUMO	0.071646266
			HOMO-8 -> LUMO+3	0.147131426
			HOMO-5 -> LUMO+3	0.037117226
			HOMO-5 -> LUMO+9	0.06050329
			HOMO-2 -> LUMO	0.092149245
			HOMO-2 -> LUMO+1	0.068346439
			HOMO-2 -> LUMO+6	0.393082978
	T_{15}	4.3356 eV	HOMO-9 -> LUMO+2	0.117738634
			HOMO-6 -> LUMO+5	0.155068805

			HOMO-3 -> LUMO+5	0.033888458
			HOMO-3 -> LUMO+11	0.103085242
			HOMO -> LUMO+8	0.397582279
			HOMO -> LUMO+9	0.031711693
	T_{16}	4.3536 eV	HOMO-10 -> LUMO+1	0.054747405
			HOMO-7 -> LUMO+4	0.09167762
			HOMO-4 -> LUMO+4	0.020317248
			HOMO-4 -> LUMO+10	0.046183683
			HOMO-1 -> LUMO	0.021499085
			HOMO-1 -> LUMO+2	0.326351205
			HOMO-1 -> LUMO+7	0.269436723