π-Functionalized 1,5-Diazocines with Diverse Intramolecular Connectivity to Maneuver Photophysical Properties and Electroluminescence

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1. General Aspects

All the commercially purchased chemicals and solvents were used without further purification. ^{1}H and ^{13}C NMR spectra were recorded using a Brucker Avance III HD 500 spectrometer. UV-vis absorption spectra were recorded on the Shimadzu UV-2600 spectrophotometer. PL studies were performed using a Flurolog Horiba Xe Lamp spectrofluorometer. Cyclic voltammetric studies of 10^{-3} M solutions of Dz 1 to Dz 6 in DCM solvent with 0.1M tetrabutylammonium hexafluorophosphate as supporting electrolyte, Ferrocene as reference, glassy carbon as working electrode, Ag/AgCl electrode as reference electrode and platinum wire as counter electrode in CH Instruments (BASI CV-50W) Thermogravimetric analysis (TGA) was performed in Shimadzu DTG-60 instrument under nitrogen atmosphere at a heating rate of 10°C/minute. Differential scanning calorimetry (DSC) was pursued using the Mettler Toledo instrument with a heating rate of 10°C/minute.

Single Crystal X-Ray Structure Determination.

The single crystal X-ray diffraction intensity data collection for the suitable crystals of Dz**s** was carried out on a Bruker APEX-II CCD detector system with Mo-sealed Siemens ceramic diffraction tube (λ = 0.7107 Å) and a highly oriented graphite monochromator operating at 50 kV and 30 mA. The data were collected in a hemisphere mode and processed with Bruker SAINT. Using Olex2, the structures were solved with the SHELXT structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimization. Hydrogens were fixed geometrically, treated as riding on their nonhydrogen, and refined isotropically, while all nonhydrogens were subjected to anisotropic refinement.

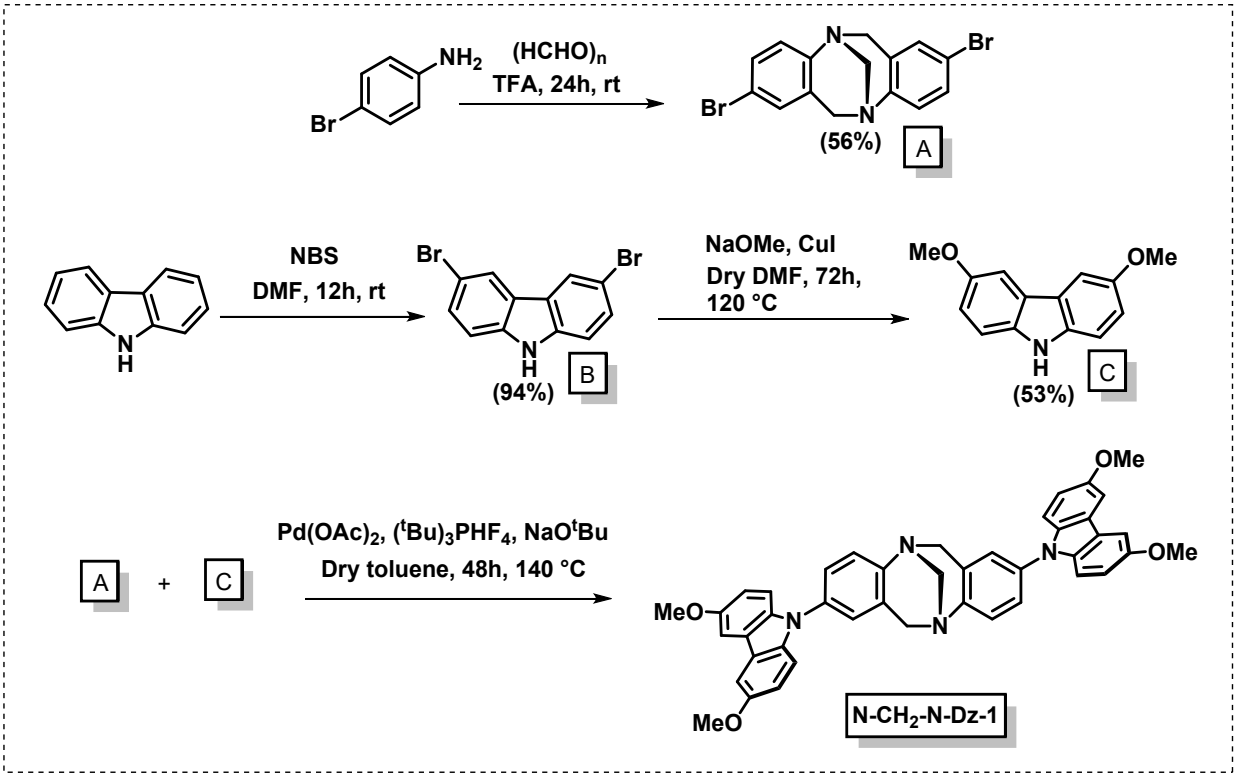
Experimental details of OLEDs

Devices were fabricated in a nitrogen glove box-integrated thermal evaporation system (Angstrom Inc.) and the film thickness was measured using Dektak XT profilometer. Indium tin oxide (ITO) substrates were purchased from Kintec Company, Hong Kong. The substrates were cleaned by using a liquid detergent followed by sequential sonication in isopropanol and de-ionized water for 15 min each. After drying, the UV-ozone treated (Novascan) substrates were loaded in thermal evaporation chamber. All the materials of the devices were deposited on the substrate by thermal evaporation under high vacuum (10^{-7} torr) conditions. After the evaporation, the devices were encapsulated inside the nitrogen filled glovebox by using a UV-curable epoxy (Epoxy Technology Inc.) The OLED characterization system consists of a SpectraScan PR-655 spectroradiometer integrated with a Keithely 2400 sourcemeter.

2. Synthesis and Characterization of Compounds

Synthesis of Dzs

Synthesis of N-CH_2-N-Dz-1



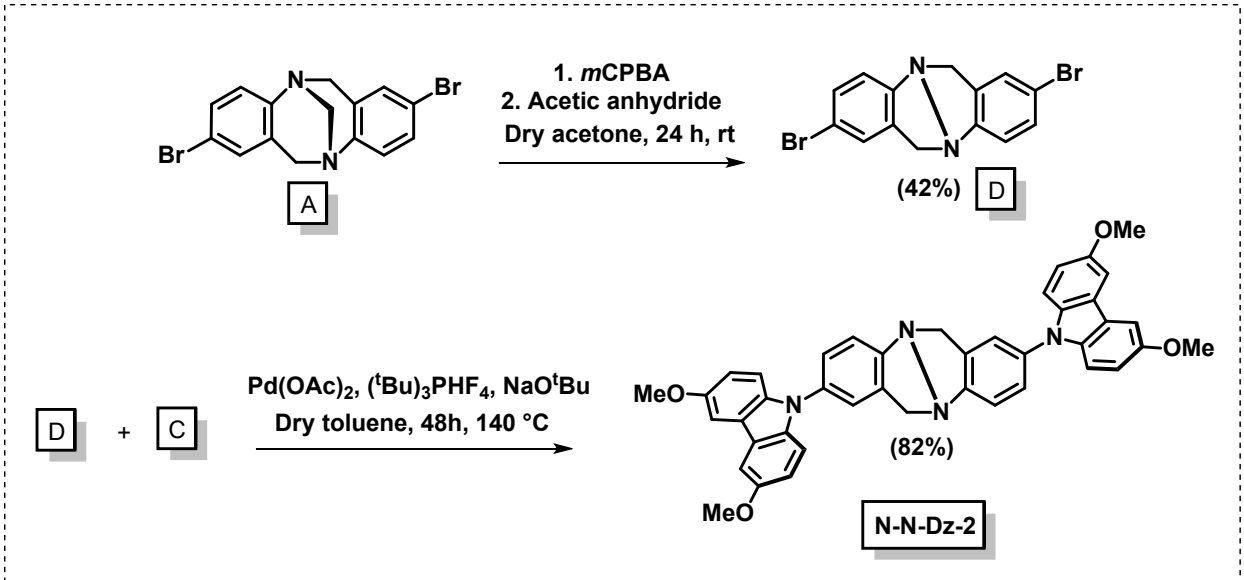
a) Synthesis of 6*H*,12*H*-5,11-Methanodibenzo[*b*,*f*][1,5]diazocine, 2,8-dibromo-) (A) [1]: To 4-bromo aniline (5 g, 29.06 mmol) and paraformaldehyde (3.5 g, 58.13 mmol) added 50 mL of TFA at -20 ℃. Then the reaction mixture was brought to rt, stirred for 24 h and then quenched by adding to 50 mL of cold ammonia solution. This was extracted with chloroform and the combined organic layer was evaporated and purified by column chromatography on silica gel with 10 % EtOAc / hexane as eluent to yield yellow solid A. Yield = 56%. ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 4.09 (d, J = 16.8 Hz, 2H), 4.25 (s, 2H), 4.63 (d, J=16.8Hz, 2H), 6.99 (d, J=8.6 Hz, 2H), 7.05 (s, 2H), 7.27 (d, J=9.7Hz, 2H).

b) Synthesis of 9*H*-Carbazole, 3,6-dibromo- (B)[2] : To carbazole (2 g, 11.96 mmol) dissolved in 15ml DMF, added NBS (4.64 g, 26.31 mmol) parts by parts by keeping in ice bath and stirred at rt for 12h. Then the reaction mixture was poured into ice, the pale white precipitate of compound B was filtered and dried. Yield = 94%. ^{1}H NMR (DMSO-d_6, 500 MHz) δ =7.47 (d, J=8.6Hz, 2H), 7.53 (dd, J=8.6, 1.6Hz, 2H), 11.60 (s, NH), 8.43 (s, 2H).

c) Synthesis of 9*H*-Carbazole, 3,6-dimethoxy- (C) [3]: dibromo compound B (1 g, 3.07 mmol) and CuI (1.17 g, 6.15 mmol), was taken in a pressure tube. NaOMe (1.02g, 18.91 mmol) dissolved in 4 ml dry methanol and 4 ml dry DMF was added to the pressure tube under nitrogen atmosphere. The pressure tube was sealed perfectly under nitrogen and refluxed at 120°C for 24h. The reaction mixture was poured to ice and filtered the crude product. Purified by column chromatography on silica gel with 10 % EtOAc / hexane as eluent to yield compound C as white solid. Yield = 53%. ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 3.93 (s,6H), 7.05 (d, J=8.9Hz, 2H), 7.31 (d, J=8.9Hz, 2H), 7.50 (s, 2H), 7.78 (br s, NH).

d) Synthesis of N-CH_2-N-Dz-1: [1] Compound A (0.5 g, 1.32 mmol), compound C (0.747 g, 3.28 mmol), NaO^{t}Bu (0.51 g, 5.26 mmol), $Pd(OAc)_2$ (0.03 g, 0.13 mmol), and $(^t Bu)_3PHF_4$ (0.114 g, 0.39 mmol) were taken in an oven-dried pressure tube and added 15 mL of dry toluene. The pressure tube was sealed under nitrogen and heated at 140 °C for 48 h. Then the contents were cooled to room temperature, toluene was removed under pressure, and purified by column chromatography on neutral alumina with 25% EtOAc/ hexane as eluent. Yield = 76%. ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 3.85 (s, 12H), 4.25 (d, J= 16.9 Hz, 2H), 4.37 (s, 2H), 4.77 (d, J= 16.9 Hz, 2H), 6.93 (d, J= 8.8 Hz, 4H), 7.09 (s, 2H), 7.21 (d, J= 8.9 Hz, 4H), 7.29 (m, 4H), 7.45 (s, 4H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ= 56.12, 58.62, 66.86, 102.84, 110.74, 115.20, 123.48, 124.91, 125.98, 126.55, 129.18, 134.09, 136.36, 146.73, 154.02. ESI-HRMS: m/z $[M + H]^+$ calculated: 673.2814; found: 673.28347.

Synthesis of N-N-Dz-2

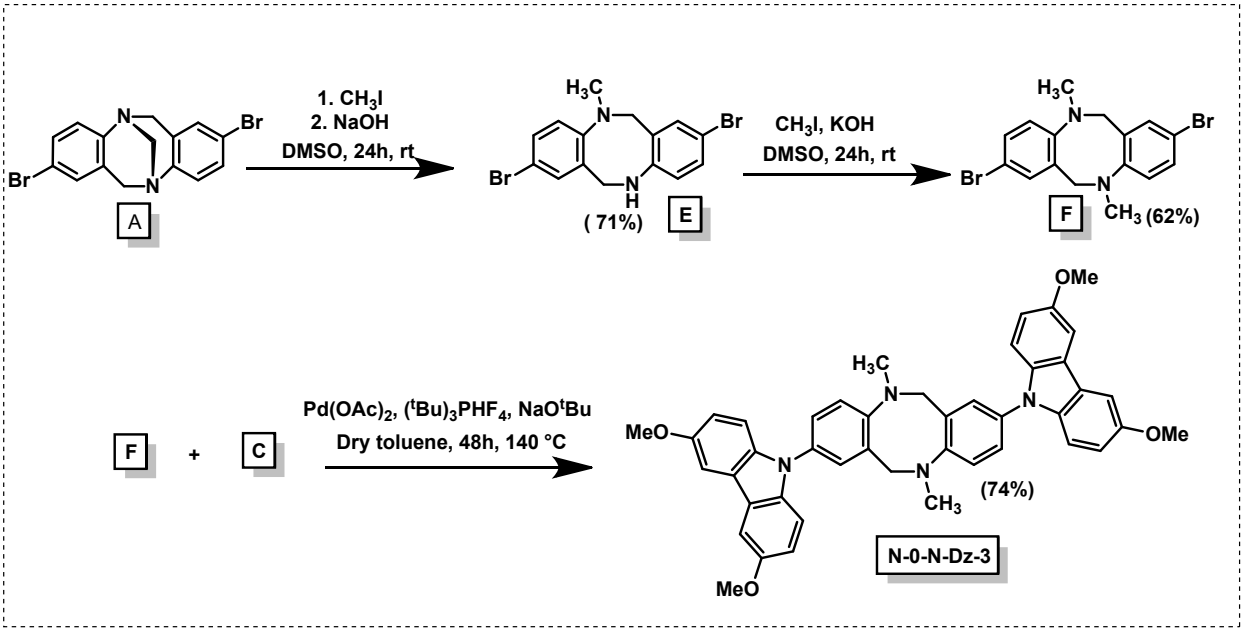


e) Synthesis of 6*H*,12*H*-Indazolo[2,1-*a*]indazole, 2,8-dibromo- (D) [4]: Compound A (0.5 g, 1.31 mmol) and *m*CPBA (0.34 g, 1.97mmol) was taken in a 2-neck rb and added dry acetone to it under nitrogen atmosphere and stirred at rt for 1 h. The formation of N-oxide was monitored using TLC and after the starting material was completely converted to N-oxide, added acetic anhydride (250 µL, 2.63 mmol). After 24h, the reaction mixture was quenched with sat. $NaHCO_3$, extracted with $CHCl_3$, combined organic layer

was evaporated and purified by column chromatography on silica gel with 10 % EtOAc / hexane as eluent. Yield= 42%. ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 4.61 (s, 4H), 6.70 (d, J=8.3 Hz, 2H), 7.20 (s, 2H), 7.24 (d, J=8.4 Hz, 2H).

f) Synthesis of N-N-Dz-2 : [1] Compound D (0.3 g, 0.819 mmol), compound C (0.465 g, 2.048 mmol), NaO^tBu (0.32 g, 3.28 mmol), $Pd(OAc)_2$ (0.018 g, 0.182 mmol), and $(^tBu)_3PHF_4$ (0.071 g, 0.24 mmol) were taken in an oven-dried pressure tube and added 10 mL of dry toluene. The pressure tube was sealed under nitrogen and heated at 140 °C for 48 h. Then the contents were cooled to room temperature, toluene was removed under pressure, and purified by column chromatography on silica gel with 25% EtOAc/ hexane as eluent. Yield = 82%. ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 3.87 (s, 12H), 4.77 (s, 4H), 6.95 (d, J= 8.9 Hz, 4H), 7.01 (d, J= 8.2 Hz, 2H), 7.18 (d, J= 8.7 Hz, 5H), 7.30 (d, J = 8.2 Hz, 2H), 7.48 (s, 5H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ= 56.17, 56.23, 102.93, 110.75, 111.51, 115.38, 121.96, 123.44, 127.28, 128.87, 133.30, 136.94, 150.64, 154.03. ESI-HRMS: m/z $[M - H]^+$ calculated: 657.2580; found: 657.2519.

Syntheis of N-o-N-Dz-3

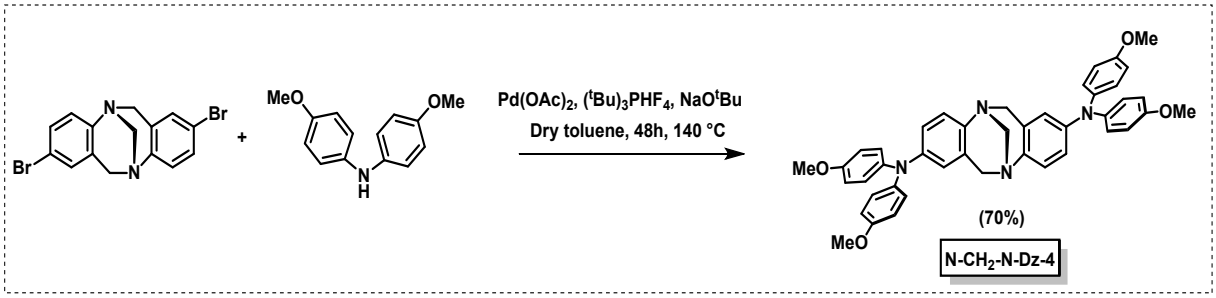


g) Synthesis of (E):[5] Compound A (0.1g, 0.263mmol) was taken in a 25 ml rb and added 2ml DMSO then stirred until it dissolved completely. Then added CH_3I (81.88µL, 1.315mmol) and kept the reaction for stirring under room temperature for 2hr. Prepared 25ml 1M saturated NaOH solution and to this the reaction mixture was added, a white precipitate was formed. The reaction mixture was kept for stirring under room temperature for another 12hrs. Product was filtered using Buchner funnel. Yield=74%.^{1}H NMR ($CDCl_3$, 500 MHz) δ= 2.86 (s, 3H), 4.17 (s, 1H), 4.26 (s,2H), 4.40 (s, 2H), 6.52 (d, J= 8.3Hz, 1H), 6.72 (d, J=8.6Hz, 1H), 7.20-7.12 (m, 3H), 7.24 (d, J=1.9Hz, 1H).

h) Synthesis of (F): Methylation reaction of (E) was carried out using a modified procedure.[5] KOH (0.87g, 15.705mmol) was taken in a 100ml rb and dissolved it by adding 15ml DMSO kept stirring for a while. To this compound E (0.4g, 1.04mmol) was added and stirred it for 2hrs. 1ml (15.70 mmol) of CH_3I was then added to the reaction mixture and kept it for stirring for 24hrs under room temperature. Reaction mixture was poured into ice and stirred for a while, yellow colored colloid like solution was formed. Workup using brine solution and $CHCl_3$ was done and then the organic layer collected was evaporated and purified by column chromatography on silica gel with 5% EtOAc/hexane as eluent. Yield =62%. ^{1}H NMR ($CDCl_3$, 500 MHz) δ= 2.70 (s, 6H), 4.12 (s, 4H), 6.62 (d, J= 8.6Hz, 2H), 7.12 (s, 2H), 7.16 (s, 2H).

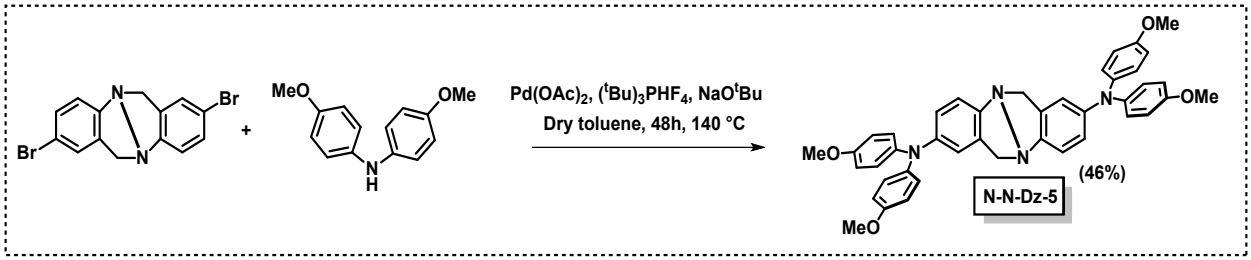
i) Synthesis of N-o-N-Dz-3 : Compound F (0.3g, 0.755mmol), compound C (0.43g, 1.88mmol), NaO^tBu (0.3g, 3.045mmol), $Pd(OAc)_2$ (0.0169g, 0.075mmol) and $(^tBu)_3PHF_4$ (0.0657g, 0.2267mmol) were taken in an oven-dried pressure tube and added 10ml of dry toluene. The pressure tube was sealed under nitrogen and kept for stirring at 140^{O}C for for 48hrs. The reaction mixture was taken to room temperature for cooling and solvent was evaporated. Purification of the compound was done by column chromatography on silica gel with 10% EtOAc /hexane and then with 25% EtOAc/hexane as eluent. Yield =74%. ^{1}H NMR ($CDCl_3$, 500 MHz) δ= 2.98 (s, 6H), 3.97 (s, 12H), 4.46 (s, 4H), 7.05 (d, J= 7.3Hz, 6H), 7.31 (d, J= 8.9Hz, 6H), 7.36 (d, J= 8.4 Hz, 2H), 7.58 (s, 4H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ= 39.30, 56.11, 58.42, 102.84, 110.72, 115.16, 123.15, 126.85, 127.20, 127.87, 130.06, 137.06, 149.33, 153.69. ESI-HRMS: m/z $[M + H]^+$ calculated: 689.3150; found: 689.31305.

Synthesis of N-CH_2-N-Dz4



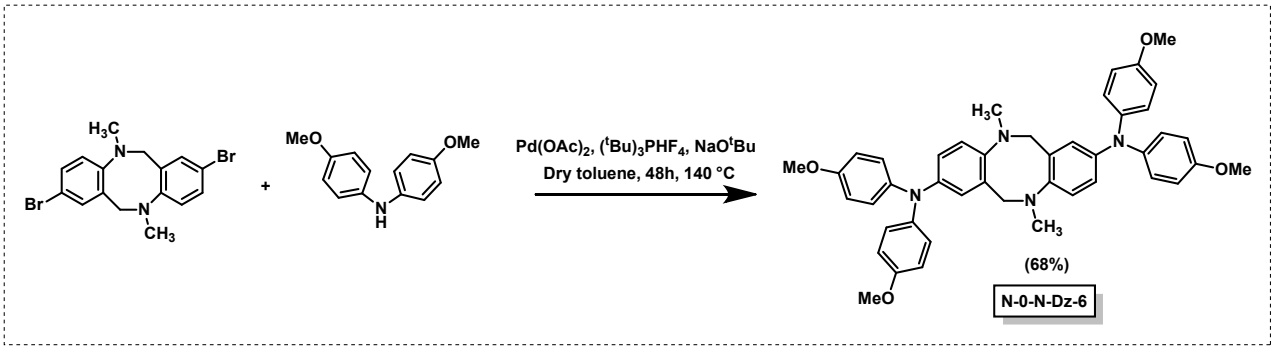
j) Synthesis of N-CH_2-N-Dz-4: Compound A (0.5 g, 1.315 mmol), 4,4'-dimethoxy diphenylamine (0.753 g, 3.28 mmol), NaO^tBu (0.505 g, 5.26 mmol), $Pd(OAc)_2$ (0.03 g, 0.13 mmol), and $(^tBu)_3PHF_4$ (0.114 g, 0.394 mmol) were taken in an oven-dried pressure tube and added 15 mL of dry toluene. The pressure tube was sealed under nitrogen and heated at 140 °C for 48 h. Then the contents were cooled to room temperature, toluene was removed under pressure, and purified by column chromatography on silica gel with 25% EtOAc/ hexane as eluent. Yield = 70.0%. ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 3.78 (s, 12H), 3.97 (d, J= 16.8 Hz, 2H), 4.30 (s, 2H), 4.54 (d, J= 16.7 Hz, 2H), 6.48 (s, 2H), 6.80 (d, J= 8.9 Hz, 10H), 6.94 (d, J= 8.6 Hz, 2H), 6.98 (d, J= 8.7 Hz, 8H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ= 55.50, 57.91, 67.14, 114.75, 117.76, 120.37, 125.31, 126.51, 140.72, 146.23, 155.90. ESI-HRMS: m/z $[M + H]^+$ calculated: 677.3150; found: 677.3132.

Synthesis of N-N-Dz5



k) Synthesis of N-N-Dz-5: Compound D (0.3 g, 0.82 mmol), 4,4'-dimethoxy diphenylamine (0.47 g, 2.04 mmol), NaO^tBu (0.31 g, 3.27 mmol), $Pd(OAc)_2$ (0.02 g, 0.08 mmol), and $(^tBu)_3PHF_4$ (0.07 g, 0.24 mmol) were taken in an oven-dried pressure tube and added 10 mL of dry toluene. The pressure tube was sealed under nitrogen and heated at 140 °C for 48 h. Then the contents were cooled to room temperature, toluene was removed under pressure, and purified by column chromatography on neutral alumina with 25% EtOAc/ hexane as eluent. Yield = 46.2%. %. ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 3.77 (s, 12H), 4.50 (s, 4H), 6.68 (d, J= 8.4 Hz, 2H), 6.77 (d, J= 7.2 Hz, 10H), 6.83 (d, J= 8.3 Hz, 2H), 6.95 (d, J = 8.1 Hz, 8H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ= 55.51, 56.36, 111.02, 114.58, 117.82, 122.83, 125.30, 128.44, 141.91, 144.38, 146.24, 155.16, ESI-HRMS: m/z $[M - H]^+$ calculated: 661.2893; found: 661.2818.

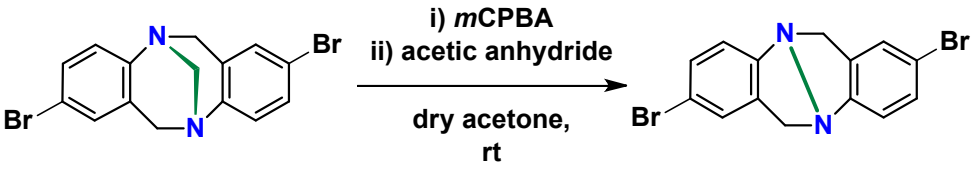
Synthesis of N-o-N-Dz-6



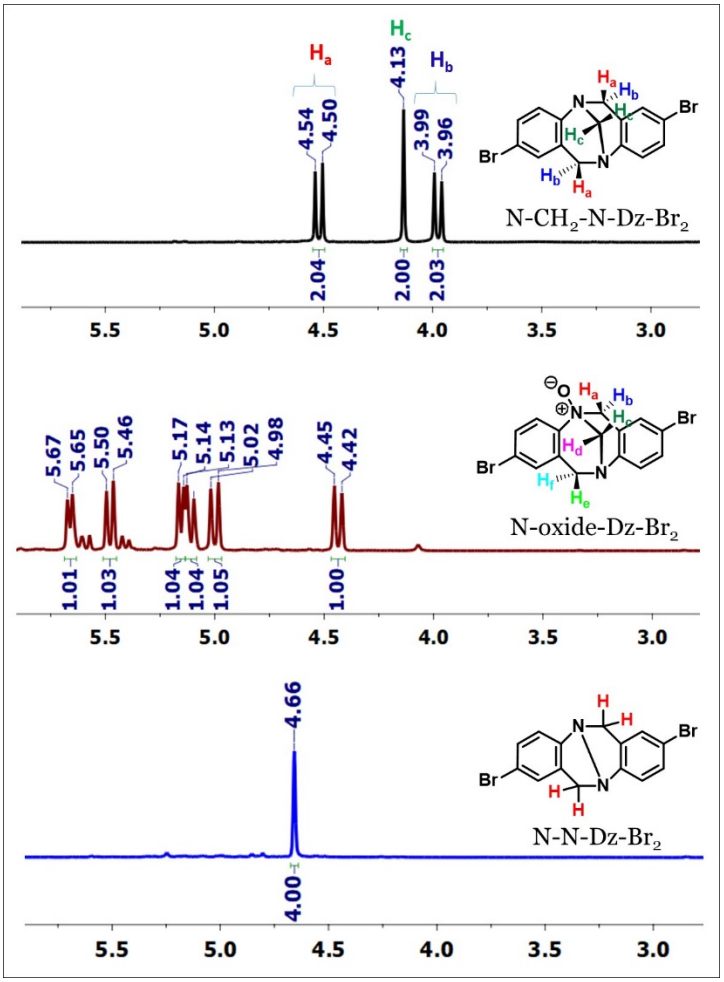
l) Synthesis of N-o-N-Dz-6: Compound F (0.1g, 0.251mmol), 4,4'-dimethoxy diphenylamine (0.144g, 0.629mmol), NaO^tBu (0.096g, 0.305mmol), $Pd(OAc)_2$ (0.005g, 0.025mmol) and $(^tBu)_3PHF_4$ (0.021g, 0.753 mmol) were taken in an oven-dried pressure tube and added 10ml of dry toluene. The pressure tube was sealed under nitrogen and kept for stirring at 140^{O}C for for 48hrs. The reaction mixture was taken to room temperature for cooling and solvent was evaporated. Purification of the compound was done by column chromatography on silica gel with 10% EtOAc /hexane and then with 25% EtOAc/hexane as eluent. Yield =68%. ^{1}H NMR (Acetone-d_6, 500 MHz) δ= 2.82 (s, 6H), 3.75 (s, 12H), 4.19 (s, 4H), 6.78 (d, J= 8.2Hz, 2H), 6.82 (d, J= 8.8Hz, 10H), 6.86 (s, 2H), 6.92 (d, J= 8.7Hz, 8H). ESI-HRMS: m/z $[M + H]^+$ calculated: 689.310; found: 689.31. ^{13}C NMR (Acetone-d_6, 125 MHz) δ= 38.73, 54.80, 58.05, 114.44, 116.04, 123.96,

124.25, 127.50, 139.41, 142.24, 146.43, 154.93. ESI-HRMS: m/z $[M + H]^+$ calculated: 693.1663; found: 693.1652.

^{1}H NMR monitoring experiment



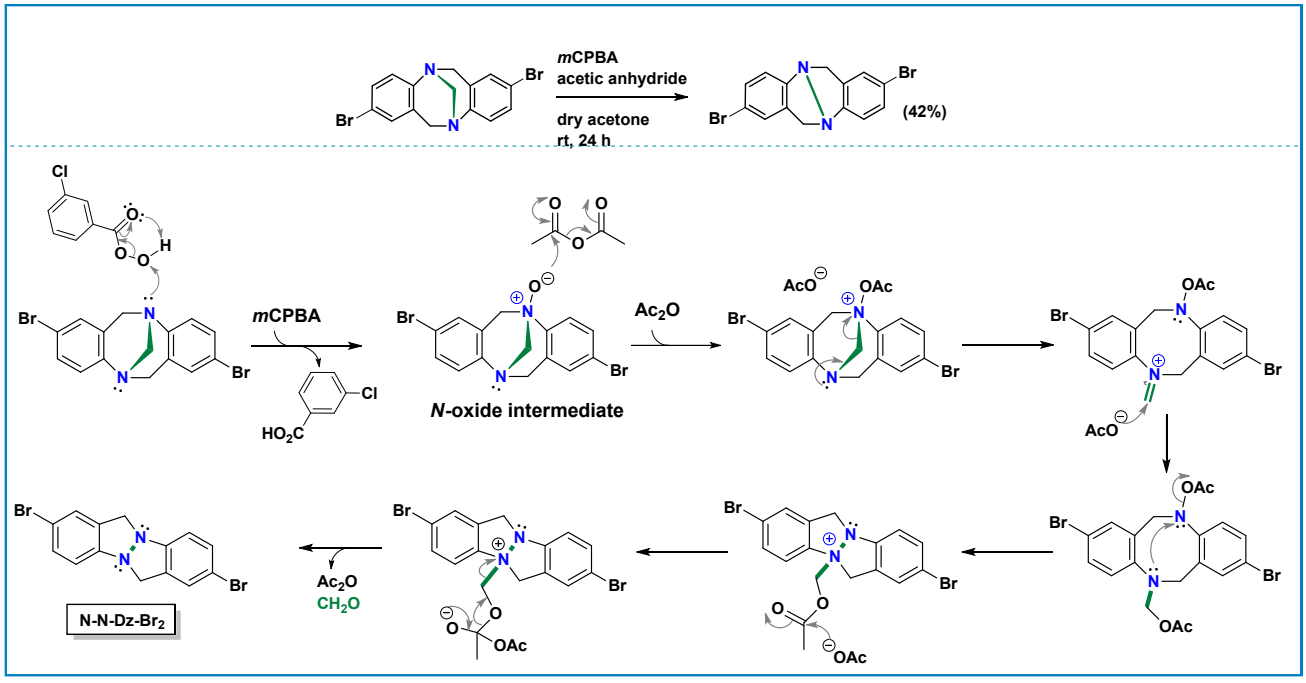
1H NMR monitoring experiment was carried out to track the one-pot conversion of N-CH_2-N-Br_2 to N-N-Br_2 via N-CH_2-N-oxide-Br_2 intermediate. In an NMR tube taken compound the N-CH_2-N-Br_2 (0.025 g, 0.065 mmol) and *m*CPBA (0.022 g, 0.098mmol), and added acetone-d_6 to it under nitrogen atmosphere and stirred at rt for 1 h. ^{1}H NMR spectrum was recorded immediately and then added acetic anhydride (12.5 µL, 0.131 mmol), stirred overnight at rt and recorded ^{1}H NMR spectrum.



Scheme S1 : ^{1}H NMR monitoring for the one-pot transformation of N-CH_2-N-Dz-Br_2 to N-N-Dz-Br_2.

	Reaction parameters	*m*CPBA-mediated conversion in this work	DMDO-mediated conversion by Harmata et al. [4]
1	Equivalents of oxidizing agent used	1.5	4
2	Time taken for conversion of N-CH_2-N-Br_2 to N-CH_2-N-oxide-Br_2	1 h	1 h
3	No of steps to obtain N-N bridged product	1	2
4	Whether isolation of N-oxide done by chromatography.	No	Yes
5	Yield	42% (two steps in one-pot)	67% (overall yield of two steps) Step- 1 yield = 86% Step-2 yield= 78%

Table S1. Comparison of reaction parameters of *m*CPBA-mediated and DMDO-mediated conversion of N-CH_2-N-Br_2 to N-N-Br_2



Scheme S2 : Plausible mechanism for the conversion of N-CH_2-N-Dz-Br2 into N-N-Dz-Br2.

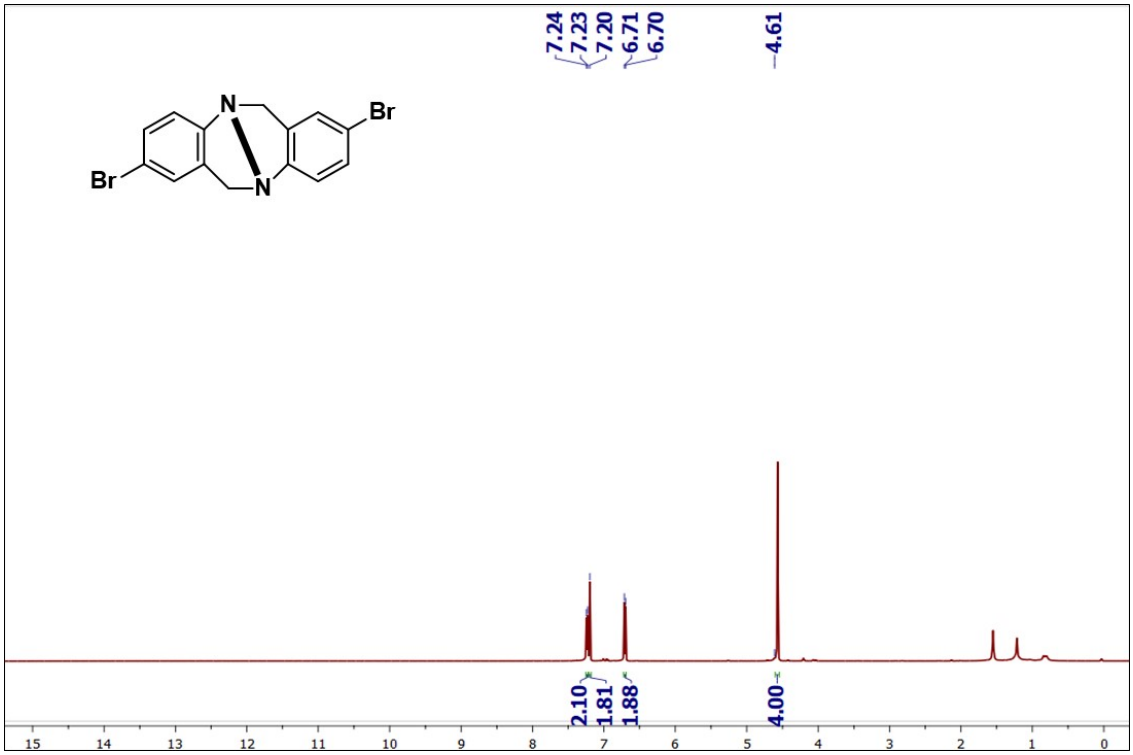


Figure S1. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of N-N-Dz-Br_2.

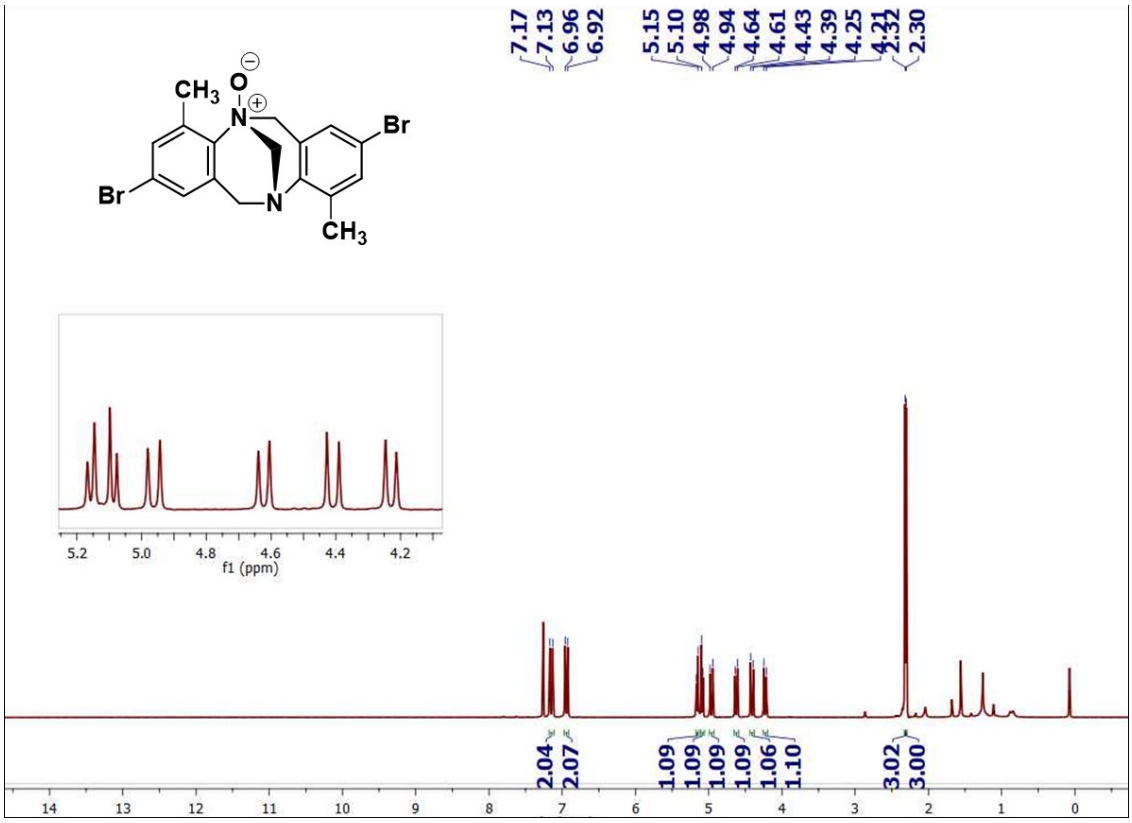


Figure S2. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of methyl-N-CH_2-N-oxide-Dz-Br_2.

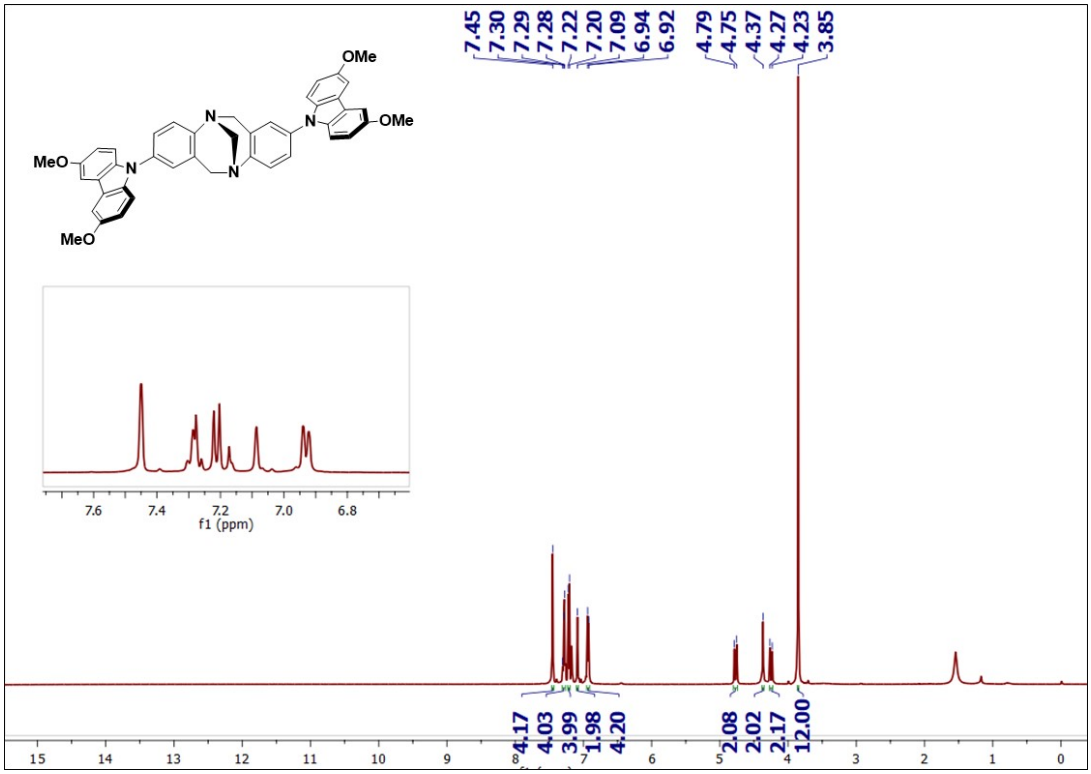


Figure S3. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of N-CH_2-N-Dz-1.

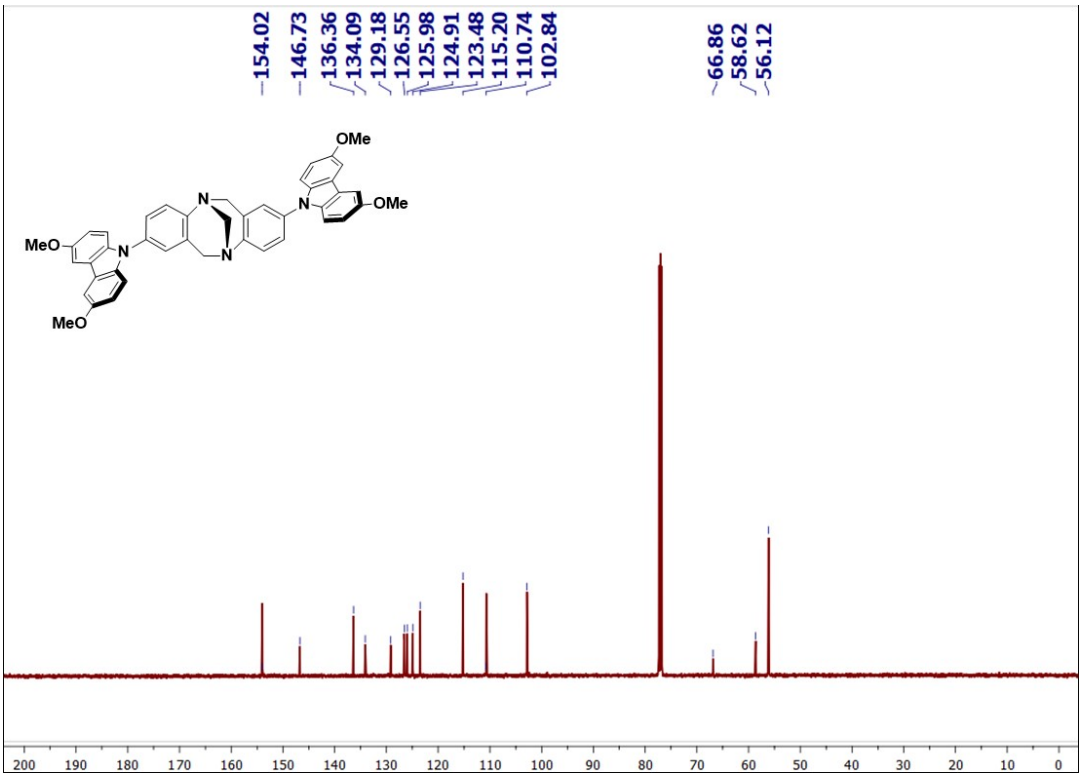


Figure S4. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of N-CH_2-N-Dz-1.

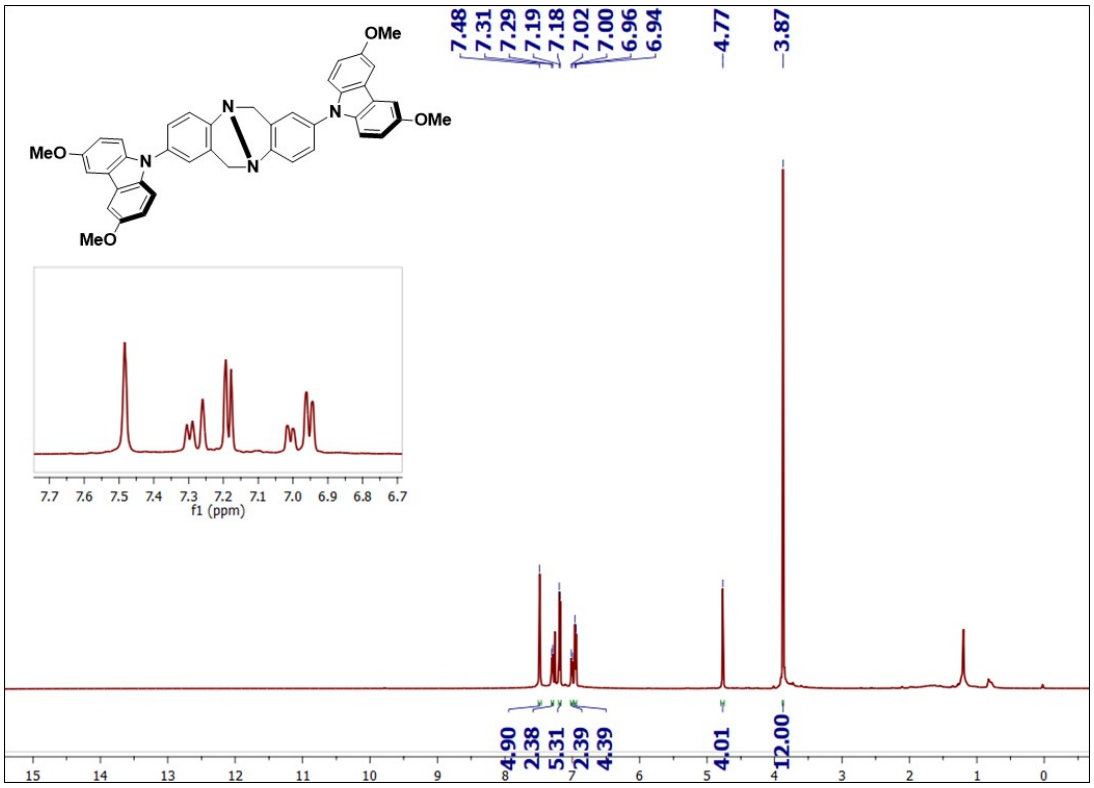


Figure S5. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of N-N-Dz-2.

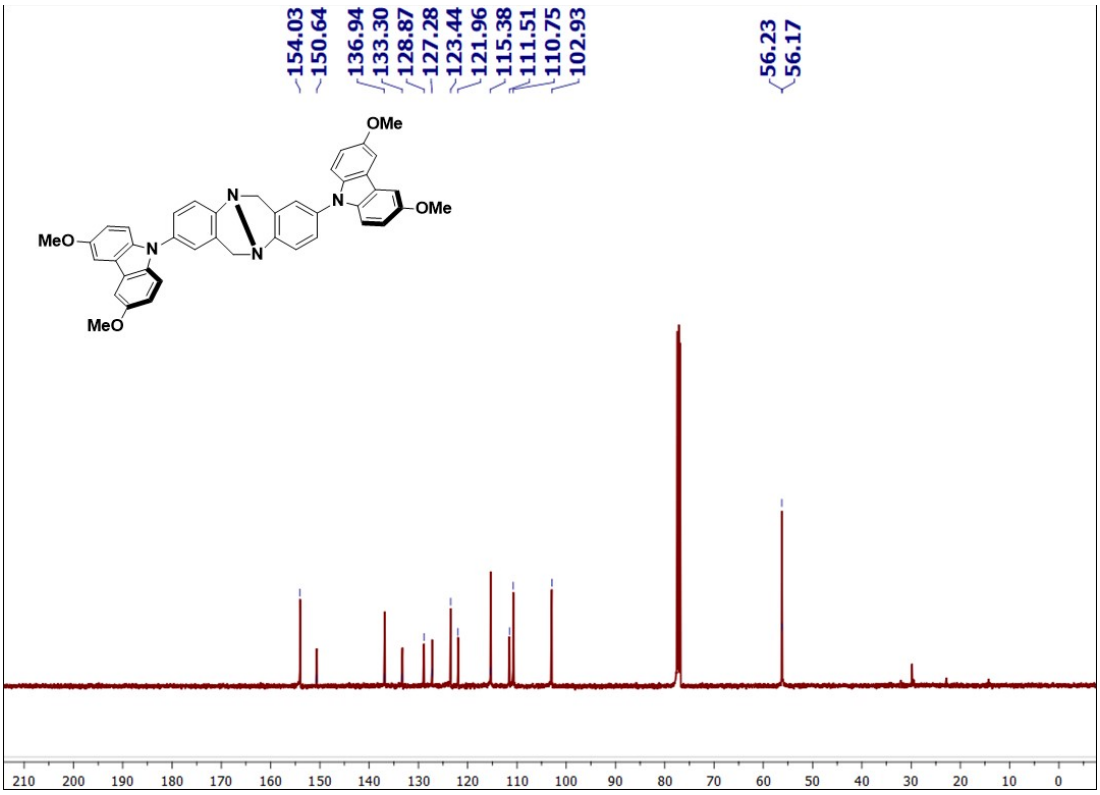


Figure S6. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of N-N-Dz-2.

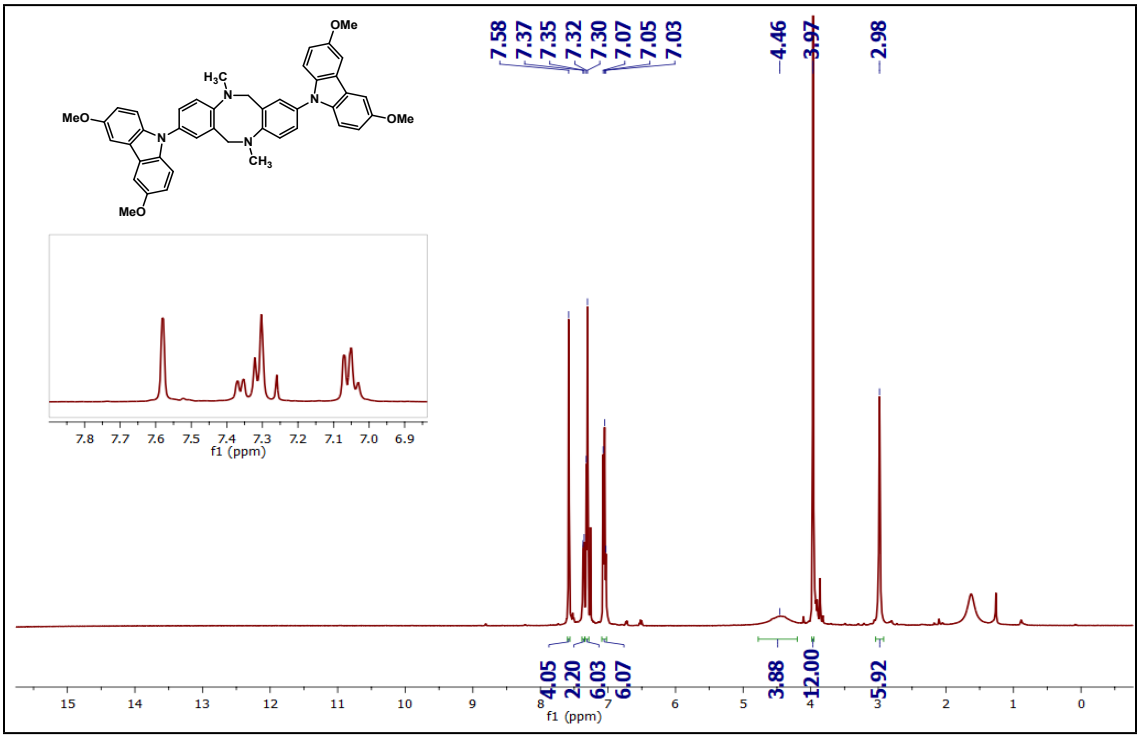


Figure S7. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of N-o-N-Dz-3.

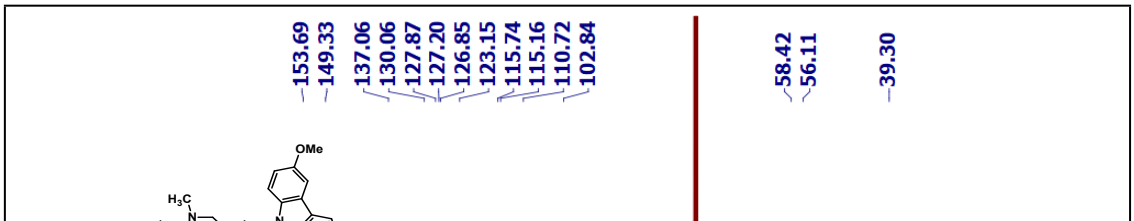


Figure S8. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of N-o-N-Dz-3.

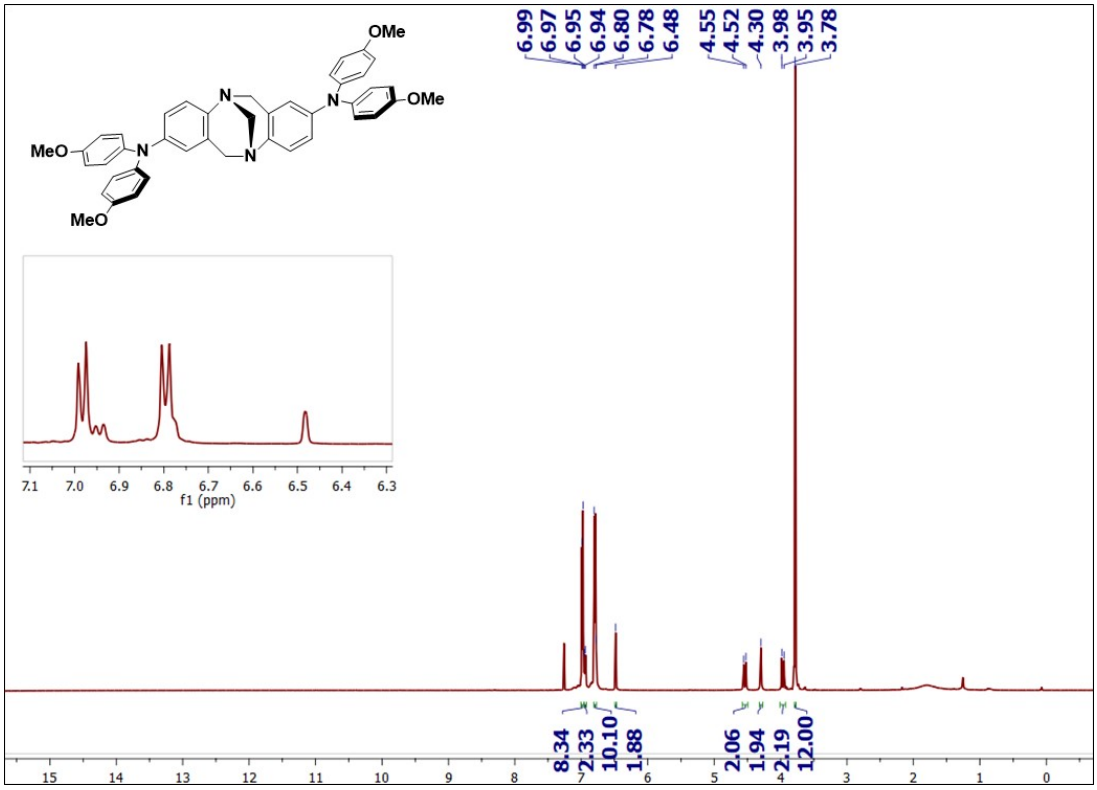


Figure S9. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of N-CH_2-N-Dz-4.

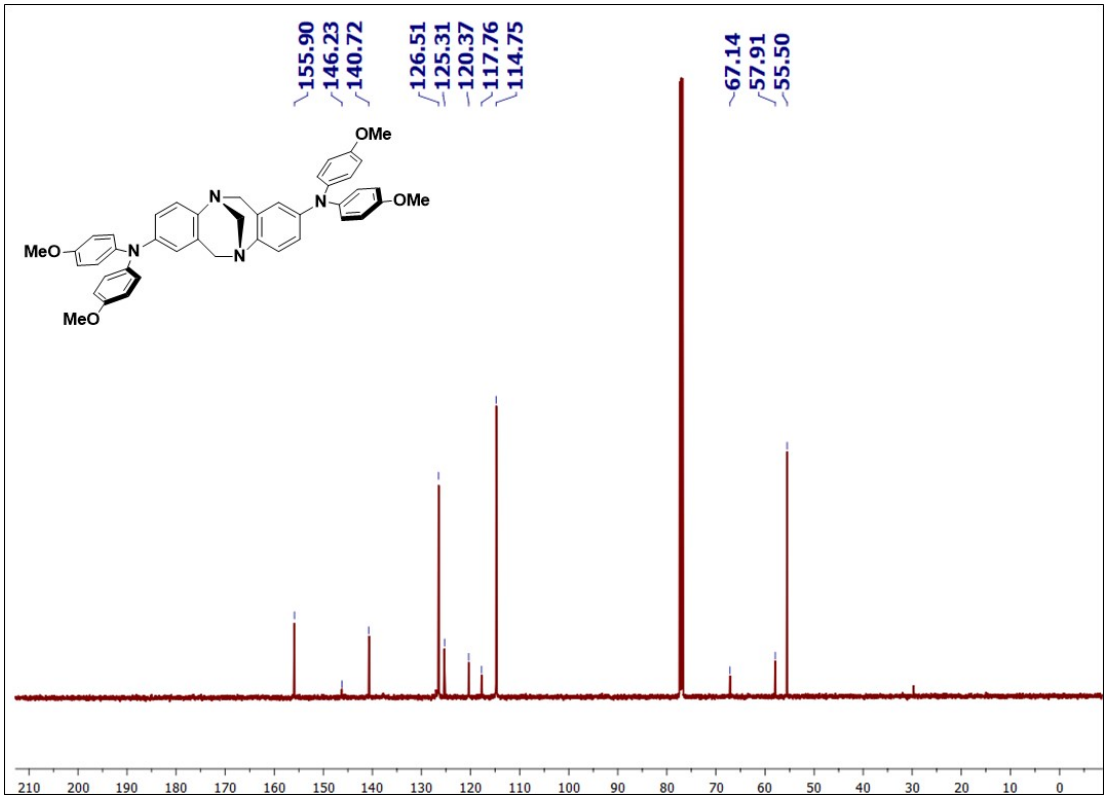


Figure S10. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of N-CH_2-N-Dz-4.

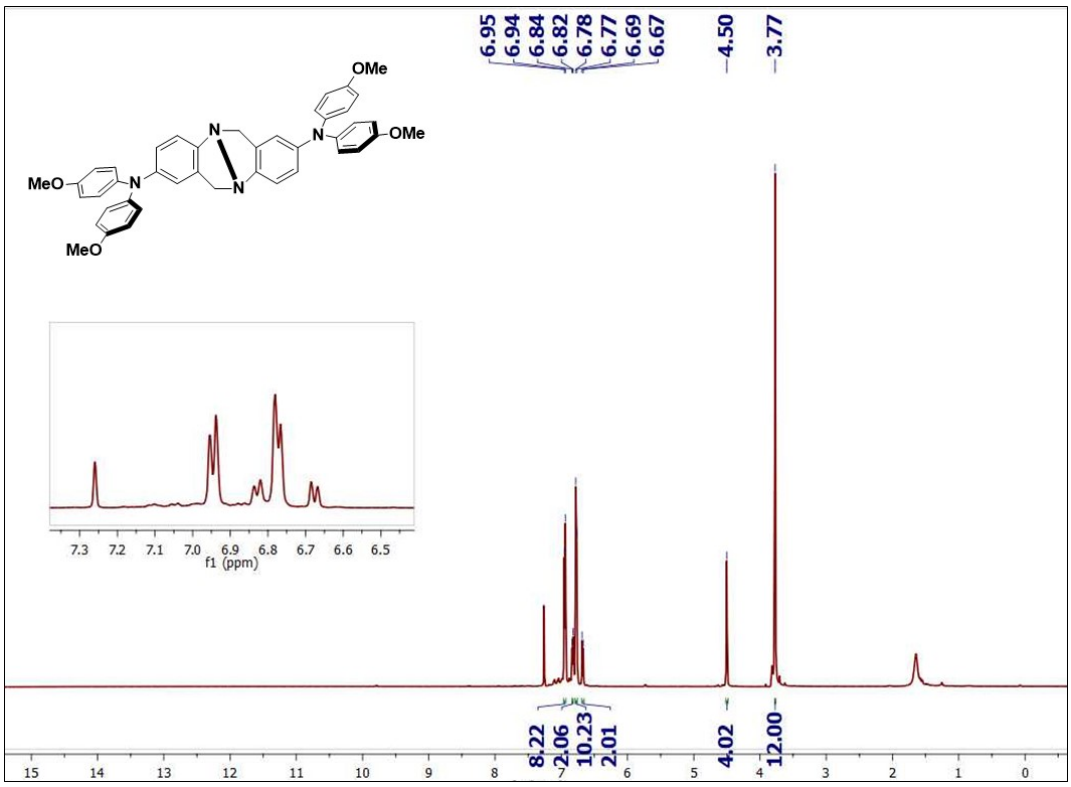


Figure S11. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of N-N-Dz-5.

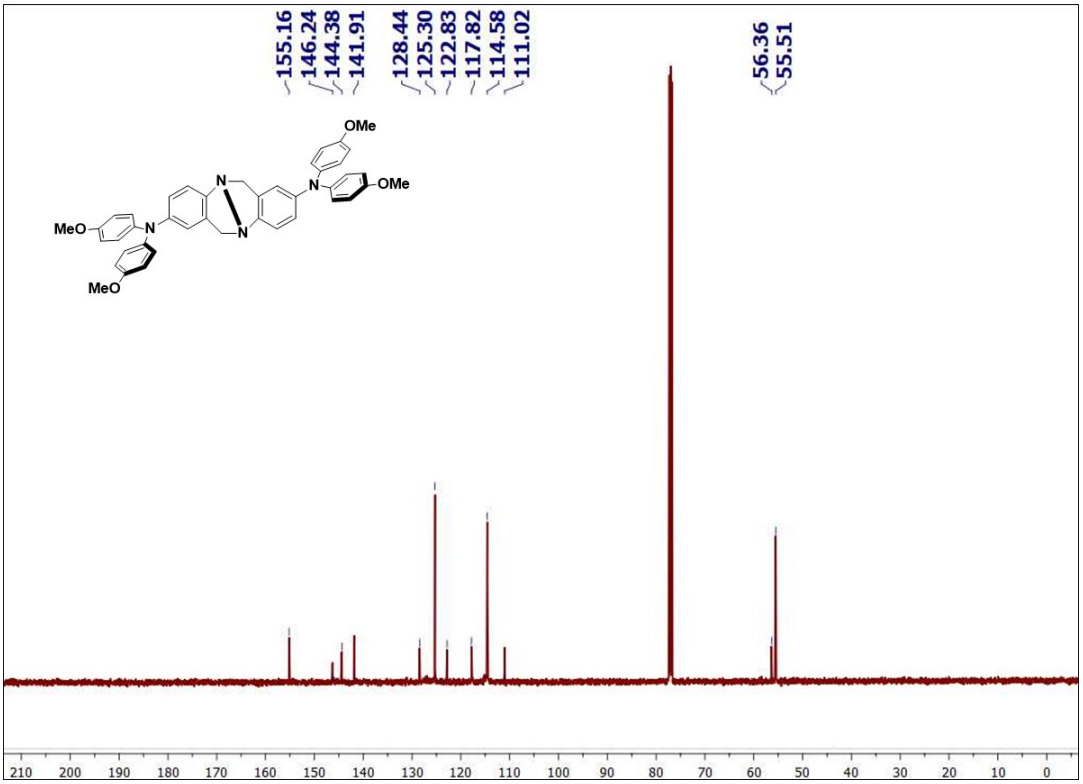


Figure S12. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of N-N-Dz-5.

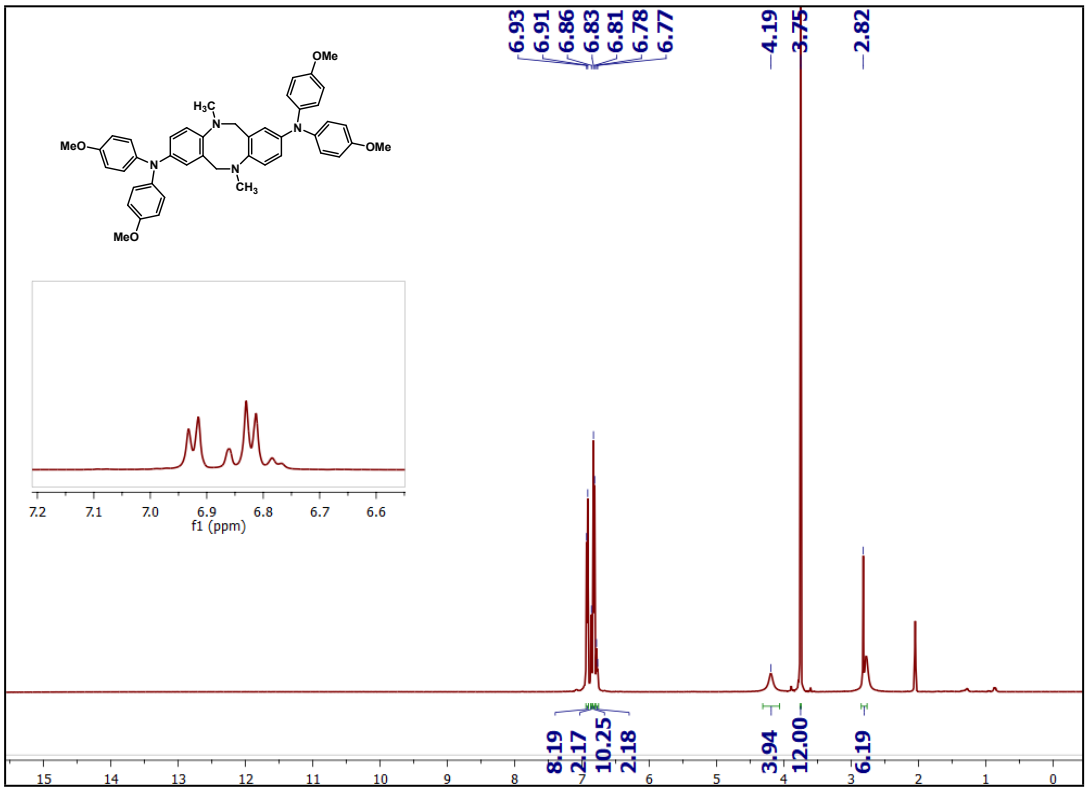


Figure S13. ^{1}H NMR (500 MHz, Acetone-d_6) spectrum of N-o-N-Dz-6.

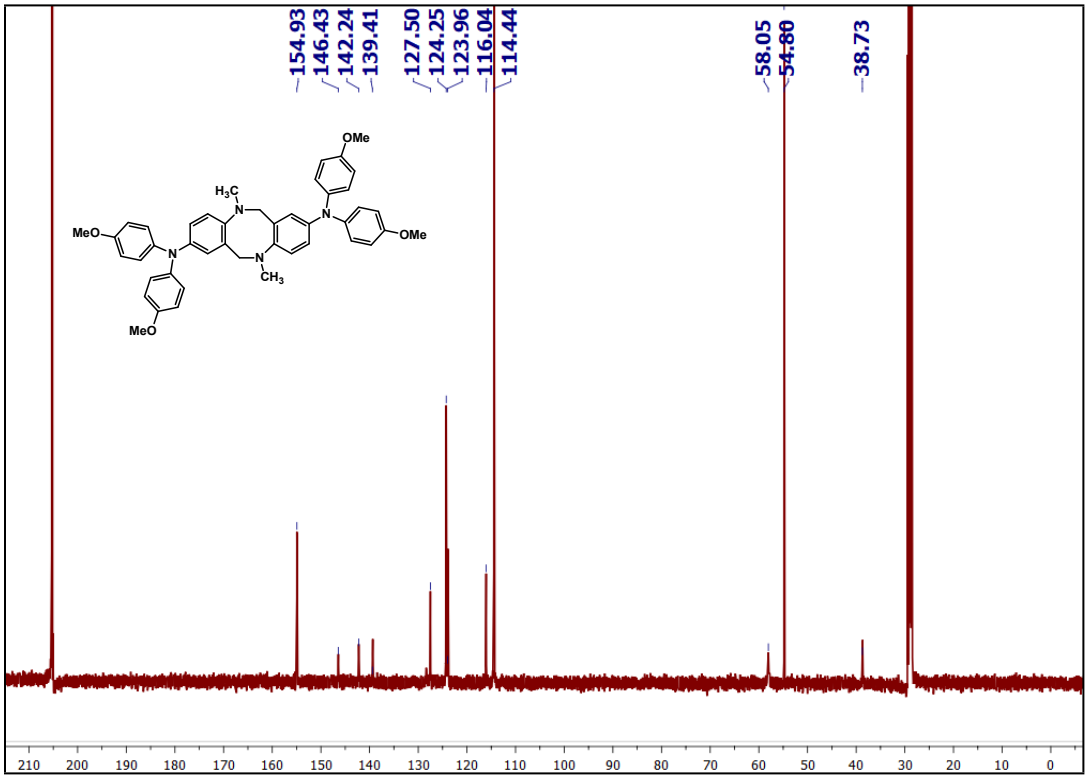


Figure S14. ^{13}C NMR (125 MHz, Acetone-d_6) spectrum of N-o-N-Dz-6.

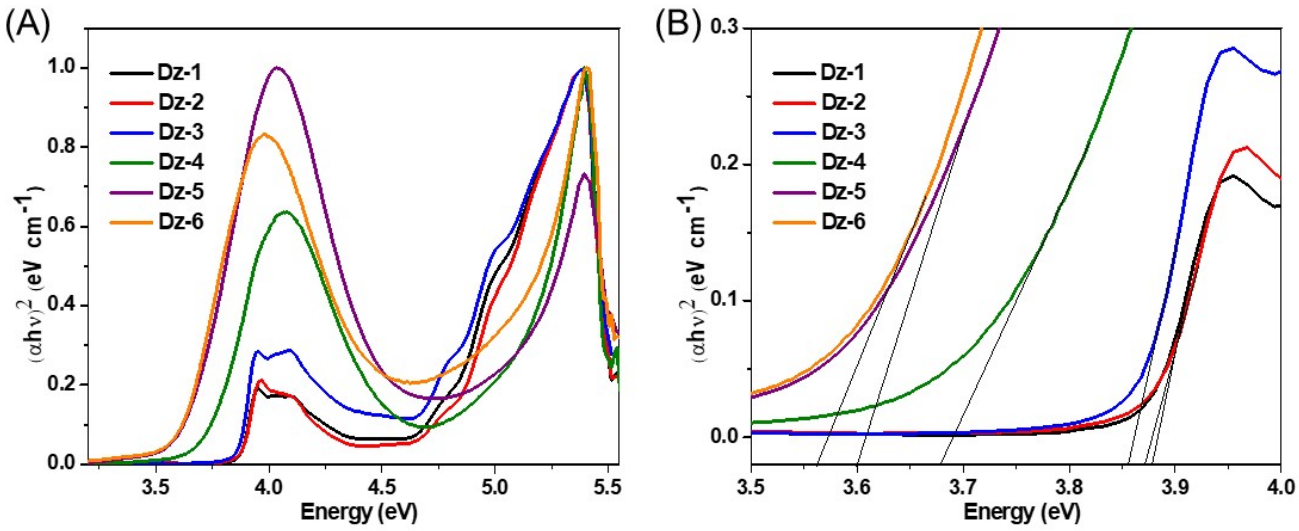


Figure S15. (A) Tauc plot of Dzs (B) Enlarged portion of (A) showing the bandgap.

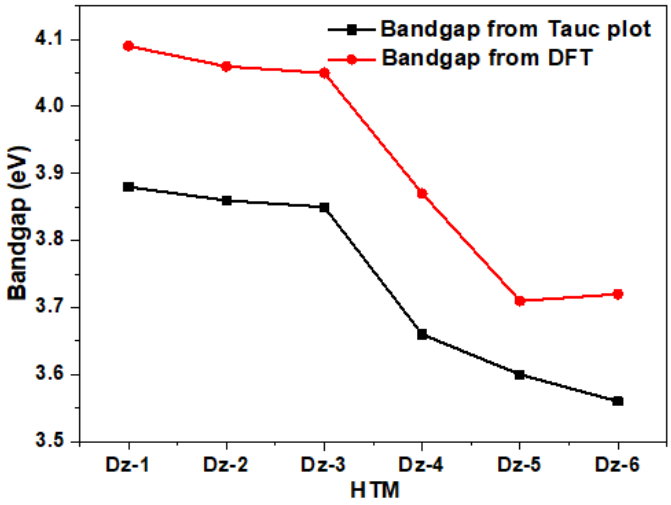


Figure S16. A comparison of bandgap values obtained from Tauc plot and DFT.

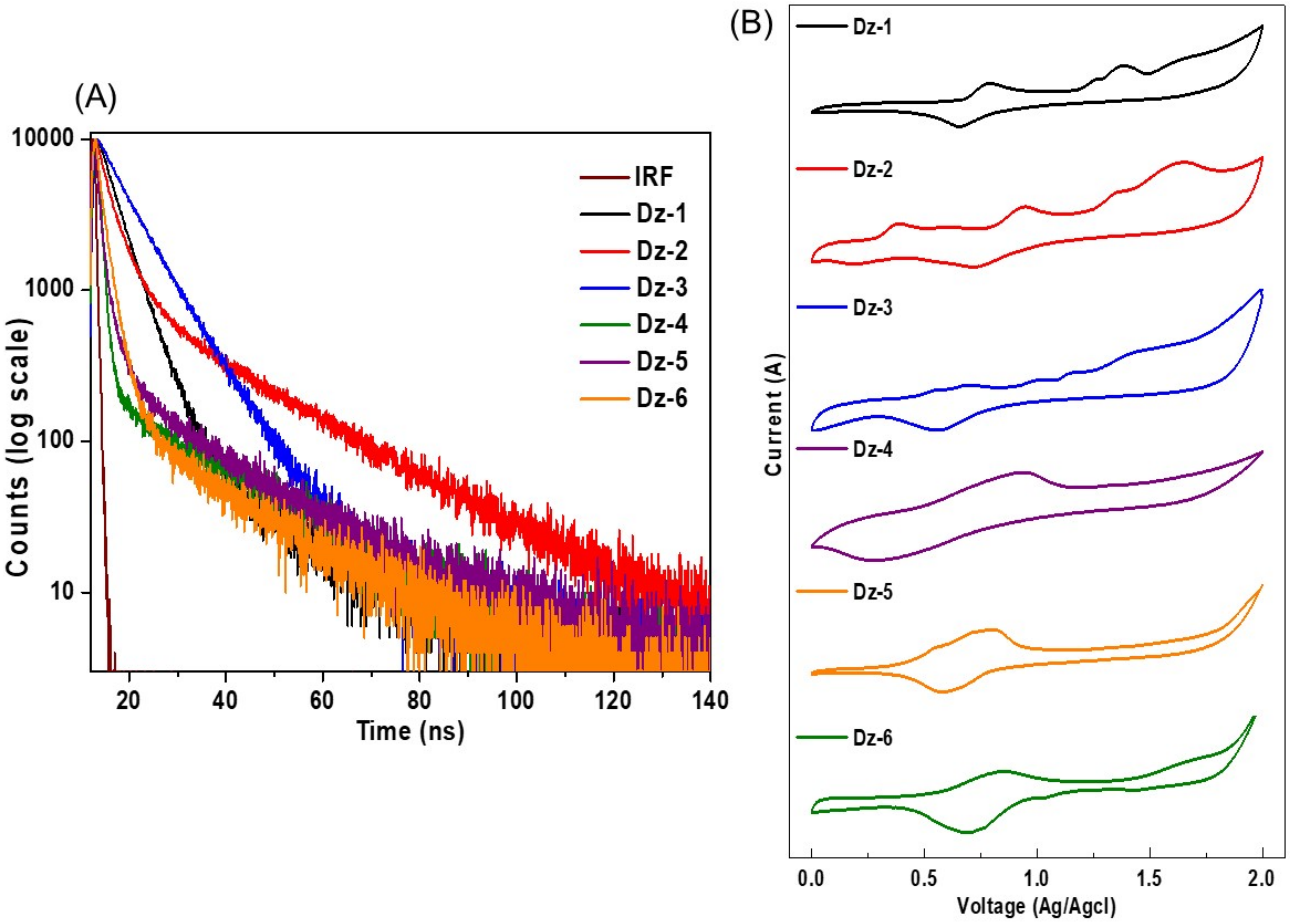


Figure S17. (A) TCSPC spectra of Dzs (B) CV profiles of Dzs.

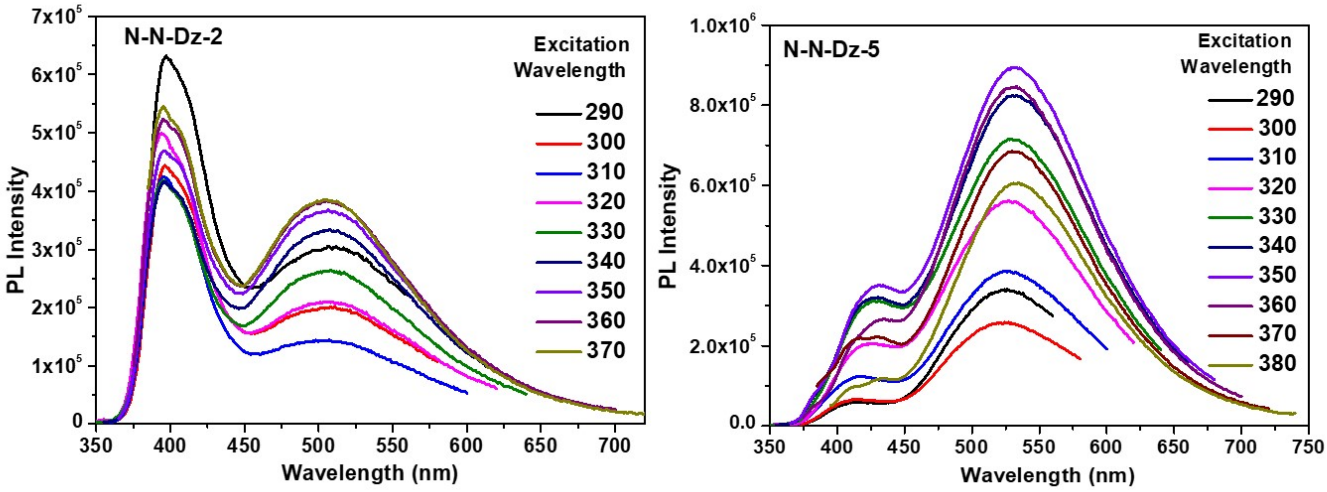


Figure S18. PL spectra of N-N-Dzs at different excitation wavelengths.

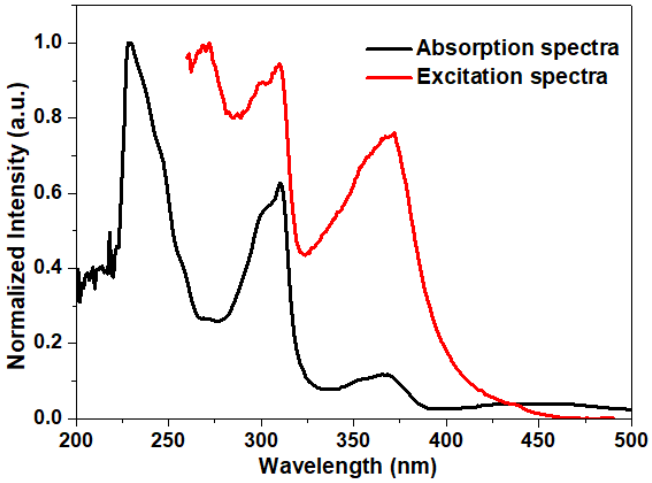


Figure S19. Absorption and excitation spectra of N-N-Dz-2.

Table S2. Comparison of fluorescence quantum yield, lifetime, radiative and non-radiative decay constants of Dzs.

Material	PL λ_{max} (nm)[a]	Φ_f[b]	τ (ns)[c]	K_r (ns^{-1})[d]	K_{nr} (ns^{-1})[e]
N-CH_2-N-Dz-1	393	0.72	4.20	0.17	0.07

N-N-Dz-2	396, 505	0.10	4.97	0.02	0.18
N-O-N-Dz-3	423	0.68	7.15	0.09	0.04
N-CH_2-N-Dz-4	404	0.06	0.95	0.07	0.99
N-N-Dz-5	430, 530	-	1.02	-	-
N-O-N-Dz-6	418	0.03	1.00	0.03	0.97

[a] PL λ_{max} obtained from photoluminescence spectra. [b]Fluorescence quantum yield calculated using anthracene as reference. [c]PL lifetime estimated using TCSPC. [d]Radiative rate constant calculated from Φ_f and τ. [e]Non-radiative rate constant calculated from Φ_f and τ_f.

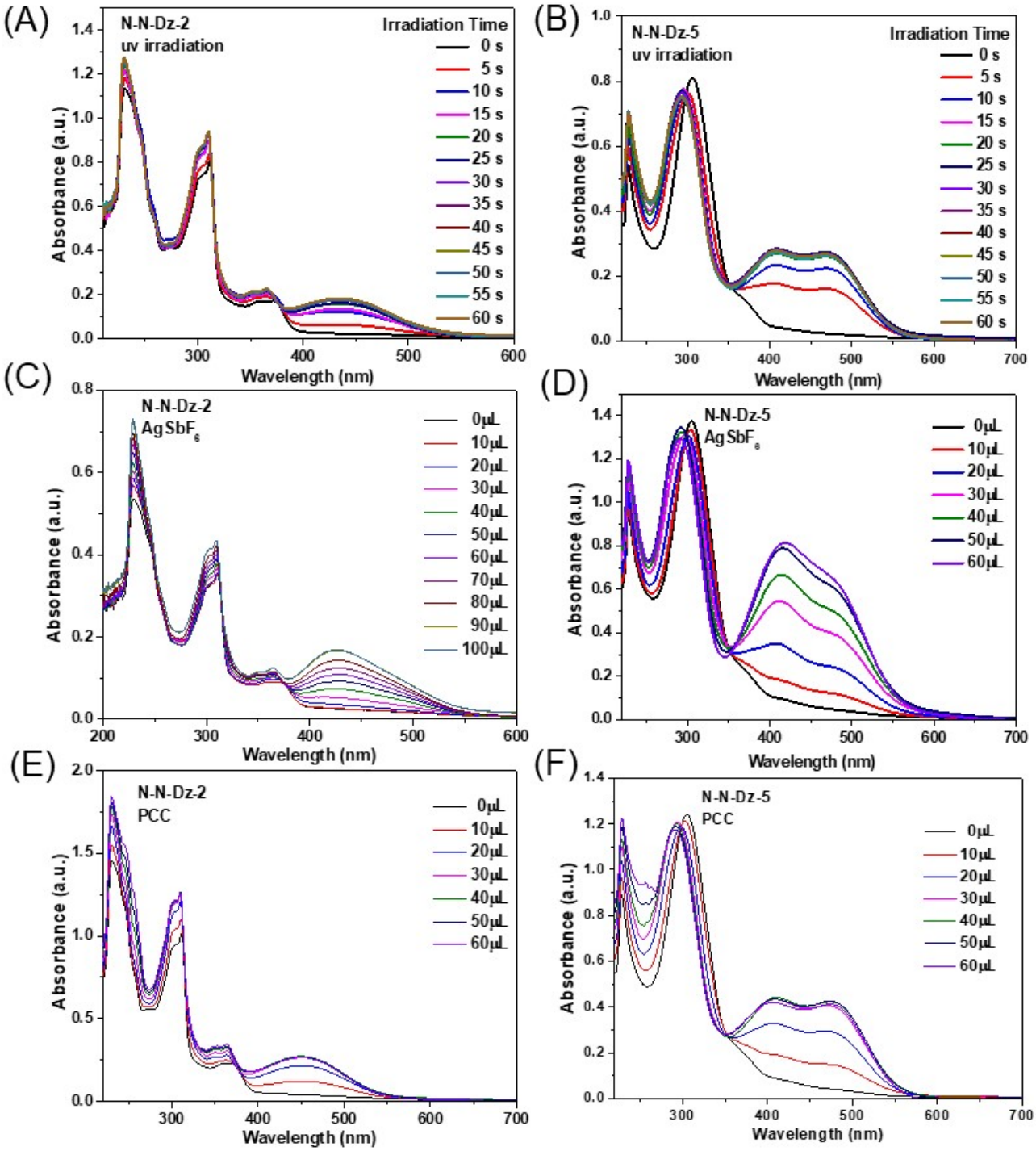


Figure S20. Change in UV absorption spectra after irradiating (A) N-N-Dz-2, (B) N-N-Dz-5 at 365 nm for different time intervals, Change in uv absorption spectra after titrating (C) N-N-Dz-2 and (D) N-N-Dz-5 with oxidizing agent $AgSbF_6$, Change in uv absorption spectra after titrating (E) N-N-Dz-2 and (F) N-N-Dz-5 upon titration with oxidizing agent PCC.

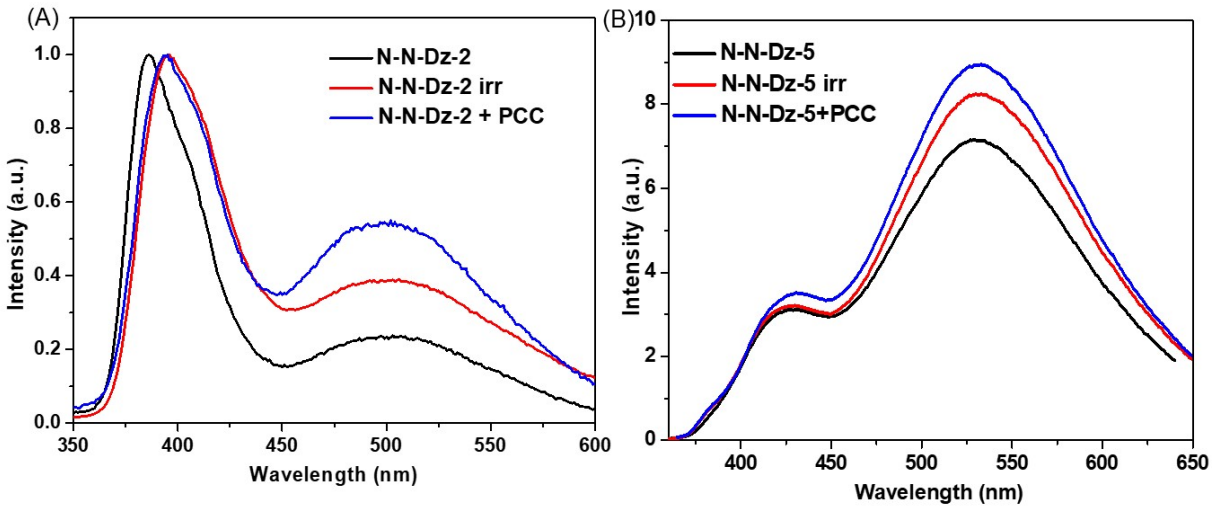


Figure S21. Change in emission spectra after irradiating N-N-Dzs at 365 nm and addition of oxidizing agent.

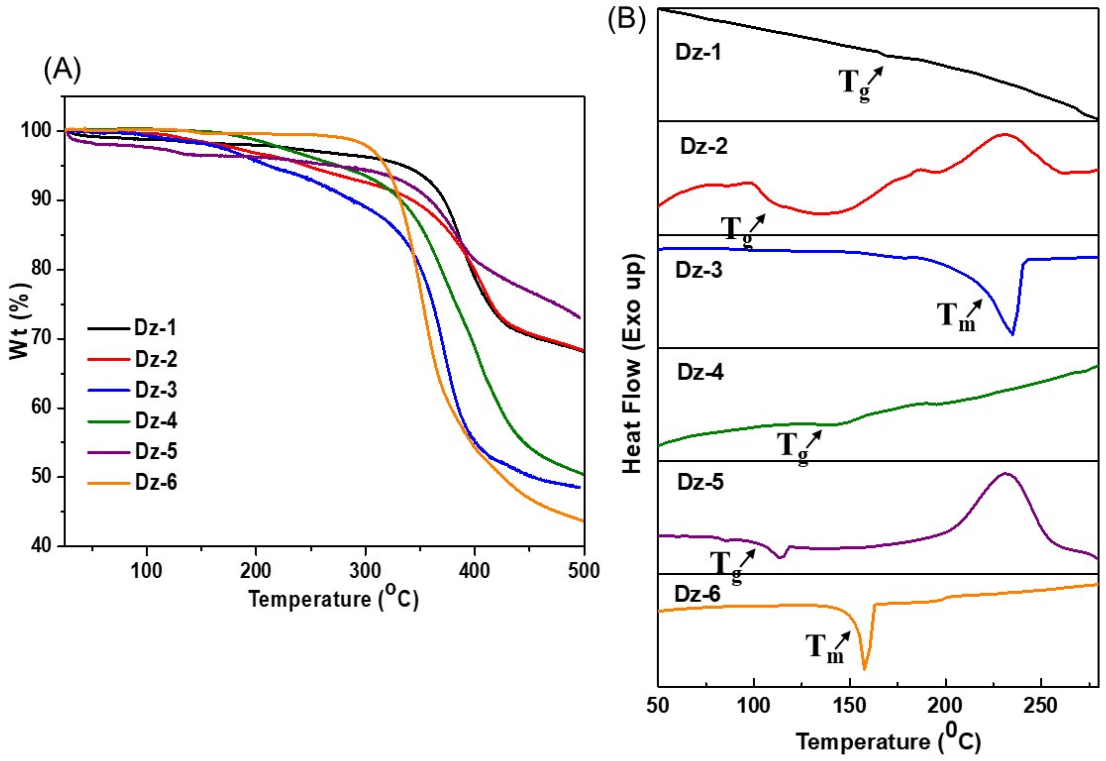


Figure S22. (A) TGA and (B) DSC profiles of Dzs.

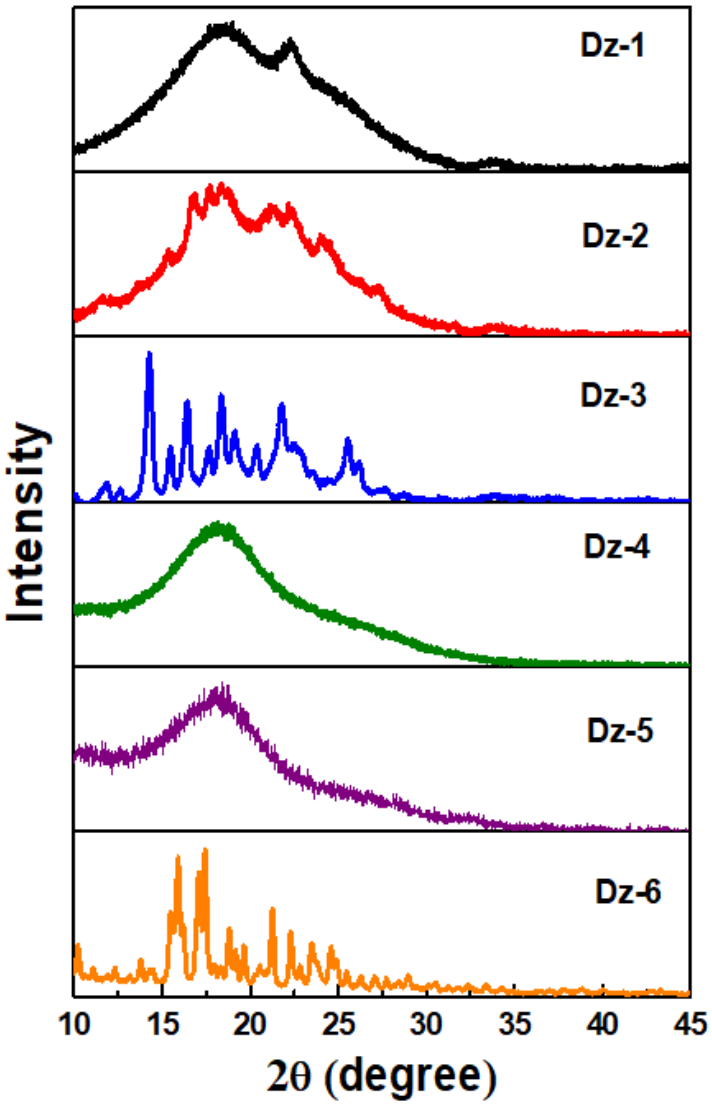


Figure S23. Powder XRD patterns of Dzs.

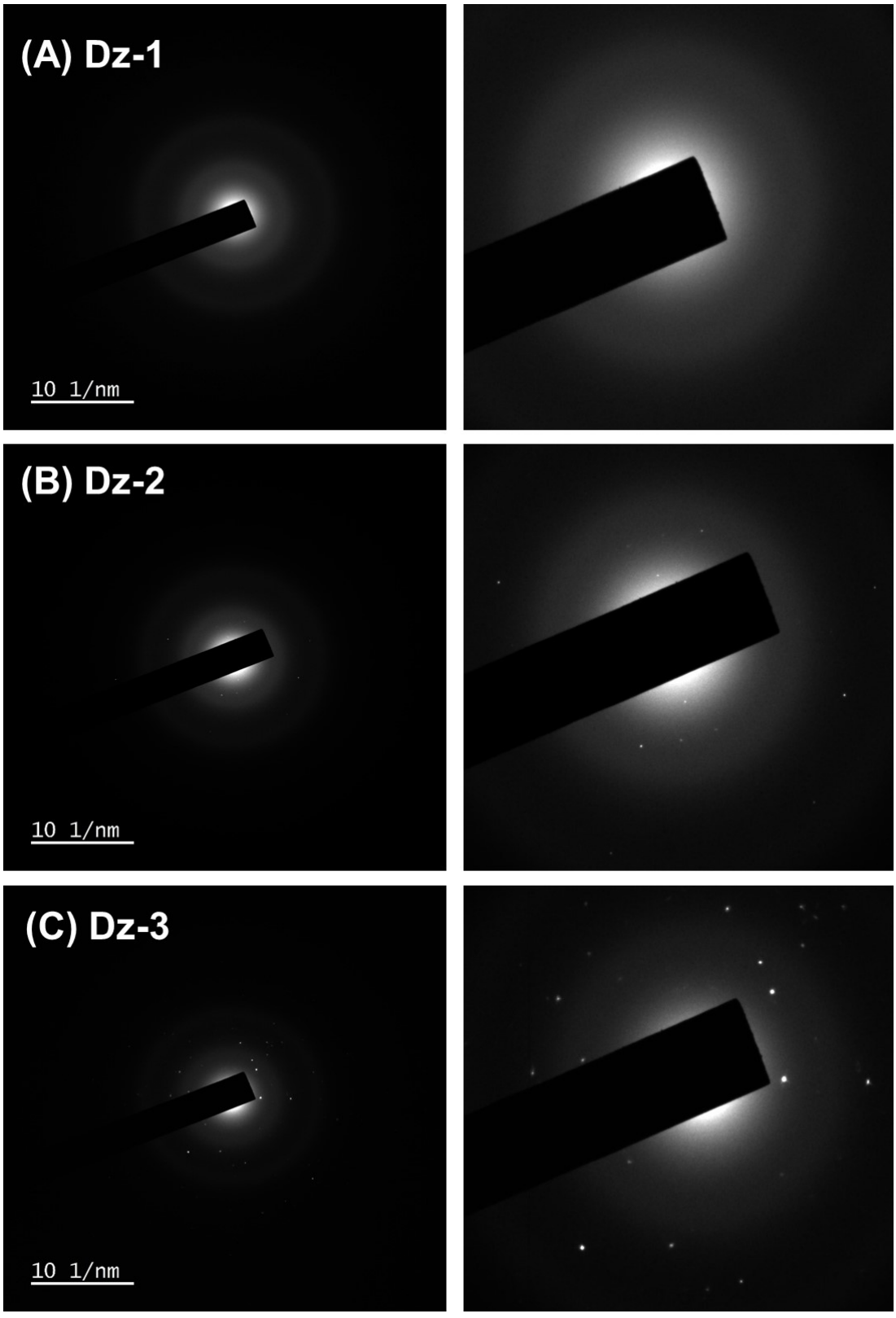


Figure S24. HR-TEM SAED images of Right : (A) Dz-1 (B) Dz-2 and (C) Dz-3. Zoomed images are shown in left.

Table S3: Crystal data of N-O-N-Dz-3	
Crystal system	Monoclinic
Space group	2P 21/c 1
a (Å)	a = 18.467(2)
b (Å)	b = 31.227(4)
c (Å)	c = 14.6308(17)
α (deg)	90.00
β (deg)	92.04
γ (deg)	90.00
Volume (Å^3)	8431.8(18)
Z	4
absorption coefficient (mm^{-1})	0.079
F(000)	3316
goodness-of-fit on F^2	1.080

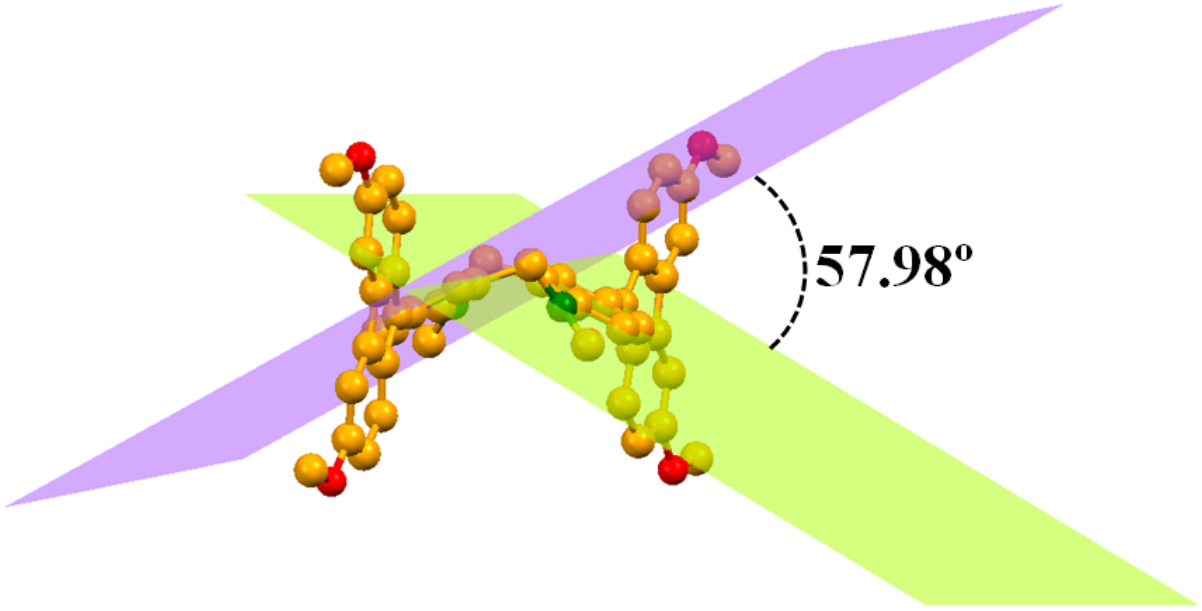


Figure S25. Interplanar angle between the aryl rings of N-O-N-Dz-3.

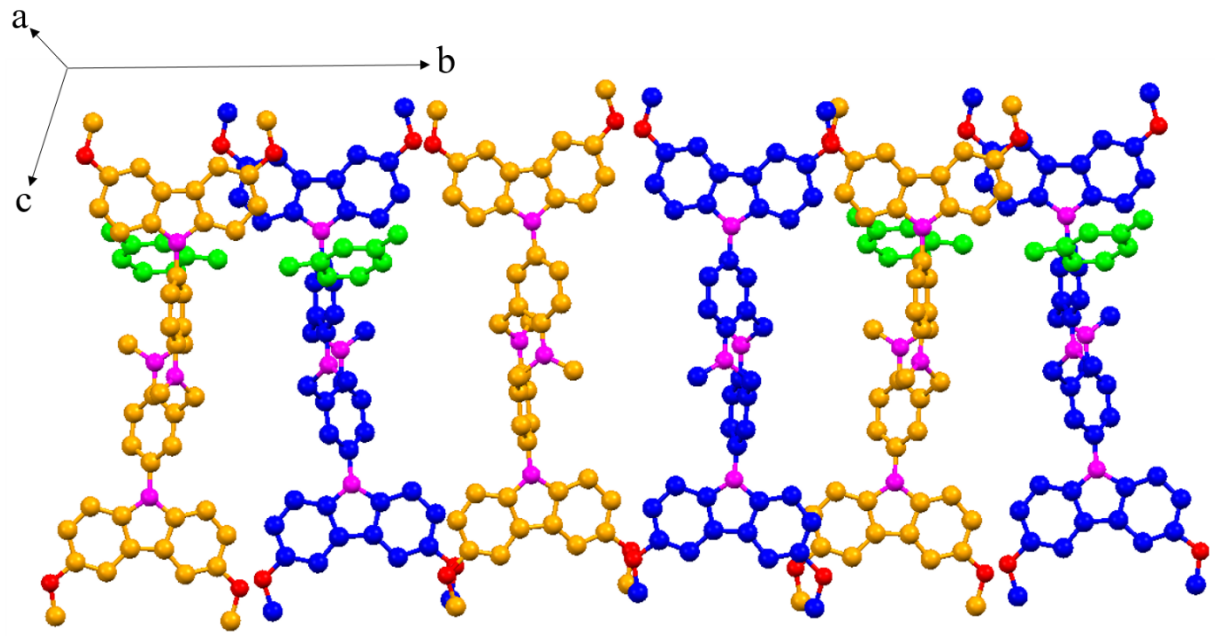


Figure S26. Packing of N-o-N-Dz-3 along b-axis and down c-axis

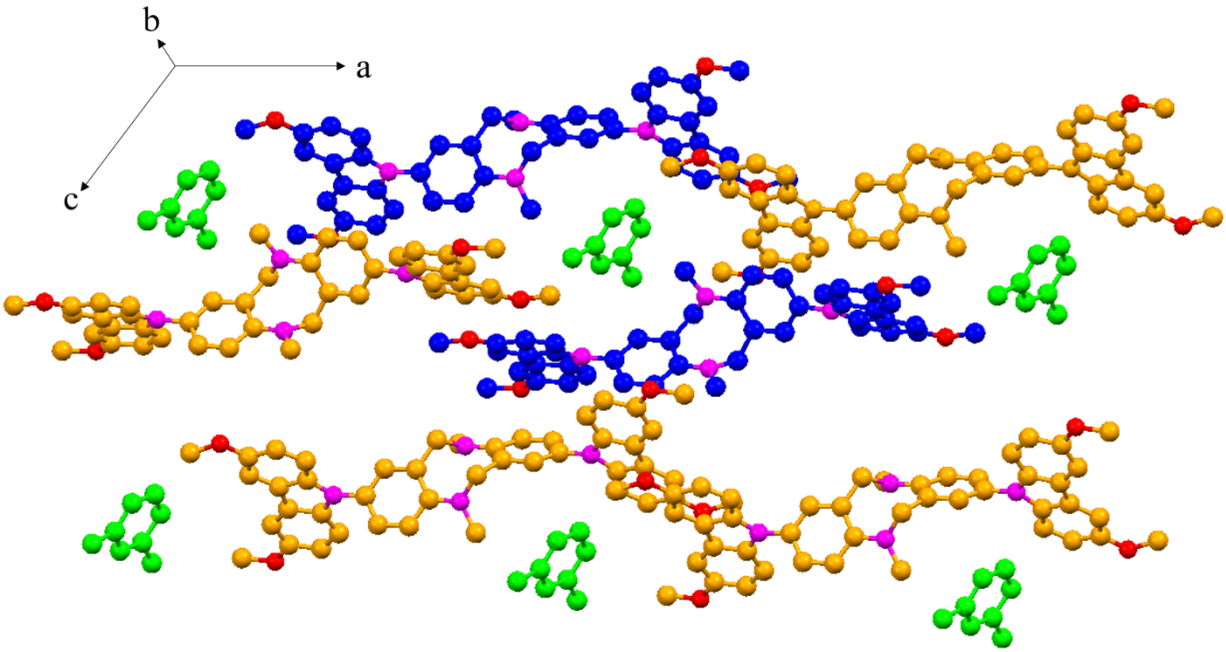


Figure S27. Packing of N-o-N-Dz-3 in ac-plane

Table S4: Crystal data of N-o-N-Dz-6	
Crystal system	Triclinic
Space group	2P-1
a (Å)	a = 9.7753(15)
b (Å)	b = 11.738(2)
c (Å)	c = 17.447(3)
α (deg)	77.325
β (deg)	82.367
γ (deg)	70.387
Volume (Å^3)	1835.9(5)
Z	2
absorption coefficient (mm^{-1})	0.081
F(000)	736
goodness-of-fit on F^2	1.005

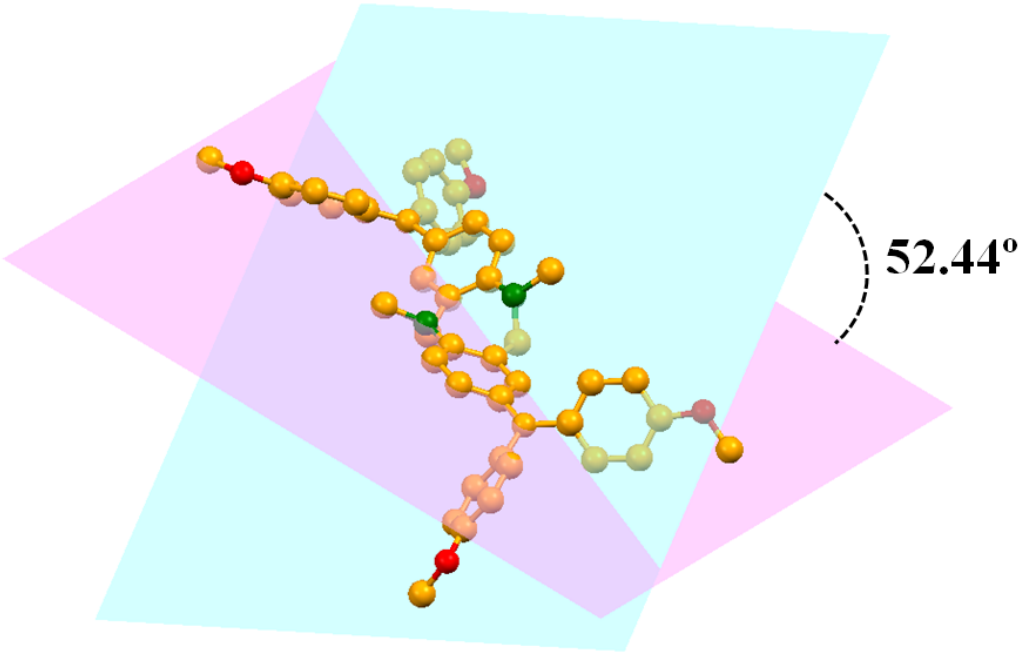


Figure S28. Interplanar angle between the aryl rings of N-o-N-Dz-6.

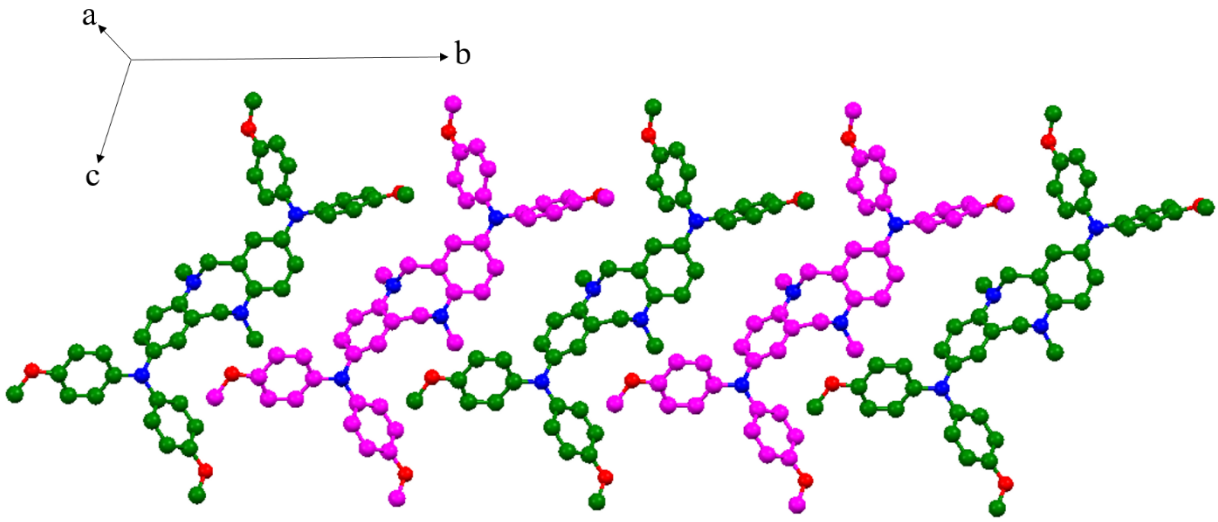


Figure S29. Packing of N-o-N-Dz-6 along b-axis and down c-axis

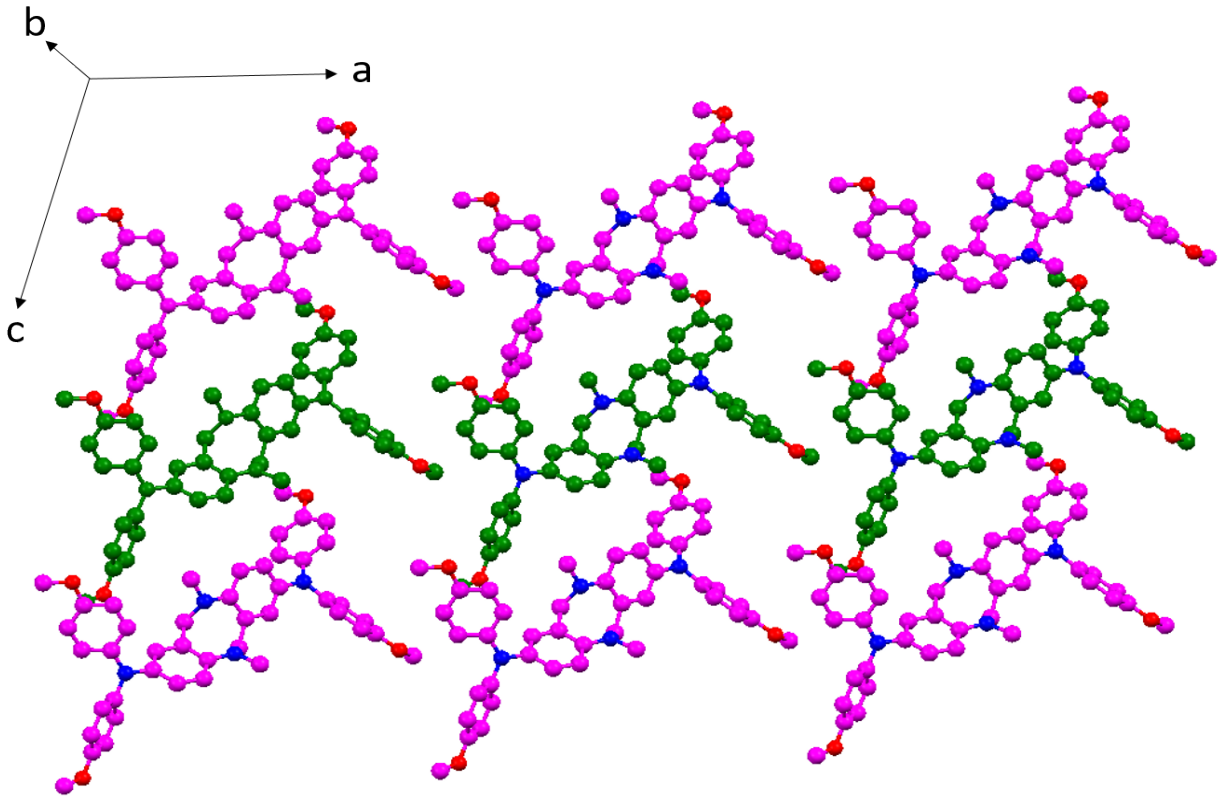


Figure S30. Packing of N-o-N-Dz-6 in ac plane

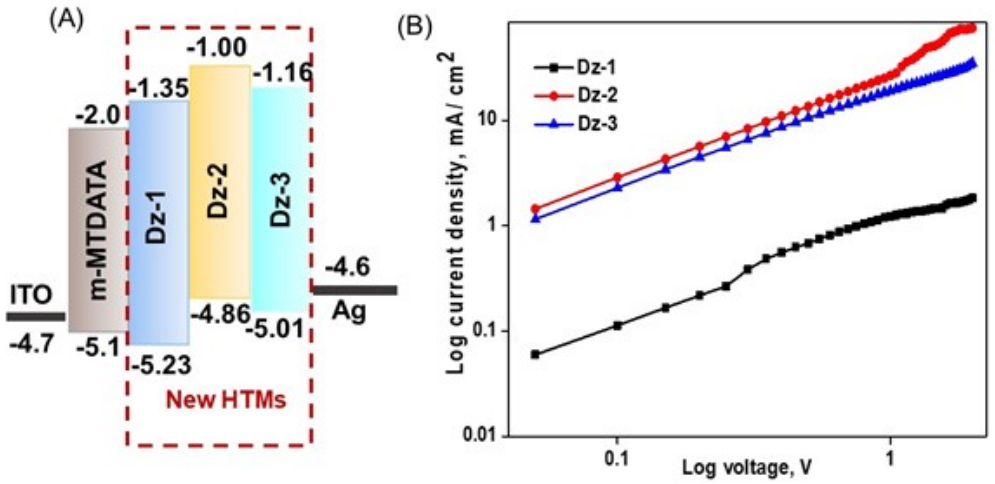


Figure 31. (A) The schematic representation of the single carrier device and (B) the J-V characteristics of the hole-only device.

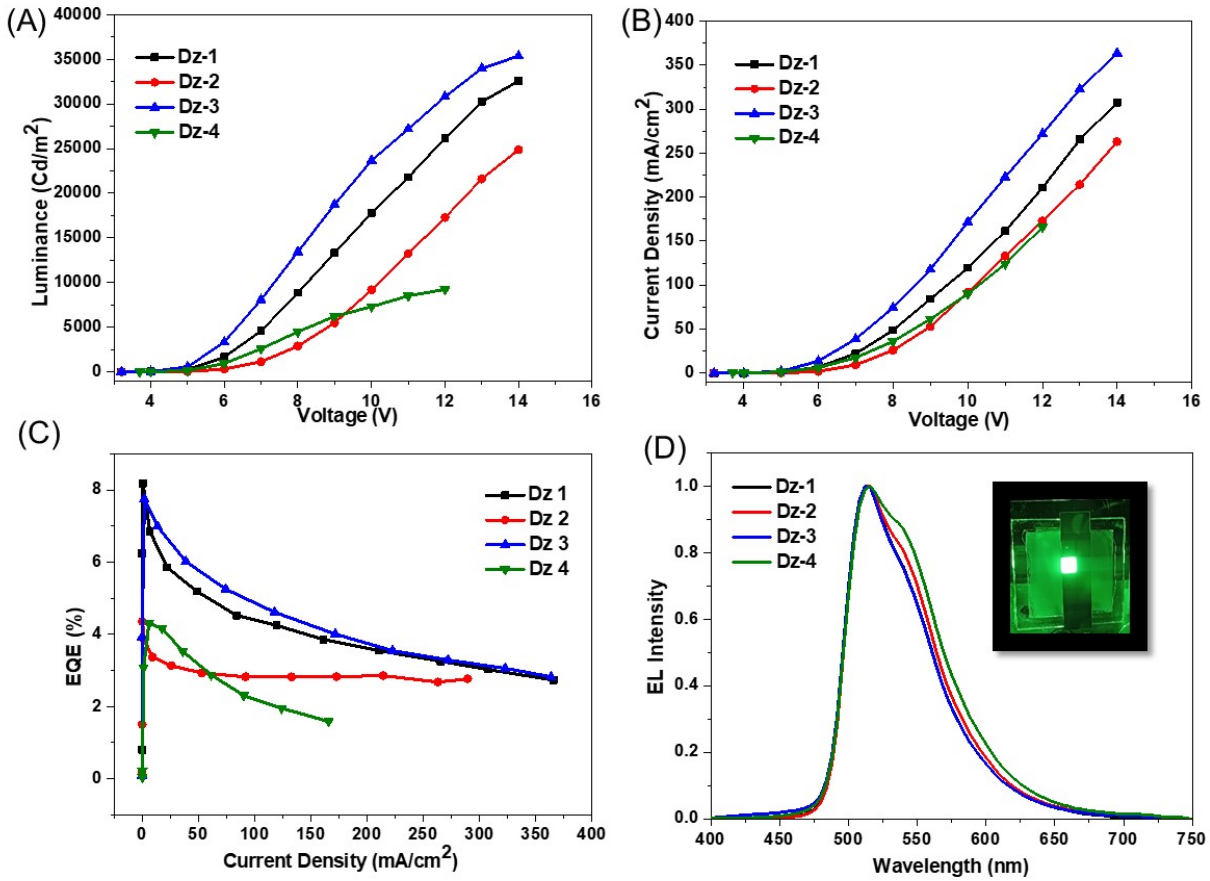


Figure S32. (A) Luminance vs. voltage graph; (B) current density vs. voltage; (C) Power efficiency vs. voltage; and (D) Current efficiency vs. voltage graph for devices employing Dz 1-4 as HTM.

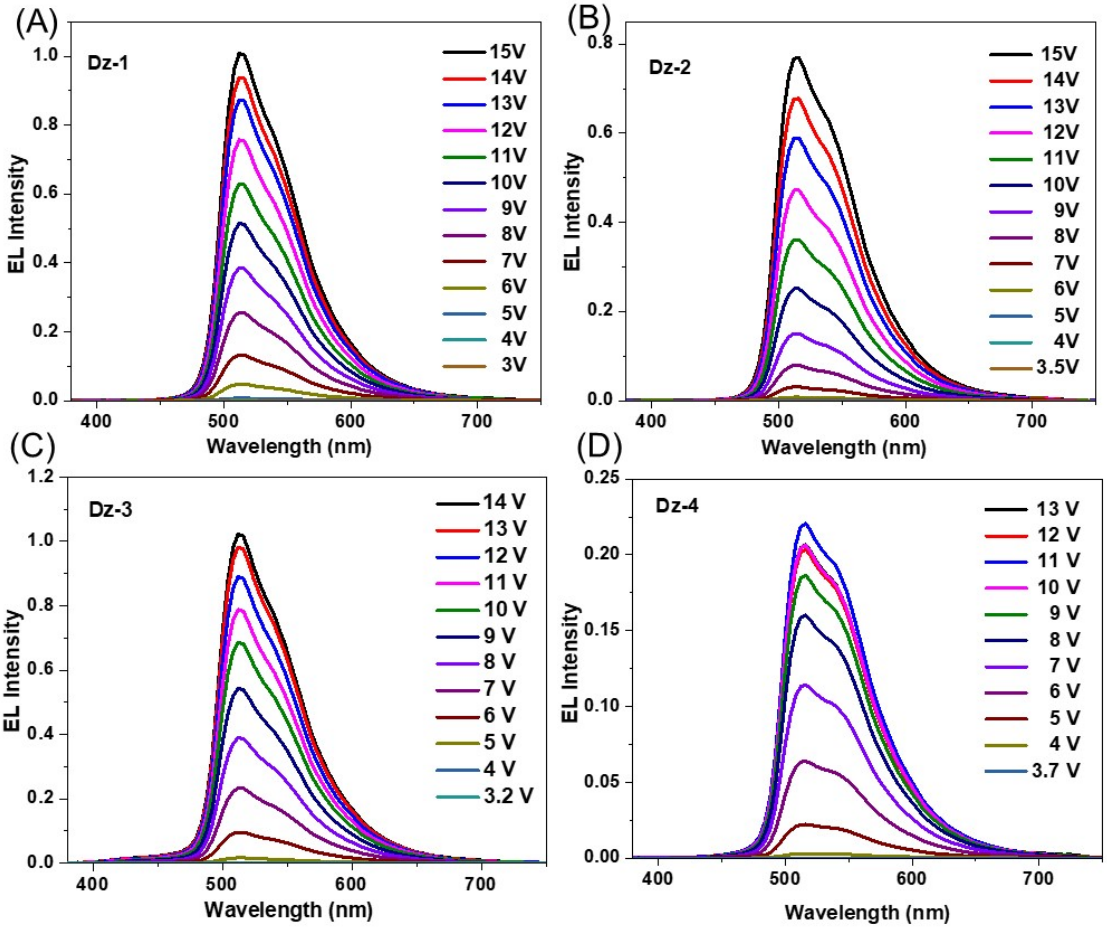


Figure S33. The EL spectra with increasing voltages for the OLED devices with (A)Dz-1; (B) Dz-2; (C) Dz-3; and (D) Dz-4 as HTMs.

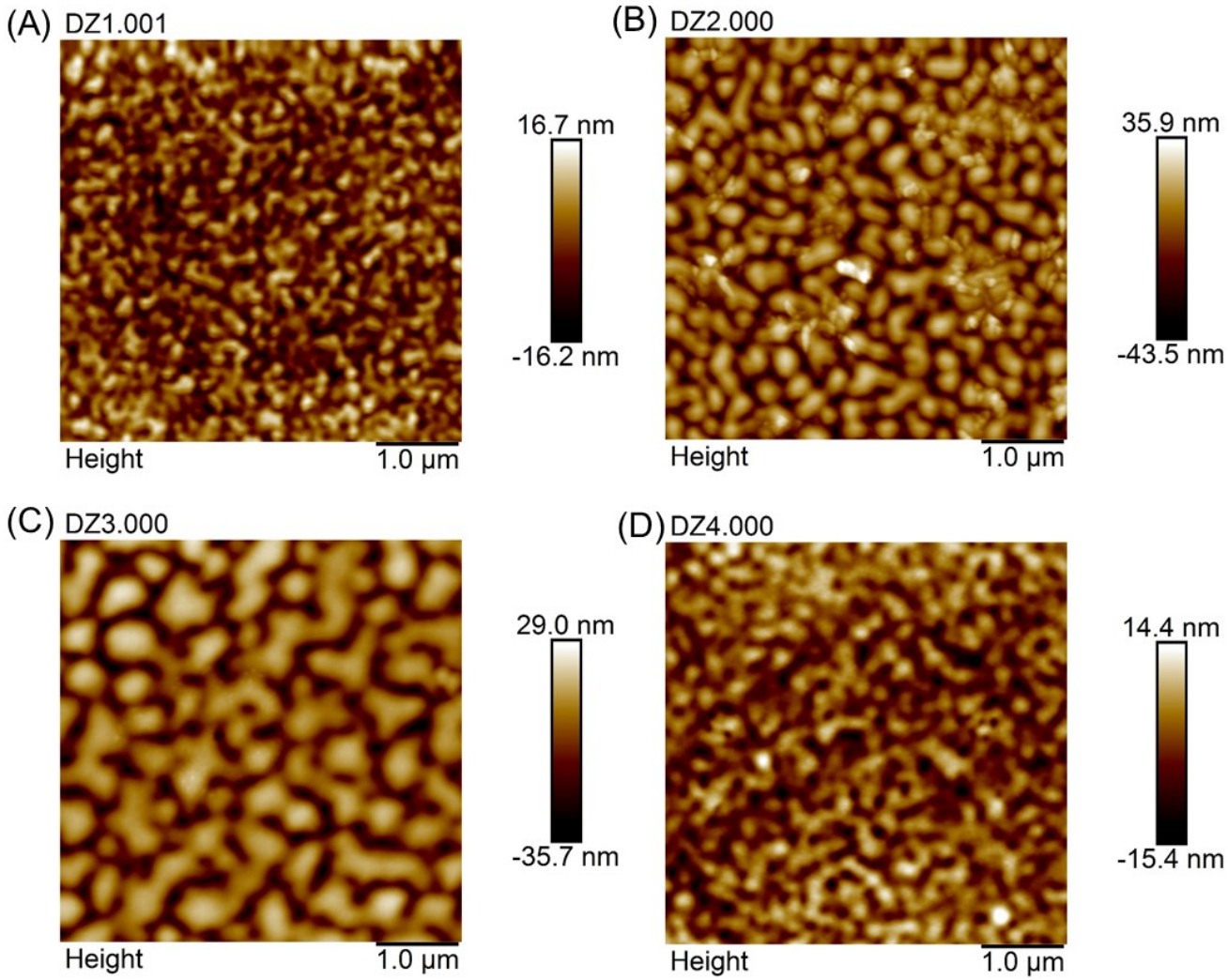


Figure S34. The AFM images of thermally evaporated films of (A)Dz-1; (B) Dz-2; (C) Dz-3; and (D) Dz-4.

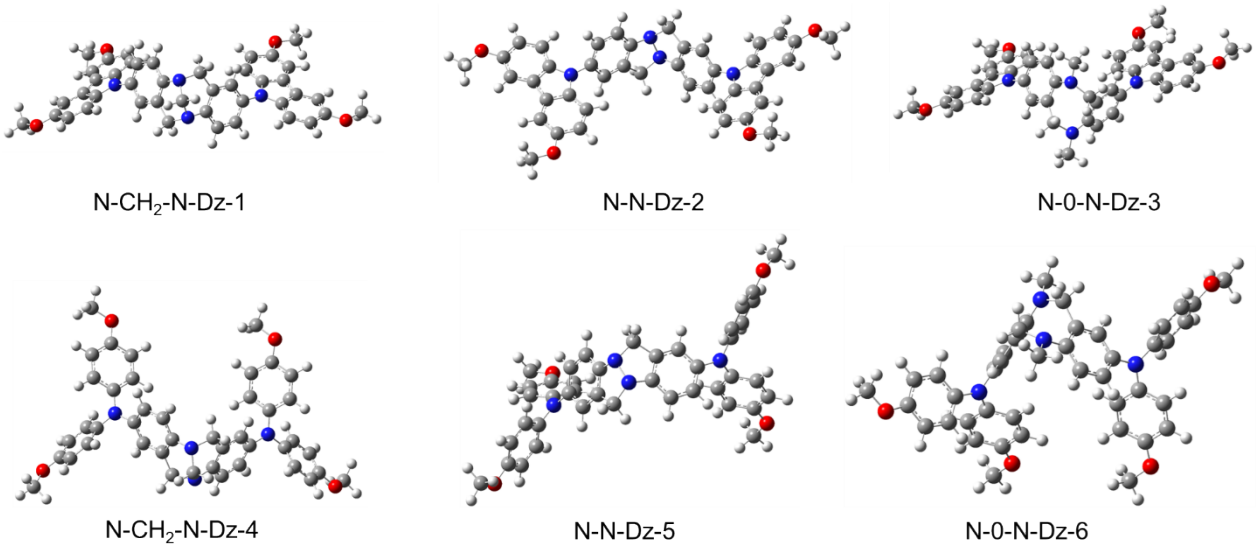


Figure S35. Optimized structures of Dzs obtained from DFT calculations.

Table S5: Energies of HOMO (E_{HOMO}), LUMO (E_{LUMO}), and HOMO-LUMO gap (ΔE_g) obtained from DFT calculations.

Dzs	E_{HOMO}(au)	E_{LUMO} (au)	ΔE_g(eV)
N-CH_2-N-Dz-1	-0.18949	-0.03934	4.09
N-N-Dz-2	-0.18812	-0.0391	4.06
N-0-N-Dz-3	-0.18473	-0.03595	4.05
N-CH_2-N-Dz-4	-0.1741	-0.03181	3.87
N-N-Dz-5	-0.16789	-0.0316	3.71
N-0-N-Dz-6	-0.16678	-0.0299	3.72

Table S6: Total electronic energies (E) and Gibbs free energies (G) of optimized structures of Dzs obtained from DFT calculations. The computed free energy includes thermal corrections to enthalpy, entropy, and zero-point energy.

Dzs	**E(au)**	**G(au)**
N-CH_2-N-Dz-1	-2180.261039	-2179.638956
N-N-Dz-2	-2140.918249	-2140.326972
N-0-N-Dz-3	-2220.769509	-2220.102902
N-CH_2-N-Dz-4	-2182.626158	-2181.967875
N-N-Dz-5	-2143.282222	-2142.654349
N-0-N-Dz-6	-2223.132471	-2222.429883

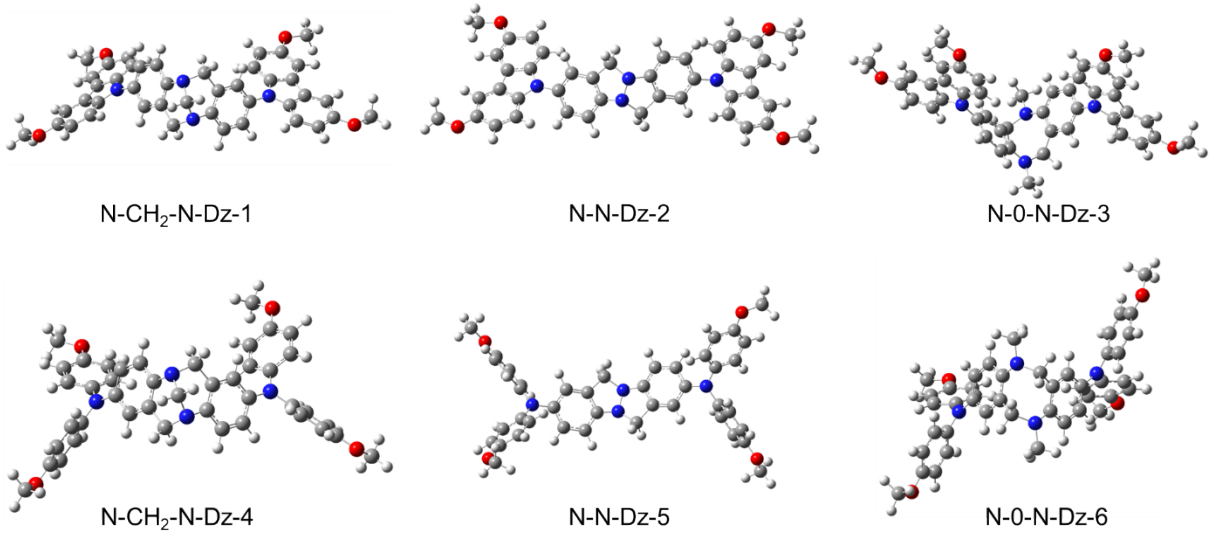


Figure S36. Optimized structures of the cations of Dzs obtained from DFT calculations.

Table S7. Total electronic energies of Dzs in the neutral molecule (E_A^0), the corresponding cation ($E_{A+}^{\ 0}$), the neutral molecule in the geometry of the cation (E_A^1), cation in the geometry of the neutral molecule ($E_{A+}^{\ 1}$), and the reorganization energy, λ_h.

Dzs	E_A^0 (au)	$E_{A+}^{\ 0}$ (au)	E_A^1 (au)	$E_{A+}^{\ 1}$ (au)	$\lambda_h\,(eV)$
N-CH_2-N-Dz-1	-2180.261039	-2180.039845	-2180.258504	-2180.037281	0.14
N-N-Dz-2	-2140.918249	-2140.701886	-2140.90743	-2140.69611	0.45
N-0-N-Dz-3	-2220.769509	-2220.552972	-2220.76627	-2220.549503	0.18
N-CH_2-N-Dz-4	-2182.626158	-2182.420197	-2182.623288	-2182.417244	0.16
N-N-Dz-5	-2143.282222	-2143.08714	-2143.267451	-2143.078906	0.63
N-0-N-Dz-6	-2223.132471	-2222.933368	-2223.128591	-2222.929304	0.22

Cartesian Coordinates

Table S8: Cartesian coordinates of all the optimized structures. The structure name with 'cation' in parentheses indicates the cation derived from the corresponding Dzs.

N-CH_2-N-Dz-1			
C	3.071	-1.947	-1.280

C	3.503	-1.259	-0.136
C	2.844	-1.465	1.078
C	1.751	-2.334	1.170
C	1.343	-3.049	0.026
C	2.012	-2.844	-1.190
N	0.270	-3.999	0.087
C	0.009	-4.411	1.468
N	-0.255	-3.254	2.326
C	-1.332	-2.462	1.805
C	-1.745	-2.583	0.463
C	-2.828	-1.821	0.010
C	-3.500	-0.941	0.862
C	-3.075	-0.813	2.193
C	-2.000	-1.567	2.653
C	1.011	-2.513	2.491
C	-0.999	-3.512	-0.489
N	4.600	-0.357	-0.213
N	-4.601	-0.180	0.384
C	4.564	1.010	0.083
C	5.855	1.560	-0.102
C	6.713	0.478	-0.531
C	5.907	-0.684	-0.588
C	-4.692	1.216	0.372
C	-5.939	1.597	-0.180
C	-6.636	0.376	-0.519
C	-5.784	-0.695	-0.158
C	3.485	1.814	0.472

C	3.719	3.166	0.689
C	5.006	3.725	0.521
C	6.080	2.931	0.121
C	8.081	0.409	-0.852
C	8.616	-0.824	-1.220
C	7.804	-1.980	-1.261
C	6.452	-1.924	-0.946
C	-3.759	2.179	0.778
C	-4.096	3.519	0.640
C	-5.342	3.912	0.102
C	-6.269	2.958	-0.315
C	-7.901	0.119	-1.078
C	-8.291	-1.206	-1.261
C	-7.437	-2.267	-0.884
C	-6.186	-2.026	-0.332
O	5.087	5.073	0.775
C	6.344	5.711	0.618
O	9.931	-1.032	-1.560
C	10.813	0.080	-1.540
O	-9.494	-1.597	-1.798
C	-10.411	-0.590	-2.194
O	-5.537	5.270	0.031
C	-6.763	5.745	-0.504
H	3.574	-1.782	-2.227
H	3.183	-0.927	1.960
H	1.695	-3.407	-2.063
H	-0.854	-5.082	1.477

H	0.876	-4.949	1.861
H	-3.141	-1.891	-1.029
H	-3.605	-0.145	2.864
H	-1.688	-1.498	3.692
H	1.636	-3.063	3.207
H	0.797	-1.538	2.938
H	-1.619	-4.384	-0.733
H	-0.789	-2.997	-1.431
H	2.490	1.402	0.597
H	2.913	3.825	0.991
H	7.070	3.347	-0.023
H	8.693	1.302	-0.806
H	8.267	-2.919	-1.545
H	5.844	-2.822	-0.977
H	-2.795	1.895	1.186
H	-3.403	4.297	0.942
H	-7.225	3.243	-0.739
H	-8.548	0.944	-1.352
H	-7.788	-3.283	-1.036
H	-5.546	-2.852	-0.040
H	6.180	6.761	0.866
H	7.096	5.290	1.298
H	6.707	5.635	-0.416
H	11.789	-0.306	-1.841
H	10.496	0.857	-2.248
H	10.889	0.514	-0.534
H	-11.283	-1.115	-2.586

H	-10.715	0.034	-1.343
H	-9.989	0.051	-2.980
H	-6.704	6.833	-0.466
H	-6.897	5.424	-1.546
H	-7.620	5.406	0.092

N-N-Dz-2			
C	3.163	-0.744	2.047
C	3.668	-0.923	0.752
C	3.008	-1.781	-0.146
C	1.862	-2.439	0.274
C	1.352	-2.241	1.564
C	1.999	-1.396	2.467
N	0.219	-3.055	1.789
N	-0.218	-3.513	0.450
C	-1.348	-2.728	0.127
C	-1.855	-2.088	1.266
C	-3.010	-1.324	1.197
C	-3.660	-1.183	-0.042
C	-3.148	-1.825	-1.178
C	-1.998	-2.617	-1.104
C	0.976	-3.448	-0.422
C	-0.974	-2.465	2.437
N	4.848	-0.242	0.345
N	-4.840	-0.395	-0.138
C	6.058	-0.841	-0.018
C	6.989	0.166	-0.373

C	6.312	1.434	-0.216
C	4.998	1.143	0.225
C	-6.119	-0.864	-0.452
C	-7.032	0.218	-0.427
C	-6.271	1.397	-0.079
C	-4.929	0.982	0.090
C	6.415	-2.195	-0.040
C	7.705	-2.527	-0.433
C	8.640	-1.533	-0.800
C	8.293	-0.183	-0.769
C	6.711	2.767	-0.422
C	5.785	3.782	-0.187
C	4.474	3.478	0.243
C	4.068	2.166	0.450
C	-6.549	-2.167	-0.737
C	-7.896	-2.368	-1.007
C	-8.816	-1.295	-0.995
C	-8.395	0.001	-0.704
C	-6.620	2.750	0.087
C	-5.617	3.660	0.417
C	-4.278	3.233	0.573
C	-3.922	1.901	0.411
O	9.875	-2.011	-1.169
C	10.872	-1.074	-1.545
O	6.043	5.123	-0.346
C	7.337	5.510	-0.780
O	-5.819	5.005	0.611

C	-7.135	5.514	0.465
O	-10.113	-1.645	-1.285
C	-11.098	-0.623	-1.291
H	3.694	-0.090	2.732
H	3.399	-1.909	-1.151
H	1.629	-1.256	3.478
H	-3.421	-0.836	2.076
H	-3.657	-1.698	-2.128
H	-1.625	-3.124	-1.989
H	0.685	-3.164	-1.437
H	1.446	-4.439	-0.463
H	-1.449	-3.221	3.074
H	-0.680	-1.621	3.066
H	5.711	-2.969	0.246
H	8.025	-3.564	-0.465
H	9.002	0.591	-1.039
H	7.717	2.984	-0.760
H	3.787	4.302	0.405
H	3.056	1.948	0.775
H	-5.856	-3.001	-0.745
H	-8.273	-3.360	-1.233
H	-9.089	0.832	-0.683
H	-7.649	3.064	-0.044
H	-3.531	3.980	0.821
H	-2.889	1.590	0.526
H	11.756	-1.662	-1.796
H	10.564	-0.489	-2.422

H	11.112	-0.390	-0.720
H	7.321	6.599	-0.837
H	8.111	5.195	-0.067
H	7.569	5.099	-1.772
H	-7.067	6.585	0.660
H	-7.517	5.354	-0.553
H	-7.826	5.057	1.186
H	-12.039	-1.115	-1.543
H	-11.190	-0.148	-0.305
H	-10.877	0.144	-2.045

N-o-N-Dz-3			
H	6.091	5.829	-0.450
H	5.736	5.646	1.296
H	5.105	7.054	0.397
H	-6.091	5.829	0.450
H	-5.736	5.646	-1.296
H	-5.106	7.054	-0.397
H	-9.852	0.785	-1.624
H	-10.209	0.975	0.120
H	-11.194	-0.127	-0.880
H	9.852	0.785	1.624
H	10.209	0.976	-0.121
H	11.195	-0.127	0.880
H	-1.292	-3.060	-3.480
H	-1.246	-4.824	-3.256

H	0.195	-3.981	-3.824
H	1.292	-3.060	3.480
H	1.246	-4.824	3.256
H	-0.195	-3.981	3.824
H	-7.982	1.511	-0.403
H	-7.820	-2.760	0.122
H	-5.378	-2.652	0.613
H	-1.747	1.616	0.859
H	-2.015	4.074	0.542
H	-6.218	3.594	-0.262
H	1.747	1.616	-0.859
H	2.015	4.074	-0.541
H	6.218	3.594	0.262
H	7.982	1.511	0.403
H	7.820	-2.759	-0.122
H	5.378	-2.652	-0.613
H	3.067	-2.099	0.970
H	2.558	-0.281	-2.874
H	0.710	-1.817	-3.361
H	-3.067	-2.099	-0.970
H	-2.558	-0.281	2.875
H	-0.710	-1.816	3.362
H	2.179	-4.252	1.303
H	1.028	-4.997	0.213
H	-2.179	-4.252	-1.303
H	-1.028	-4.997	-0.213
C	5.337	5.990	0.332

O	4.115	5.343	0.015
C	-5.337	5.990	-0.332
O	-4.115	5.343	-0.015
C	-10.190	0.266	-0.718
O	-9.373	-0.858	-0.428
C	10.190	0.266	0.717
O	9.373	-0.858	0.428
C	-0.663	-3.905	-3.150
C	0.663	-3.905	3.150
C	-7.424	0.607	-0.192
C	-8.039	-0.643	-0.177
C	-7.295	-1.810	0.113
C	-5.934	-1.750	0.383
C	-2.718	2.039	0.622
C	-2.866	3.408	0.444
C	-4.121	3.976	0.129
C	-5.251	3.173	-0.015
C	2.718	2.039	-0.622
C	2.866	3.408	-0.443
C	4.121	3.976	-0.129
C	5.250	3.173	0.015
C	7.424	0.607	0.191
C	8.039	-0.643	0.177
C	7.295	-1.810	-0.113
C	5.934	-1.750	-0.383
C	-3.852	1.228	0.487
C	-5.113	1.784	0.164

C	-6.045	0.681	0.081
C	-5.309	-0.496	0.358
C	3.852	1.228	-0.487
C	5.113	1.784	-0.164
C	6.045	0.681	-0.081
C	5.309	-0.496	-0.358
N	3.975	-0.160	-0.604
N	-3.975	-0.160	0.604
C	2.539	-2.044	0.022
C	2.923	-1.069	-0.905
C	2.263	-1.020	-2.135
C	1.222	-1.903	-2.411
C	-2.539	-2.044	-0.022
C	-2.923	-1.069	0.905
C	-2.263	-1.020	2.135
C	-1.222	-1.903	2.411
N	0.206	-3.792	1.772
C	1.254	-4.070	0.751
C	1.524	-2.964	-0.249
C	0.824	-2.887	-1.481
N	-0.206	-3.792	-1.772
C	-1.254	-4.070	-0.751
C	-1.524	-2.964	0.249
C	-0.824	-2.887	1.481

N-CH$_2$-N-Dz-4			
C	3.222	-2.032	-0.343

C	3.581	-0.901	0.416
C	2.841	-0.611	1.570
C	1.757	-1.402	1.963
C	1.424	-2.547	1.214
C	2.171	-2.846	0.065
N	0.352	-3.419	1.612
C	0.017	-3.222	3.024
N	-0.302	-1.820	3.309
C	-1.354	-1.350	2.449
C	-1.683	-2.021	1.256
C	-2.737	-1.549	0.466
C	-3.473	-0.413	0.830
C	-3.129	0.257	2.019
C	-2.085	-0.209	2.810
C	0.947	-1.040	3.203
C	-0.883	-3.244	0.823
N	4.664	-0.073	0.019
N	-4.541	0.052	0.017
H	3.780	-2.277	-1.239
H	3.102	0.264	2.160
H	1.919	-3.734	-0.506
H	-0.843	-3.850	3.271
H	0.864	-3.522	3.647
H	-2.981	-2.063	-0.460
H	-3.693	1.132	2.324
H	-1.844	0.293	3.743
H	1.539	-1.222	4.110

H	0.699	0.025	3.194
H	-1.490	-4.153	0.936
H	-0.619	-3.168	-0.236
C	-5.439	-0.875	-0.584
C	-5.816	-0.739	-1.933
C	-5.971	-1.943	0.148
C	-6.699	-1.636	-2.521
H	-5.412	0.081	-2.519
C	-6.844	-2.864	-0.442
H	-5.696	-2.063	1.191
C	-7.217	-2.710	-1.782
H	-6.989	-1.530	-3.562
H	-7.230	-3.679	0.159
C	-4.731	1.447	-0.186
C	-6.008	2.017	-0.127
C	-3.637	2.290	-0.462
C	-6.203	3.385	-0.347
H	-6.865	1.386	0.085
C	-3.820	3.653	-0.660
H	-2.639	1.867	-0.518
C	-5.105	4.213	-0.608
H	-7.209	3.785	-0.298
H	-2.976	4.302	-0.873
O	-8.070	-3.544	-2.456
C	-8.626	-4.649	-1.757
H	-9.261	-5.169	-2.477
H	-7.845	-5.334	-1.402

H	-9.236	-4.321	-0.906
O	-5.179	5.564	-0.828
C	-6.457	6.184	-0.789
H	-6.281	7.242	-0.992
H	-7.126	5.774	-1.557
H	-6.926	6.076	0.197
C	4.568	1.342	0.146
C	3.414	2.028	-0.250
C	5.639	2.087	0.672
C	3.314	3.417	-0.115
H	2.577	1.471	-0.661
C	5.557	3.470	0.789
H	6.543	1.574	0.986
C	4.391	4.147	0.401
H	2.401	3.909	-0.429
H	6.384	4.045	1.194
C	5.836	-0.648	-0.547
C	6.433	-0.093	-1.685
C	6.433	-1.784	0.033
C	7.599	-0.640	-2.232
H	5.989	0.783	-2.147
C	7.578	-2.346	-0.517
H	5.989	-2.226	0.918
C	8.175	-1.777	-1.653
H	8.033	-0.177	-3.110
H	8.037	-3.223	-0.071
O	4.405	5.507	0.566

O	9.307	-2.399	-2.110
C	3.251	6.245	0.189
H	3.479	7.289	0.407
H	3.037	6.136	-0.882
H	2.371	5.937	0.768
C	9.953	-1.865	-3.257
H	10.818	-2.505	-3.437
H	9.296	-1.888	-4.136
H	10.293	-0.836	-3.084

N-N-Dz-5			
H	4.725717	5.865513	-4.9004
H	-9.83141	-3.326	-1.65512
H	-8.67013	-3.79491	-2.93561
H	-10.271	-3.13829	-3.37516
H	7.196272	2.476418	-3.48858
H	3.133876	3.556829	-2.57139
H	2.953815	1.617172	-1.07887
H	5.807029	-2.66042	-0.02613
H	7.631165	-3.2082	1.566273
H	8.076788	0.973898	2.472895
H	-2.79435	1.894599	0.686265
H	-2.9725	4.086255	1.838715
H	-7.05813	3.203389	2.857219
H	-8.01693	0.609144	-2.70067
H	-7.59186	-3.27838	-0.90674
H	-5.74794	-2.43863	0.478486
H	6.250202	1.505963	0.923846
H	6.99698	0.497278	-2.00232
H	-6.86596	1.024713	1.746015
H	-6.12852	1.443562	-1.32039
H	-3.41855	-1.32243	-1.43156
H	-3.43122	-0.41098	2.773982

H	-1.409	-1.79408	3.115205
H	3.506346	-1.13946	1.563389
H	3.534816	-1.06517	-2.73902
H	1.469202	-2.42463	-2.81086
H	-0.80411	-2.57765	-2.14797
H	-1.57278	-4.00915	-1.43235
H	0.855364	-2.14768	2.502809
H	1.576502	-3.71416	2.080544
C	-6.19659	5.476759	3.66564
O	-5.00978	5.030805	3.0248
C	9.67873	-0.59095	3.716872
O	8.975629	-1.57629	2.973399
C	4.34025	5.12264	-4.20075
O	5.403211	4.205772	-3.98231
C	-9.45342	-3.07862	-2.65553
O	-8.9794	-1.74068	-2.71564
C	6.272816	2.27818	-2.95379
C	5.18898	3.151334	-3.13331
C	3.98909	2.900982	-2.45808
C	3.885838	1.796299	-1.60526
C	6.298843	-1.86702	0.527469
C	7.317986	-2.17957	1.418228
C	7.977157	-1.16502	2.129238
C	7.590747	0.166245	1.938258
C	-3.72467	2.179508	1.166936
C	-3.81805	3.406239	1.811964
C	-5.01757	3.79775	2.426095
C	-6.11798	2.934225	2.390274
C	-7.51219	-0.04829	-1.99988
C	-7.93599	-1.38262	-1.90237
C	-7.28729	-2.24349	-1.00993
C	-6.2367	-1.76543	-0.21854
C	5.89106	-0.53311	0.334079
C	6.548113	0.4708	1.055879
C	6.155062	1.171514	-2.12234
C	4.957741	0.913244	-1.42812

C	-4.82016	1.295278	1.132845
C	-6.00914	1.69062	1.757724
C	-6.45423	0.412572	-1.22646
C	-5.79916	-0.43913	-0.31653
N	-4.71791	0.038835	0.474807
N	4.843682	-0.21984	-0.57542
C	-2.97759	-1.42972	-0.44509
C	-3.55958	-0.76704	0.654748
C	-2.97901	-0.91525	1.926266
C	-1.83037	-1.6892	2.119997
C	3.058888	-1.42132	0.615084
C	3.657597	-1.00462	-0.59084
C	3.068109	-1.37936	-1.81116
C	1.895875	-2.13945	-1.85396
N	0.184219	-3.37237	-0.449
C	-1.05279	-3.07013	-1.20353
C	-1.84967	-2.21159	-0.24736
C	-1.26568	-2.33293	1.018687
N	-0.1632	-3.22538	0.987485
C	1.085399	-2.82155	1.672554
C	1.905137	-2.19035	0.569823
C	1.314133	-2.53743	-0.64951
H	3.46659	4.626283	-4.64279
H	4.042382	5.62126	-3.2693
H	10.41778	-1.13364	4.307852
H	10.19245	0.119469	3.056212
H	9.008039	-0.04146	4.390123
H	-5.9671	6.465812	4.064493
H	-7.03049	5.555831	2.956089
H	-6.48255	4.810349	4.48972

N-o-N-Dz-6			
H	2.457	7.272	-2.039
H	-9.660	-2.747	0.106

H	-8.774	-3.736	-1.096
H	-10.325	-2.969	-1.536
H	1.422	-2.712	3.408
H	1.353	-4.481	3.249
H	-0.064	-3.603	3.825
H	-1.349	-2.853	-3.447
H	-1.302	-4.614	-3.205
H	0.127	-3.780	-3.817
H	5.531	4.112	-2.440
H	1.555	3.964	-0.805
H	1.858	1.585	-0.282
H	5.325	-2.176	-1.405
H	7.430	-3.001	-0.380
H	7.545	0.477	2.149
H	-1.705	1.627	0.107
H	-1.396	4.048	0.564
H	-5.410	4.258	2.097
H	-7.532	0.393	-2.233
H	-7.346	-2.870	0.564
H	-5.225	-2.000	1.440
H	5.447	1.270	1.157
H	5.819	1.698	-1.939
H	-5.697	1.859	1.678
H	-5.370	1.250	-1.365
H	-3.062	-1.843	-0.926
H	-2.377	0.113	2.827
H	-0.545	-1.431	3.299

H	3.149	-1.854	0.848
H	2.490	-0.054	-2.987
H	0.633	-1.588	-3.390
H	-2.194	-3.992	-1.239
H	-1.026	-4.723	-0.155
H	2.244	-3.974	1.255
H	1.062	-4.731	0.205
C	-4.112	6.467	2.124
O	-3.098	5.650	1.557
C	9.491	-1.162	2.454
O	8.793	-1.870	1.441
C	2.283	6.251	-1.697
O	3.476	5.535	-1.987
C	-9.408	-2.850	-0.957
O	-8.780	-1.679	-1.458
C	0.775	-3.561	3.125
C	-0.713	-3.696	-3.123
C	4.734	3.548	-1.966
C	3.533	4.205	-1.659
C	2.494	3.486	-1.058
C	2.666	2.130	-0.758
C	5.807	-1.600	-0.622
C	6.984	-2.068	-0.051
C	7.632	-1.329	0.951
C	7.074	-0.118	1.375
C	-2.512	2.203	0.548
C	-2.334	3.557	0.803

C	-3.372	4.321	1.358
C	-4.588	3.700	1.663
C	-7.018	-0.121	-1.427
C	-7.590	-1.289	-0.900
C	-6.931	-1.968	0.131
C	-5.722	-1.472	0.633
C	5.227	-0.389	-0.197
C	5.876	0.335	0.811
C	4.889	2.196	-1.685
C	3.857	1.463	-1.069
C	-3.727	1.562	0.860
C	-4.753	2.331	1.425
C	-5.807	0.353	-0.939
C	-5.138	-0.313	0.107
N	-3.900	0.176	0.605
N	4.020	0.080	-0.781
C	-2.500	-1.752	-0.001
C	-2.846	-0.736	0.901
C	-2.131	-0.658	2.103
C	-1.091	-1.546	2.370
C	2.588	-1.794	-0.080
C	2.950	-0.825	-1.027
C	2.232	-0.789	-2.230
C	1.178	-1.670	-2.457
N	-0.221	-3.569	-1.759
C	-1.254	-3.808	-0.712
C	-1.487	-2.675	0.267

C	-0.742	-2.571	1.469
N	0.281	-3.493	1.758
C	1.308	-3.796	0.721
C	1.560	-2.712	-0.307
C	0.815	-2.650	-1.511
H	1.423	5.830	-2.233
H	2.072	6.259	-0.620
H	10.371	-1.763	2.687
H	9.810	-0.171	2.105
H	8.880	-1.048	3.359
H	-3.686	7.469	2.192
H	-5.007	6.496	1.489
H	-4.391	6.123	3.129

N-CH_2-N-Dz-1 (cation)			
C	3.070724	-1.9421	-1.17634
C	3.516765	-1.22465	-0.05435
C	2.852013	-1.36252	1.168052
C	1.747776	-2.21035	1.292242
C	1.326666	-2.96201	0.17347
C	1.989567	-2.80515	-1.05493
N	0.258046	-3.90401	0.276272
C	-0.008958	-4.258	1.671868
N	-0.274088	-3.05415	2.461212
C	-1.339867	-2.28801	1.896985
C	-1.766793	-2.49853	0.567584
C	-2.863841	-1.78328	0.080446
C	-3.525357	-0.84872	0.884485
C	-3.078665	-0.61578	2.194971
C	-1.996392	-1.3321	2.689763
C	0.996529	-2.32129	2.616203
C	-1.010201	-3.46946	-0.33654
N	4.637236	-0.35656	-0.16499
N	-4.641704	-0.13396	0.372671

C	4.65832	1.000027	0.169037
C	5.951649	1.518997	-0.08606
C	6.749405	0.417766	-0.60136
C	5.902126	-0.71726	-0.6353
C	-4.766825	1.256344	0.321414
C	-6.014925	1.587275	-0.26177
C	-6.674371	0.330123	-0.57817
C	-5.795089	-0.70377	-0.17166
C	3.622946	1.824052	0.633621
C	3.907051	3.160766	0.867081
C	5.199824	3.687297	0.635943
C	6.230834	2.867442	0.148977
C	8.083755	0.31539	-1.00157
C	8.556534	-0.93547	-1.43163
C	7.704064	-2.0655	-1.4432
C	6.380513	-1.97149	-1.04403
C	-3.85717	2.251477	0.708217
C	-4.224036	3.576081	0.528435
C	-5.474926	3.920766	-0.03624
C	-6.377609	2.92394	-0.44223
C	-7.915823	0.021432	-1.13883
C	-8.264835	-1.33179	-1.28224
C	-7.384509	-2.35447	-0.85503
C	-6.15261	-2.0547	-0.29553
O	5.337156	5.008719	0.910579
C	6.602182	5.637612	0.704609
O	9.82398	-1.17156	-1.85031
C	10.766689	-0.09957	-1.86989
O	-9.433323	-1.7683	-1.81286
C	-10.39847	-0.81637	-2.26104
O	-5.703975	5.252608	-0.1496
C	-6.938031	5.705496	-0.70681
H	3.571317	-1.82017	-2.13099
H	3.202091	-0.80244	2.031312
H	1.659739	-3.38929	-1.90872
H	-0.872855	-4.9257	1.708087
H	0.853529	-4.7769	2.096332
H	-3.185591	-1.92098	-0.94864
H	-3.606867	0.088225	2.829332
H	-1.678196	-1.19574	3.718809
H	1.606462	-2.84741	3.361268

H	0.790361	-1.32541	3.017599
H	-1.617994	-4.36103	-0.53607
H	-0.802093	-3.00009	-1.30178
H	2.623593	1.438261	0.799945
H	3.14053	3.837508	1.228222
H	7.218884	3.264699	-0.04903
H	8.733384	1.181598	-0.97097
H	8.120124	-3.01233	-1.7692
H	5.744356	-2.84925	-1.0444
H	-2.891044	2.002135	1.132025
H	-3.556988	4.381676	0.814748
H	-7.330798	3.177482	-0.88989
H	-8.590492	0.81128	-1.44579
H	-7.706483	-3.38333	-0.97181
H	-5.496032	-2.84821	0.042714
H	6.463058	6.678588	0.994835
H	7.375902	5.182424	1.333792
H	6.900103	5.588318	-0.34924
H	11.695089	-0.53243	-2.24113
H	10.43987	0.700245	-2.54457
H	10.9273	0.302285	-0.86269
H	-11.235287	-1.40306	-2.6387
H	-10.739529	-0.18227	-1.43444
H	-9.993509	-0.19446	-3.06786
H	-6.887439	6.793689	-0.68582
H	-7.051722	5.364373	-1.74242
H	-7.789702	5.366846	-0.10548

N-N-Dz-2 (cation)			
C	3.622206	0.467028	1.831686
C	4.152078	-0.22798	0.726102
C	3.334228	-1.12372	0.000088
C	2.022257	-1.29728	0.395134
C	1.506913	-0.59779	1.503149
C	2.301055	0.290232	2.235244
N	0.195118	-0.97745	1.734991
N	-0.21642	-1.84964	0.695262
C	-1.51625	-1.53263	0.336912
C	-2.02357	-0.53705	1.193142
C	-3.33366	-0.11162	1.081509
C	-4.151	-0.6779	0.078634

C	-3.62396	-1.66312	-0.78237
C	-2.31183	-2.11042	-0.6579
C	0.926037	-2.16989	-0.18176
C	-0.93691	-0.13449	2.168035
N	5.488847	-0.02952	0.34233
N	-5.48421	-0.25719	-0.06437
C	6.419898	-1.04045	0.041748
C	7.64814	-0.44226	-0.32013
C	7.45865	0.99558	-0.24187
C	6.123973	1.214461	0.167653
C	-6.60421	-1.09698	-0.20854
C	-7.76433	-0.29948	-0.33199
C	-7.33576	1.086192	-0.26465
C	-5.9324	1.076787	-0.09869
C	6.29449	-2.43336	0.129767
C	7.397682	-3.21283	-0.18848
C	8.623442	-2.62638	-0.57854
C	8.758681	-1.23372	-0.6364
C	8.306311	2.076622	-0.51177
C	7.797148	3.373723	-0.37367
C	6.45227	3.579576	0.010083
C	5.60661	2.511994	0.276683
C	-6.69139	-2.4952	-0.16864
C	-7.94434	-3.07782	-0.29555
C	-9.10899	-2.29094	-0.44762
C	-9.02627	-0.89333	-0.45595
C	-8.03301	2.296672	-0.36155
C	-7.30679	3.491814	-0.29839
C	-5.90024	3.469642	-0.1611
C	-5.20341	2.272879	-0.06703
O	9.616155	-3.50983	-0.86605
C	10.89487	-3.01154	-1.25356
O	8.510453	4.509694	-0.59687
C	9.875648	4.402039	-0.99424
O	-7.85685	4.733806	-0.37263
C	-9.26925	4.855376	-0.52513
O	-10.266	-2.9956	-0.56624
C	-11.4946	-2.28747	-0.71372
H	4.269557	1.125429	2.399797
H	3.731831	-1.62821	-0.87408
H	1.918505	0.807024	3.108826

H	-3.74472	0.629509	1.758473
H	-4.25103	-2.06299	-1.57106
H	-1.92424	-2.87523	-1.32251
H	0.677773	-1.93347	-1.22409
H	1.164642	-3.23824	-0.11554
H	-1.19775	-0.35895	3.2093
H	-0.66222	0.925697	2.100054
H	5.37375	-2.90636	0.451692
H	7.345424	-4.29477	-0.13507
H	9.698939	-0.76936	-0.90747
H	9.327321	1.902304	-0.82858
H	6.095172	4.600839	0.085367
H	4.573836	2.696084	0.549476
H	-5.81699	-3.12052	-0.02981
H	-8.05799	-4.15612	-0.2729
H	-9.91211	-0.2764	-0.54492
H	-9.10814	2.296324	-0.49318
H	-5.37607	4.418856	-0.13922
H	-4.12237	2.283132	0.012244
H	11.51248	-3.8916	-1.43157
H	10.82683	-2.42038	-2.17471
H	11.34233	-2.40685	-0.45563
H	10.23203	5.425944	-1.10501
H	10.47107	3.888535	-0.22979
H	9.968792	3.877415	-1.95278
H	-9.47151	5.925823	-0.55619
H	-9.60783	4.392708	-1.46002
H	-9.79934	4.407892	0.324257
H	-12.2675	-3.05159	-0.7938
H	-11.695	-1.65586	0.160167
H	-11.4914	-1.67418	-1.62287

N-o-N-Dz-3 (cation)			
H	6.455896	5.691156	-1.16423
H	5.948835	5.787344	0.555033
H	5.462021	7.061171	-0.59671
H	-6.4559	5.691156	1.164229
H	-5.94884	5.787344	-0.55503
H	-5.46202	7.06117	0.596712
H	-9.74243	0.815492	-1.95716
H	-10.2583	0.736035	-0.23952

H	-11.0724	-0.27049	-1.46851
H	9.742431	0.815493	1.957155
H	10.2583	0.736036	0.239522
H	11.07236	-0.27049	1.468506
H	-1.33206	-2.99754	-3.49336
H	-1.27533	-4.75612	-3.23699
H	0.157048	-3.91857	-3.82922
H	1.332063	-2.99753	3.493358
H	1.275336	-4.75611	3.236991
H	-0.15705	-3.91857	3.829219
H	-8.0156	1.45344	-0.46932
H	-7.66013	-2.84262	-0.51084
H	-5.28669	-2.69811	0.221836
H	-1.92406	1.662893	1.361446
H	-2.3072	4.122389	1.368472
H	-6.39402	3.567419	0.112571
H	1.924059	1.662892	-1.36145
H	2.307195	4.122389	-1.36847
H	6.394015	3.567419	-0.11257
H	8.0156	1.453441	0.469318
H	7.660125	-2.84262	0.510842
H	5.286691	-2.69811	-0.22184
H	3.099062	-2.07981	0.93087
H	2.600985	-0.2749	-2.93209
H	0.736258	-1.78163	-3.40035
H	-3.09906	-2.07981	-0.93087
H	-2.60099	-0.2749	2.932088
H	-0.73626	-1.78163	3.400355
H	2.179779	-4.20926	1.277899
H	0.99609	-4.93765	0.219294
H	-2.17978	-4.20926	-1.2779
H	-0.99609	-4.93765	-0.21929
C	5.654416	5.994897	-0.48058
O	4.42703	5.344387	-0.80653
C	-5.65442	5.994897	0.480574
O	-4.42703	5.344387	0.806525
C	-10.1196	0.160811	-1.16256
O	-9.24579	-0.94707	-0.95105
C	10.11959	0.160812	1.16256
O	9.245786	-0.94707	0.951044
C	-0.69786	-3.83234	-3.15509

C	0.69786	-3.83234	3.155088
C	-7.42117	0.557186	-0.34015
C	-7.96745	-0.71689	-0.55565
C	-7.18734	-1.87954	-0.35265
C	-5.86256	-1.79622	0.048273
C	-2.89713	2.067435	1.107165
C	-3.10671	3.4382	1.106226
C	-4.36356	3.988492	0.761255
C	-5.43298	3.156556	0.397006
C	2.897133	2.067435	-1.10716
C	3.106709	3.4382	-1.10623
C	4.363562	3.988492	-0.76126
C	5.432981	3.156557	-0.39701
C	7.421167	0.557187	0.340144
C	7.967452	-0.71689	0.555648
C	7.187341	-1.87954	0.352652
C	5.862558	-1.79622	-0.04827
C	-3.97256	1.234358	0.766112
C	-5.22974	1.773396	0.399881
C	-6.08494	0.648062	0.061351
C	-5.3079	-0.52223	0.237997
C	3.972556	1.234358	-0.76611
C	5.229735	1.773397	-0.39988
C	6.084943	0.648063	-0.06135
C	5.307901	-0.52223	-0.238
N	4.024668	-0.15972	-0.6635
N	-4.02467	-0.15972	0.663495
C	2.568664	-2.01694	-0.01474
C	2.958669	-1.04884	-0.94884
C	2.291615	-0.99337	-2.18014
C	1.243558	-1.86332	-2.44714
C	-2.56866	-2.01694	0.014744
C	-2.95867	-1.04884	0.948835
C	-2.29162	-0.99337	2.180144
C	-1.24356	-1.86332	2.447137
N	0.237626	-3.68427	1.777656
C	1.251594	-4.00885	0.738494
C	1.531461	-2.91339	-0.27097
C	0.821109	-2.82768	-1.50153
N	-0.23763	-3.68427	-1.77766
C	-1.25159	-4.00885	-0.73849

C	-1.53146	-2.91339	0.270966
C	-0.82111	-2.82768	1.501526

N-CH_2-N-Dz-4 (cation)			
C	3.16839	-1.97262	-0.34373
C	3.591864	-0.85052	0.403007
C	2.859181	-0.48517	1.54628
C	1.747184	-1.21834	1.958976
C	1.365736	-2.37223	1.236762
C	2.076242	-2.71586	0.072705
N	0.304822	-3.21245	1.687985
C	-0.0198	-2.95602	3.091251
N	-0.32427	-1.53802	3.283977
C	-1.36149	-1.10568	2.404799
C	-1.74186	-1.87607	1.282143
C	-2.82566	-1.47071	0.505627
C	-3.53737	-0.29438	0.801697
C	-3.12245	0.492964	1.897074
C	-2.05216	0.088643	2.679056
C	0.936225	-0.77935	3.175911
C	-0.93933	-3.11988	0.90314
N	4.720943	-0.10747	-0.00117
N	-4.63682	0.096372	0.009074
H	3.708126	-2.25793	-1.23953
H	3.159786	0.391052	2.113164
H	1.777487	-3.59848	-0.48499
H	-0.88196	-3.56503	3.372975
H	0.826927	-3.22681	3.726133
H	-3.10611	-2.05147	-0.36875
H	-3.66892	1.395055	2.148921
H	-1.77389	0.666096	3.555546
H	1.50962	-0.93234	4.09875
H	0.708666	0.287949	3.111575
H	-1.52871	-4.02799	1.081843
H	-0.693	-3.09903	-0.16169
C	-5.52931	-0.88131	-0.50807
C	-5.9743	-0.80633	-1.84366
C	-5.99113	-1.92978	0.301987
C	-6.85139	-1.75304	-2.34683
H	-5.61981	-0.00493	-2.48325
C	-6.8698	-2.88916	-0.19978

H	-5.67162	-1.9886	1.337292
C	-7.30894	-2.80579	-1.53132
H	-7.19223	-1.70782	-3.37571
H	-7.2164	-3.6797	0.454509
C	-4.85914	1.468404	-0.28372
C	-6.15516	2.004528	-0.24298
C	-3.78529	2.312926	-0.63161
C	-6.38509	3.34723	-0.53942
H	-6.99015	1.368327	0.030845
C	-4.0064	3.649735	-0.92029
H	-2.78013	1.908259	-0.68571
C	-5.30862	4.182879	-0.8778
H	-7.39686	3.730697	-0.49117
H	-3.18747	4.304151	-1.19957
O	-8.16313	-3.67752	-2.11954
C	-8.67929	-4.76978	-1.35727
H	-9.3308	-5.31894	-2.03634
H	-7.87224	-5.4266	-1.01254
H	-9.26155	-4.41235	-0.50023
O	-5.41647	5.499937	-1.17983
C	-6.70777	6.111564	-1.17278
H	-6.54091	7.151828	-1.45072
H	-7.37196	5.638557	-1.90514
H	-7.15993	6.067137	-0.17535
C	4.759595	1.303037	0.175764
C	3.659742	2.100958	-0.17068
C	5.915667	1.923551	0.690384
C	3.698355	3.485586	-0.00414
H	2.77092	1.637116	-0.58608
C	5.962836	3.298314	0.853531
H	6.770978	1.316855	0.968472
C	4.854786	4.095116	0.508551
H	2.836756	4.075723	-0.29171
H	6.845299	3.782922	1.257516
C	5.837028	-0.76113	-0.58869
C	6.48503	-0.20284	-1.70101
C	6.323964	-1.97205	-0.05424
C	7.591502	-0.828	-2.27392
H	6.116813	0.724842	-2.12634
C	7.418124	-2.60196	-0.62317
H	5.84588	-2.40602	0.817572

C	8.065233	-2.03736	-1.7394
H	8.065377	-0.3742	-3.13565
H	7.806055	-3.52771	-0.21174
O	5.003934	5.428086	0.706436
O	9.126849	-2.73004	-2.21638
C	3.928756	6.306186	0.374494
H	4.281819	7.307778	0.618482
H	3.690429	6.252642	-0.69421
H	3.035193	6.078668	0.967705
C	9.848403	-2.21612	-3.33731
H	10.64791	-2.93237	-3.52418
H	9.205133	-2.14623	-4.222
H	10.28071	-1.23468	-3.11118

N-N-Dz-5(cation)			
H	-8.78346	-5.3116	4.228616
H	9.030958	-4.28692	-3.05819
H	7.562176	-5.28416	-2.79961
H	9.159923	-5.88965	-2.28328
H	-9.15761	-3.01567	0.484492
H	-6.05306	-3.0089	3.4686
H	-4.82271	-1.3108	2.184965
H	-5.70156	0.862416	-2.61515
H	-6.9545	2.909779	-3.26162
H	-8.27476	3.372622	0.810716
H	4.652068	1.425464	2.249727
H	5.861065	3.184615	3.523899
H	9.114475	2.967782	0.711696
H	8.138727	-3.39983	1.207868
H	7.057495	-2.97624	-2.93882
H	5.806147	-0.92861	-2.40356
H	-7.01735	1.358837	1.448423
H	-7.89961	-1.31029	-0.81828
H	7.905584	1.243079	-0.55568
H	6.85709	-1.33643	1.745613
H	3.731985	-1.76398	-0.37952
H	4.292985	2.518831	-0.48496
H	1.956311	2.845948	-1.19605
H	-3.7583	1.740194	-0.55617
H	-4.32078	-2.54372	-0.50722
H	-1.96393	-2.89855	-1.13272

H	0.66077	-2.17991	-0.3253
H	1.164053	-2.26151	-2.03088
H	-0.68766	2.157182	-0.4284
H	-1.14639	2.173256	-2.14842
C	9.426021	4.648395	2.627371
O	8.131804	4.16008	2.978765
C	-9.13727	5.145503	-0.83429
O	-8.34081	4.381826	-1.73949
C	-8.01492	-4.60163	3.923694
O	-8.46169	-4.06013	2.681949
C	8.538155	-5.00072	-2.38757
O	8.407049	-4.46582	-1.0716
C	-8.20628	-2.63548	0.841315
C	-7.69447	-3.13182	2.053654
C	-6.46491	-2.65471	2.531435
C	-5.76503	-1.69026	1.801491
C	-6.24902	1.424549	-1.8648
C	-6.94743	2.565683	-2.2327
C	-7.6867	3.285197	-1.27645
C	-7.71105	2.841143	0.053792
C	5.620773	1.776157	1.907278
C	6.290494	2.757812	2.623625
C	7.557604	3.202398	2.205342
C	8.139181	2.646613	1.056367
C	7.618022	-2.85146	0.42998
C	7.68006	-3.33271	-0.8901
C	7.014008	-2.63787	-1.9107
C	6.301522	-1.47484	-1.60647
C	-6.25721	0.98145	-0.52969
C	-6.99497	1.69816	0.417734
C	-7.49918	-1.6861	0.117825
C	-6.26612	-1.20399	0.589801
C	6.191565	1.225056	0.746108
C	7.452237	1.667717	0.334324
C	6.899549	-1.7016	0.724463
C	6.228941	-1.00012	-0.29261
N	5.510491	0.199907	0.013733
N	-5.55353	-0.20638	-0.15136
C	3.343116	-0.76901	-0.56452
C	4.185063	0.361434	-0.38345
C	3.649362	1.6561	-0.60773

C	2.330409	1.846249	-1.00148
C	-3.36543	0.738518	-0.68892
C	-4.21443	-0.38384	-0.49099
C	-3.67268	-1.68655	-0.64436
C	-2.34274	-1.89193	-0.98977
N	-0.20262	-0.70703	-1.57568
C	0.927331	-1.58052	-1.20485
C	2.031766	-0.5762	-0.94438
C	1.52147	0.717177	-1.1627
N	0.206946	0.637514	-1.59844
C	-0.93168	1.524538	-1.29108
C	-2.04346	0.530983	-1.02132
C	-1.52828	-0.76987	-1.17322
H	-7.05905	-5.12616	3.806407
H	-7.91794	-3.81896	4.685472
H	-9.56564	5.952412	-1.42845
H	-9.94369	4.537721	-0.40749
H	-8.52576	5.569672	-0.02908
H	9.676041	5.390408	3.385368
H	10.17051	3.843765	2.643849
H	9.41517	5.124387	1.639736

N-o-N-Dz-6 (cation)			
H	3.58655	7.004816	-3.41747
H	-9.56923	-2.73357	-0.95178
H	-8.49916	-3.60203	-2.10055
H	-9.97122	-2.78241	-2.6902
H	1.414215	-2.57176	3.467341
H	1.36515	-4.33879	3.275127
H	-0.05876	-3.48991	3.873957
H	-1.38387	-2.68176	-3.4302
H	-1.36092	-4.43991	-3.16607
H	0.075035	-3.63787	-3.79943
H	6.247425	3.527099	-2.92836
H	2.150483	4.098276	-1.72995
H	2.109088	1.830026	-0.7868
H	5.385927	-2.30588	-1.0119
H	7.332451	-3.06524	0.331642
H	7.290448	0.66585	2.482904
H	-1.93592	1.86144	0.635432
H	-1.92126	4.206148	1.457985

H	-6.05498	3.820398	2.598517
H	-7.18301	0.63104	-2.62411
H	-7.33777	-2.89793	-0.16029
H	-5.38617	-2.10336	1.102653
H	5.35479	1.405994	1.164359
H	6.196765	1.228951	-1.98941
H	-6.06005	1.498432	1.805903
H	-5.19915	1.423575	-1.35284
H	-3.12003	-1.80148	-0.86439
H	-2.52574	0.112457	2.936777
H	-0.66322	-1.37902	3.39916
H	3.168374	-1.82249	0.869316
H	2.617113	-0.06019	-3.01239
H	0.724037	-1.52954	-3.41223
H	-2.19129	-3.91384	-1.19373
H	-0.98233	-4.6167	-0.14714
H	2.205103	-3.89909	1.282952
H	0.989013	-4.62563	0.262172
C	-4.99412	6.114272	3.062245
O	-3.85775	5.461723	2.495129
C	9.142388	-0.98031	3.166209
O	8.502055	-1.77518	2.167696
C	3.238979	6.096389	-2.9261
O	4.349861	5.200854	-2.94267
C	-9.15693	-2.73487	-1.96756
O	-8.46671	-1.51687	-2.2449
C	0.778288	-3.42278	3.175787
C	-0.76049	-3.52944	-3.10478
C	5.350742	3.141721	-2.45478
C	4.211663	3.966445	-2.3974
C	3.038291	3.481524	-1.79894
C	3.013585	2.192648	-1.26427
C	5.793384	-1.66634	-0.23557
C	6.880458	-2.09521	0.509901
C	7.4382	-1.26378	1.499279
C	6.883547	0.005262	1.727087
C	-2.83063	2.288895	1.076006
C	-2.81665	3.597915	1.53194
C	-3.97575	4.172893	2.084636
C	-5.14838	3.407415	2.173425
C	-6.77678	0.043925	-1.80724

C	-7.39145	-1.18079	-1.48747
C	-6.87657	-1.95809	-0.43853
C	-5.76676	-1.50764	0.278994
C	5.224828	-0.39764	-0.00714
C	5.783379	0.426458	0.978982
C	5.316467	1.860168	-1.92963
C	4.143421	1.364864	-1.32594
C	-4.00076	1.509222	1.169958
C	-5.15229	2.086823	1.72306
C	-5.66986	0.48031	-1.09548
C	-5.14787	-0.29174	-0.03992
N	-4.01874	0.168157	0.697912
N	4.115971	0.051385	-0.7803
C	-2.56362	-1.69899	0.061707
C	-2.94785	-0.70224	0.977997
C	-2.24371	-0.62708	2.195532
C	-1.18983	-1.48761	2.459021
C	2.614505	-1.74726	-0.06071
C	3.021211	-0.7992	-1.01917
C	2.318171	-0.76001	-2.24005
C	1.247627	-1.60849	-2.46754
N	-0.26307	-3.3835	-1.73979
C	-1.25561	-3.69816	-0.6745
C	-1.52185	-2.58633	0.318878
C	-0.78329	-2.47611	1.53106
N	0.282147	-3.32592	1.806311
C	1.27201	-3.69128	0.755831
C	1.555004	-2.62272	-0.28033
C	0.819105	-2.54822	-1.49805
H	2.389027	5.682438	-3.48142
H	2.93461	6.330062	-1.89905
H	9.963174	-1.58922	3.544261
H	9.54119	-0.05366	2.737447
H	8.453799	-0.745	3.986197
H	-4.66198	7.122826	3.307303
H	-5.82019	6.165566	2.343407
H	-5.32655	5.606869	3.975335

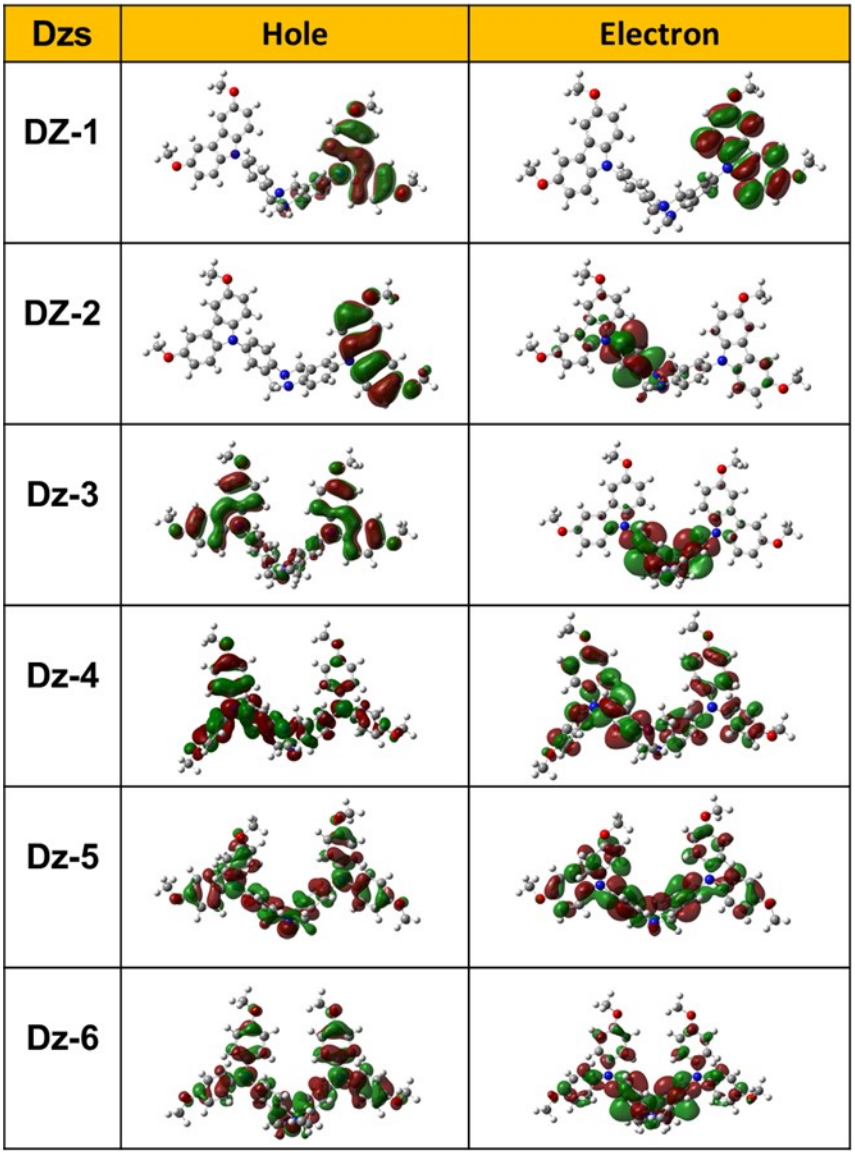


Figure S37. The hole and electron NTOs for Dz-1 - Dz-6 for the singlet excited state with the highest oscillator strength (isovalue=0.02 au).The Multiwfn program was used to perform the NTO analysis.[6-7]

Table S9. Excitation wavelength and the oscillator strength for the first excited state ($^{S}1$).

Dzs	Excitation wavelength, λ_{max} (nm)	Oscillator strength (f)
Dz-1	350	0.048
Dz-2	351	0.032
Dz-3	353	0.067
Dz-4	380	0.045
Dz5	395	0.068
Dz-6	393	0.008

Table S10. The excitation wavelength and the oscillator strength for the excited state correspond to the highest oscillator strength. The TD-DFT calculation was performed for a 40 singlet excited states (TD (nstates=40) keyword was used in Gaussian TD-DFT calculations).

Dzs	State	Excitation wavelength, λ_{max} (nm)	Oscillator strength (f)
Dz-1	S_{36}	260	0.2287
Dz-2	S_{36}	260	0.1530
Dz-3	S_{8}	316	0.1859
Dz-4	S_{5}	330	0.3596
Dz5	S_{5}	344	0.3332
Dz-6	S_{5}	334	0.4054

The complete reference to the Gaussian 16 program package:

Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

REFERENCE

1. Neogi, I.; Jhulki, S.; Ghosh, A.; Chow, T. J.; Moorthy, J. N., Amorphous Host Materials Based on Tröger's Base Scaffold for Application in Phosphorescent Organic Light-Emitting Diodes. *ACS Applied Materials & Interfaces* **2015,** *7* (5), 3298-3305.
2. Jin, M.; Zhu, Z.; Liao, Q.; Li, Q.; Li, Z., Dendronized Polymers with High FTC-chromophore Loading Density: Large Second-order Nonlinear Optical Effects, Good Temporal and Thermal Stability. *Chinese Journal of Polymer Science* **2019,** *38*, 118-125.
3. Holzapfel, M.; Lambert, C., Photoinduced Charge Separation and Recombination in Acridine−Triarylamine-Based Redox Cascades. *The Journal of Physical Chemistry C* **2008,** *112* (4), 1227-1243.
4. Gao, X.; Hampton, C. S.; Harmata, M., Demethylenation of Tröger's Bases with Concomitant Hydrazine Formation. *European Journal of Organic Chemistry* **2012,** *2012* (36), 7053-7056.
5. Inoue, K.; Ishiwari, F.; Fukushima, T., Selective synthesis of diazacyclooctane -containing flexible ladder polymers with symmetrically or unsymmetrically substituted side chains. *Polymer Chemistry* **2020,** *11* (22), 3690-3694.
6. Lu, T. and Chen, F. Multiwfn: A multifunctional wavefunction analyzer. J. Comput. Chem., **2012**, 33, 580-592.
7. Tian Lu; A comprehensive electron wavefunction analysis toolbox for chemists, Multiwfn. *J. Chem. Phys.* **2024**, 161 (8), 082503.