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Multicolour- and high-colour-contrast switches in response to force and acid vapour by introducing asymmetric D-π-A-π-D structure

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Table S1. Photophysical data of PAN and DPIAN obtained by quantum chemical calculations.

	Transition assignment	Transition energy (eV)	Maximal absorption (nm)	Oscillator strength
PAN	HOMO-1→ LUMO (2.64%) HOMO→ LUMO (95.01%)	**2.9241**	**424.00**	**0.7004**
	HOMO-1→ LUMO (94.21%) HOMO→ LUMO (3.10%)	3.4729	357.01	0.2964
	HOMO-2→ LUMO (18.91%) HOMO-1→ LUMO+1 (5.25%) HOMO→ LUMO+1 (69.54%)	3.9682	312.44	0.0154
DPIAN	HOMO-1→ LUMO+1 (3.74%) HOMO→ LUMO (94.21%)	**2.6957**	**459.93**	**1.4078**
	HOMO-1→ LUMO (91.53%) HOMO→ LUMO+1 (2.54%)	2.9418	421.45	0.0505
	HOMO-2→ LUMO (13.053%) HOMO-1→ LUMO (4.27%) HOMO-1→ LUMO+1 (2.42%) HOMO→ LUMO+1 (72.82%)	3.3520	369.88	0.1670

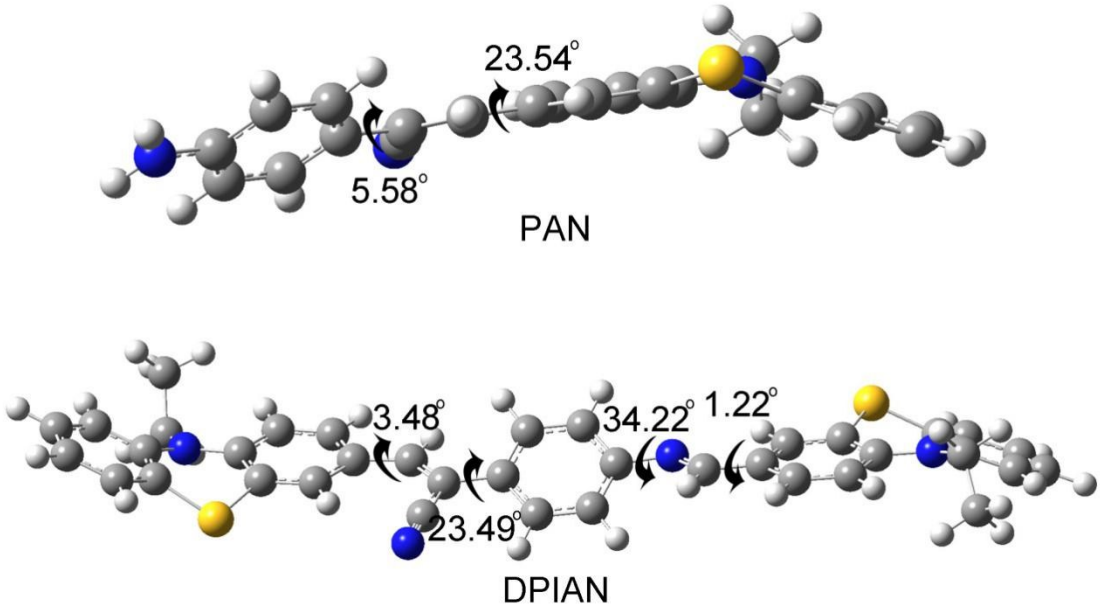

Fig. S1 Optimized conformations of PAN and DPIAN by DFT calculations.

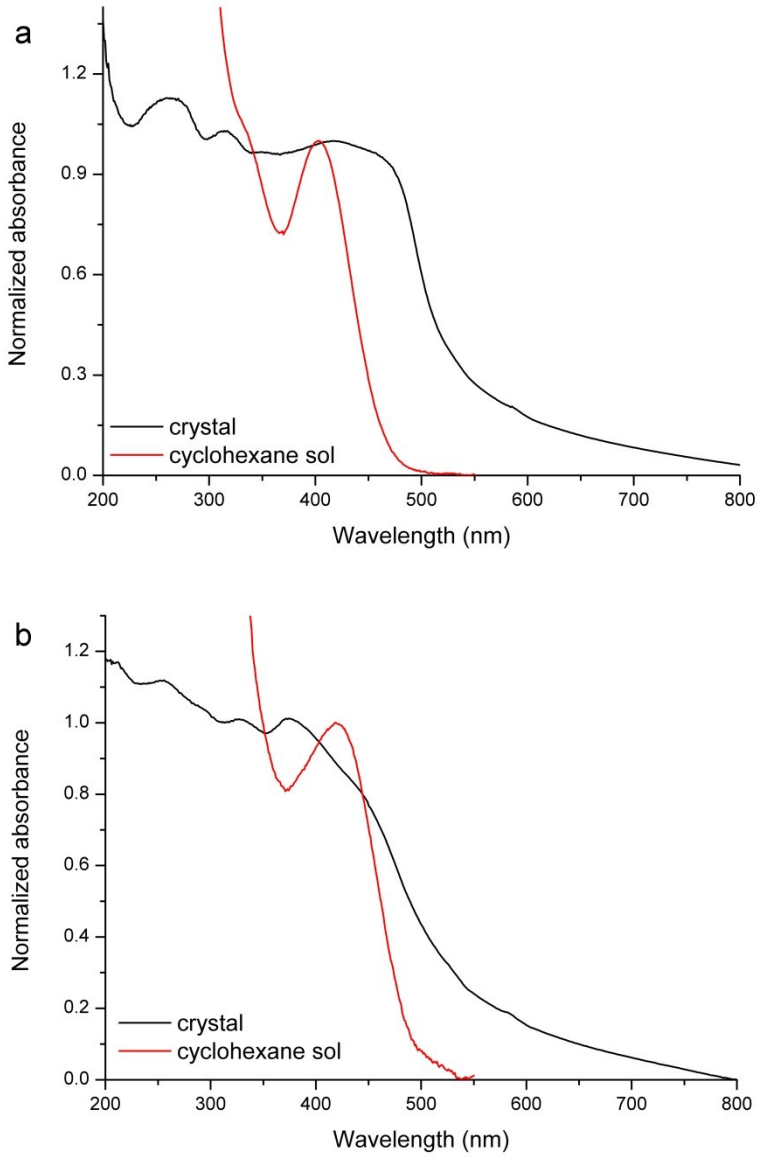

Fig. S2 Normalized absorption spectra of (a) PAN and (b) DPIAN in cyclohexane solutions (c = 10^{-4} M) and crystal state.

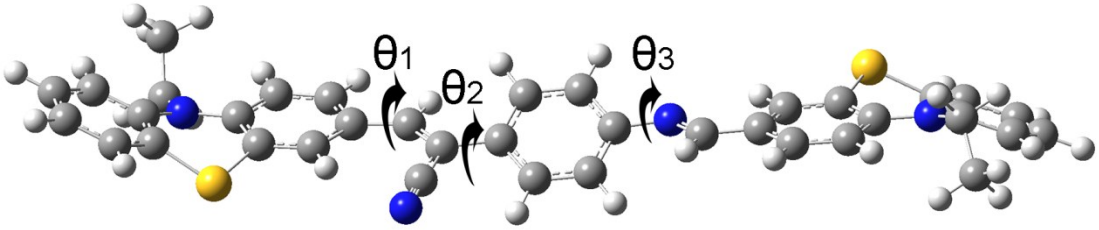

Table S2. Energy levels of frontier orbitals and electron transitions of DPIAN with different twisted angles.

	θ_1; θ_2; θ_3	E_{HOMO} (eV)	E_{LUMO} (eV)	Electron transition (nm)
1	3.48; 23.43;34.22	-5.00	-2.04	459.93
2	3.48; 50; 34.22	-5.01	-1.92	434.76
3	3.48; 70; 34.22	-5.05	-1.82	417.06
4	3.48; 50.0; 50.0	-5.27	-1.81	426.68
5	50; 70; 34.22	-5.29	-1.70	408.76

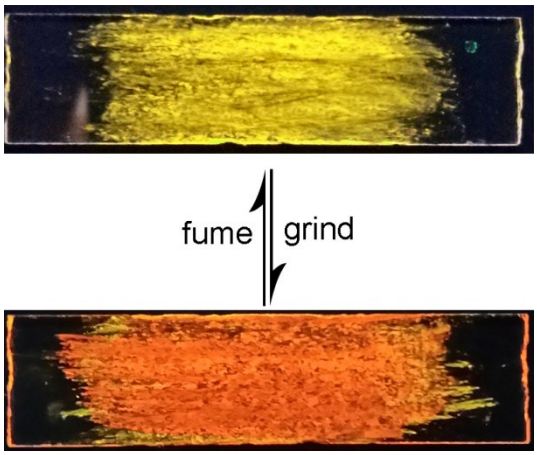

Fig. S3 Photos of PAN in different states under 365 nm light.

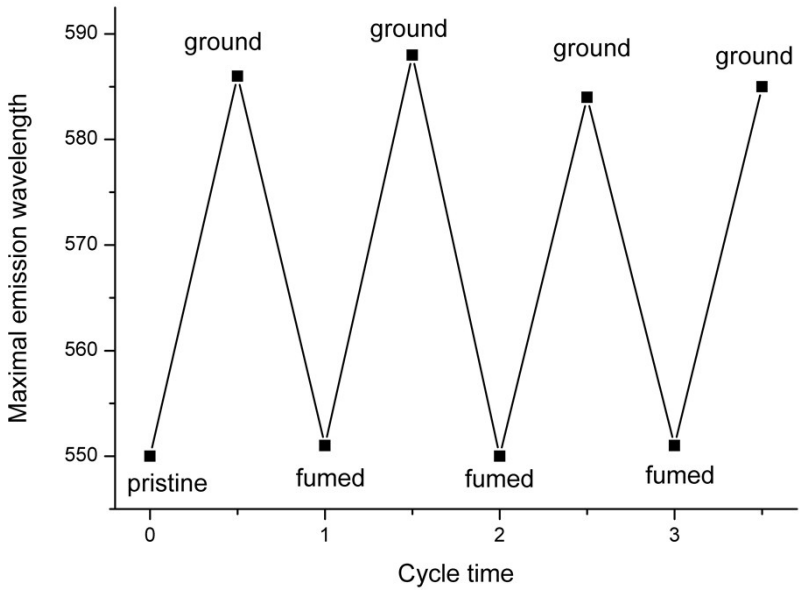

Fig. S4 Reversible MFC process of PAN.

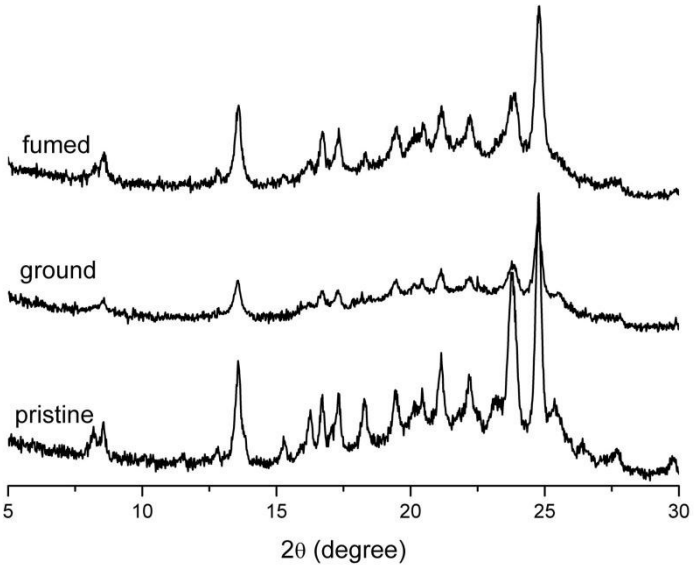

Fig. S5 XRD patterns of PAN in different states.

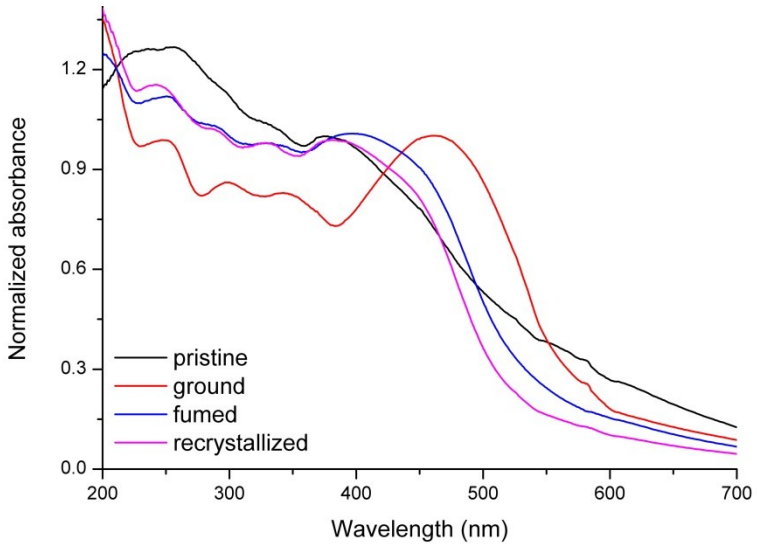

Fig. S6 Absorption spectra of DPIAN solids in different states.

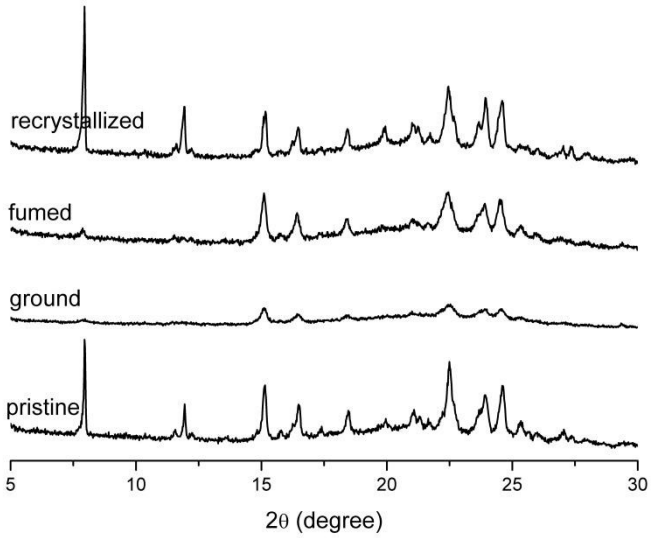

Fig. S7 XRD patterns of DPIAN in different states.

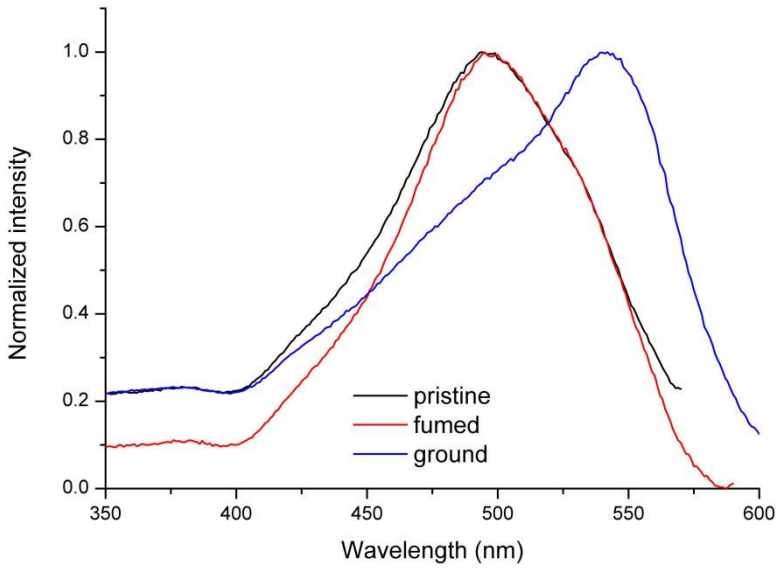

Fig. S8 Excited spectra of DPIAN in pristine, fumed and ground states. Excitation wavelengths are 580, 600 and 620 nm, respectively.

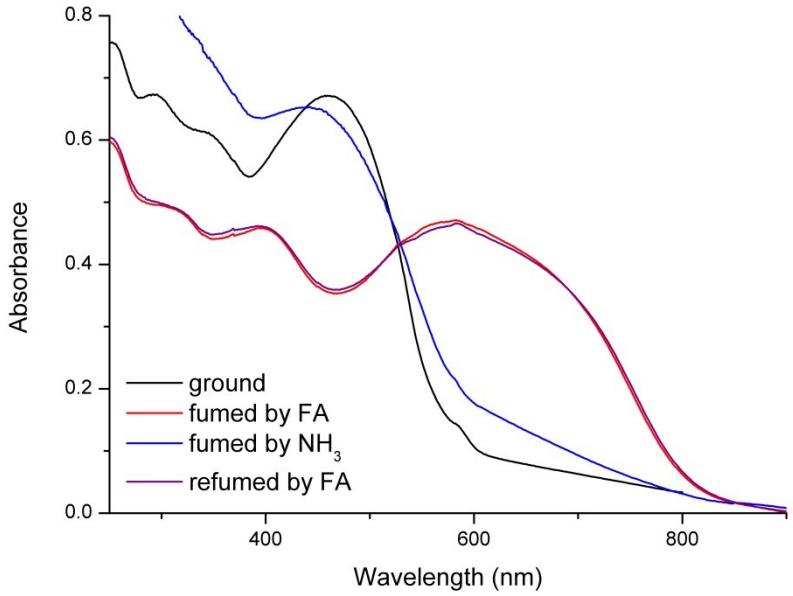

Fig. S9 Absorption spectra of DPIAN-R in response to formic acid and NH_3 vapors.

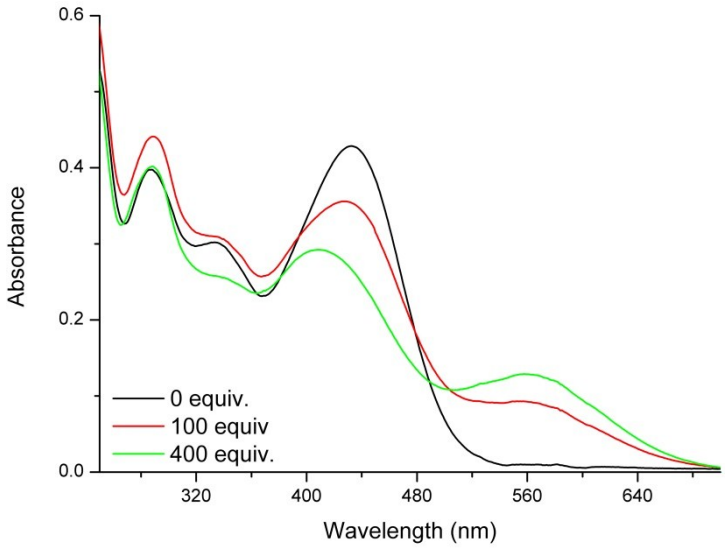

Fig. S10 Absorption spectra of DPIAN after adding formic acid.

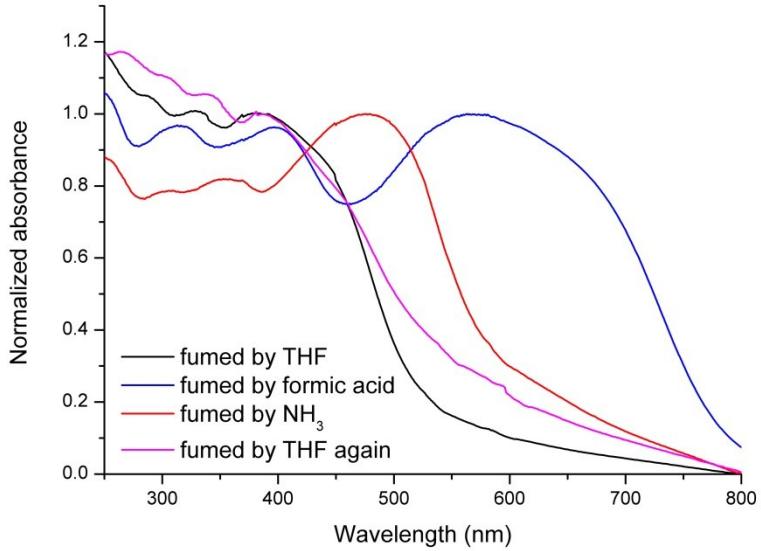

Fig. S11 Absorption spectra of DPIAN-O in response to formic acid, NH_3 and THF vapors.

Table S3. Photophysical data of protonated DPIAN obtained by quantum chemical calculation.

	Transition assignment	Transition energy (eV)	Maximal absorption (nm)	Oscillator strength
DPIAN+H	HOMO-2→ LUMO (4.23%) HOMO-1→ LUMO (3.79%) HOMO→ LUMO (87.14%) HOMO→ LUMO+1 (3.58%)	**2.0023**	**619.21**	**1.0049**

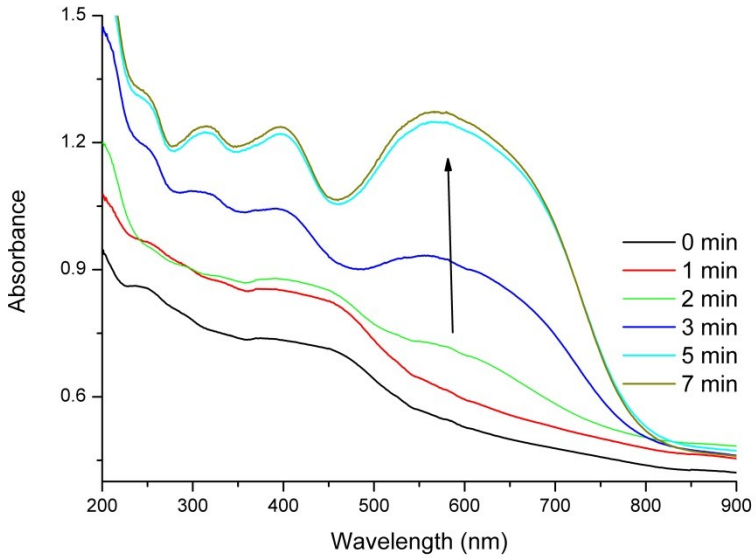

Fig. S12 Absorption spectral change of DPIAN-O upon exposure to formic acid saturated vapor.

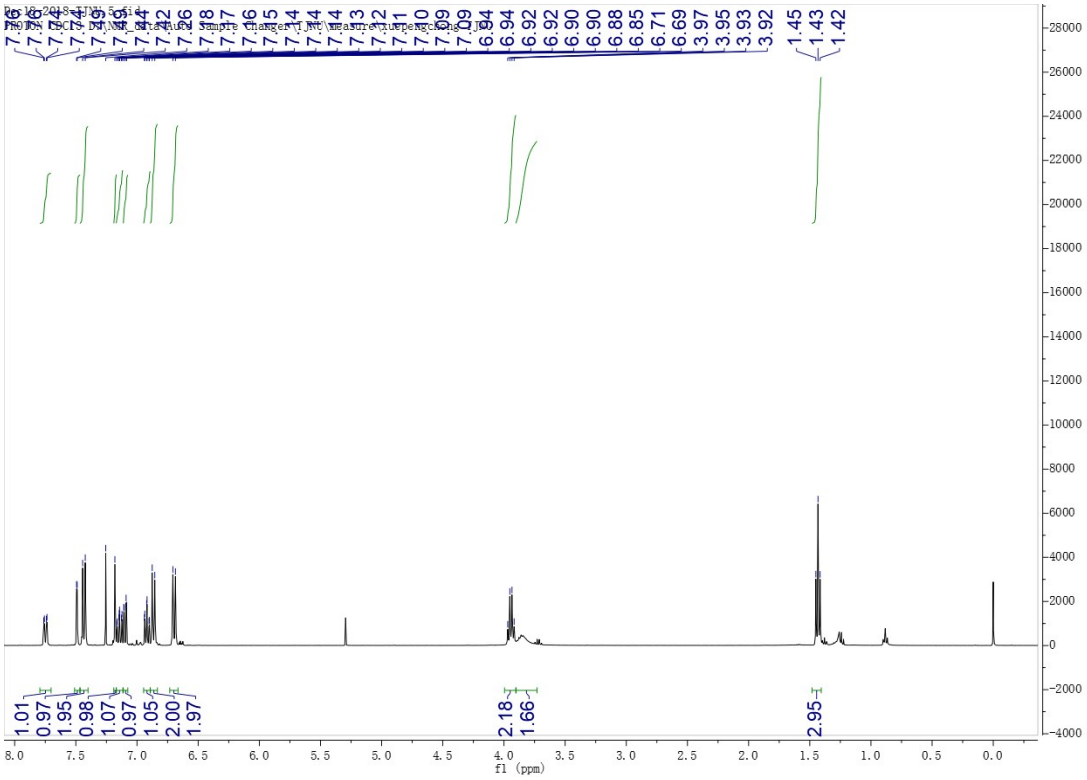

Fig. S13 ^{1}H NMR spectrum of PAN in $CDCl_3$.

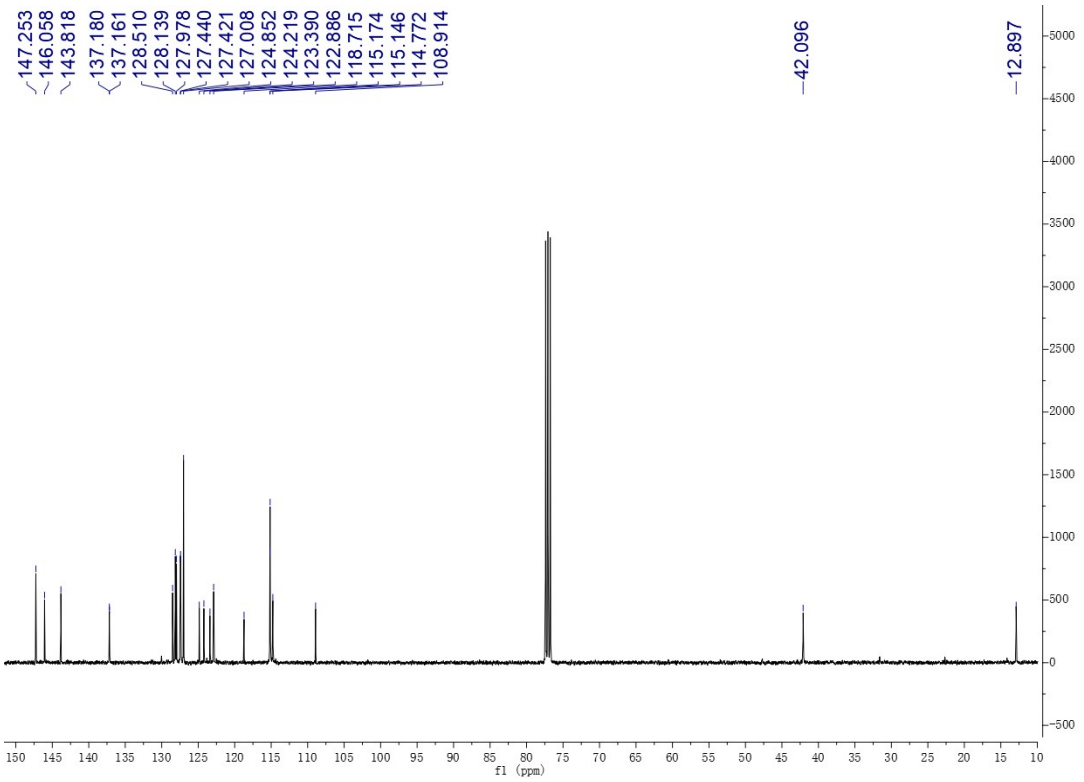

Fig. S14 ^{13}C NMR spectrum of PAN in $CDCl_3$.

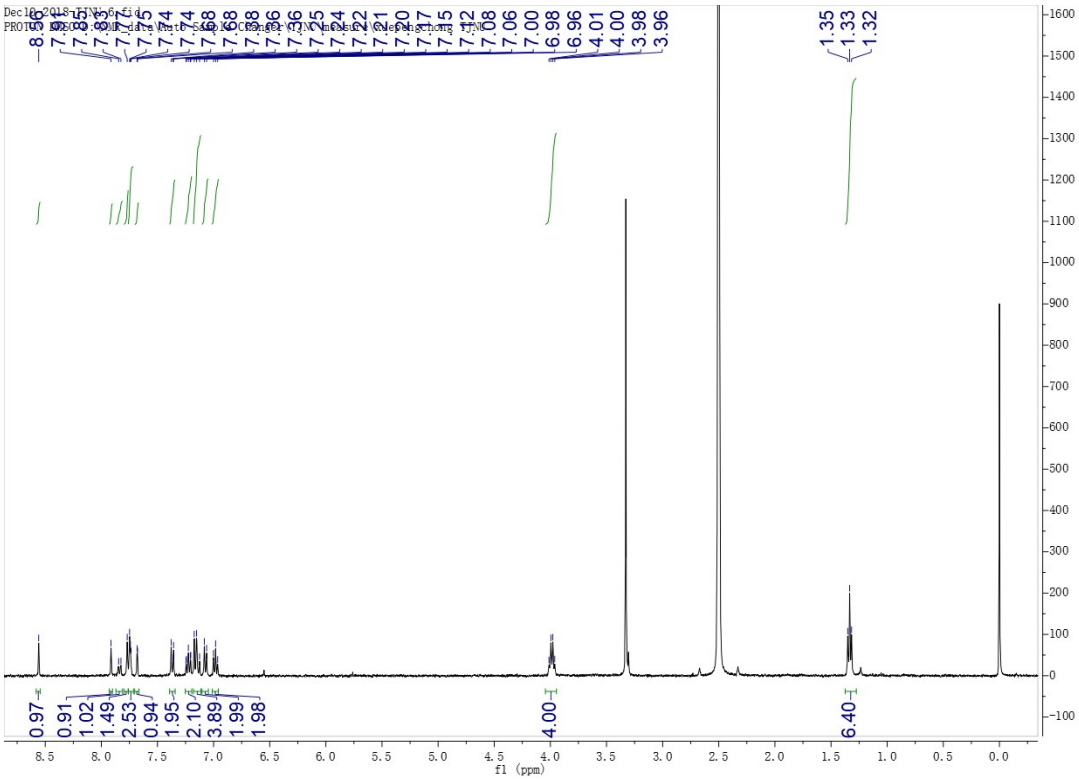

Fig. S15 ^{1}H NMR spectrum of DPIAN in d6-DMSO.

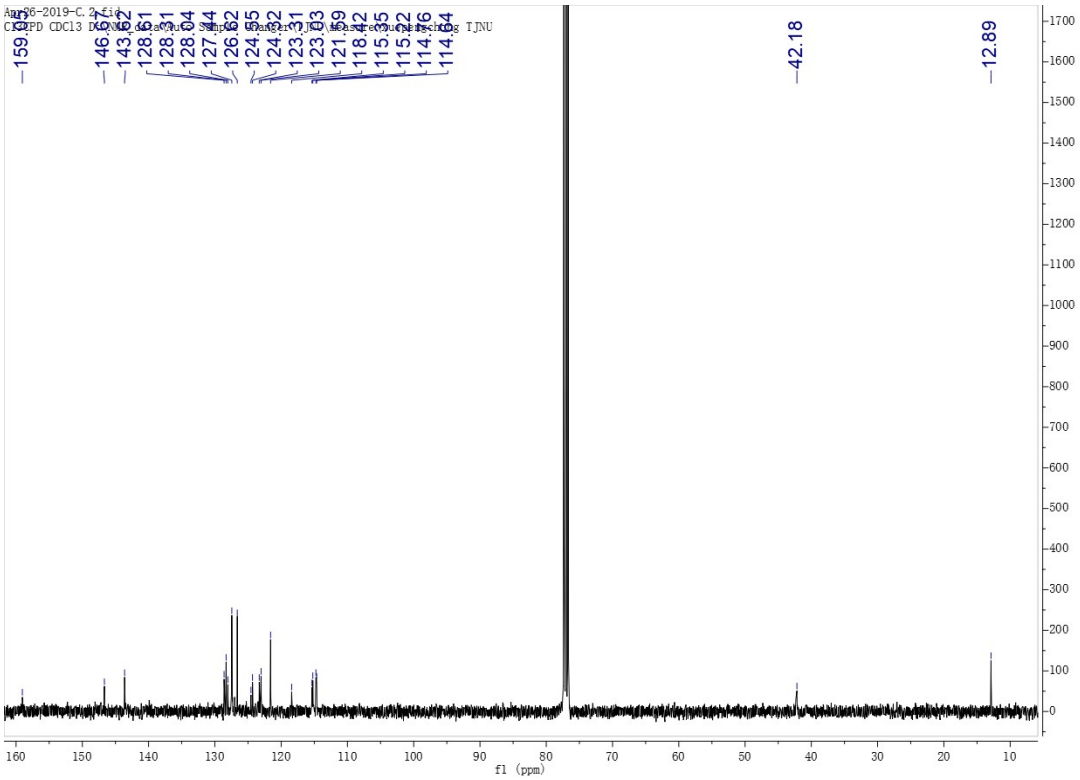

Fig. S16 ^{13}C NMR spectrum of DPIAN in $CDCl_3$.

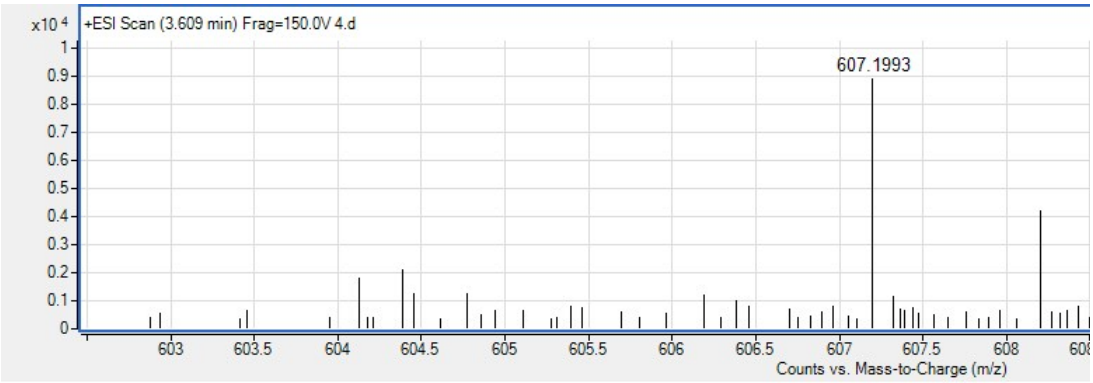

Fig. S17 MS spectrum of DPIAN.