Electronic Supplementary Material (ESI) for CrystEngComm.

Spacer group-controlled luminescence and response of C3-symmetric triphenylamine derivatives to force

Yanning Han, Tong Zhang, Xinyu Chen, Qiao Chen, Pengchong Xue*

Tianjin Key Laboratory of Structure and Performance for Functional Molecules
College of Chemistry, Tianjin Normal University
No. 393 Bin Shui West Road, Tianjin, P. R. China.
E-mail: xuepengchong@126.com; hxxyxpc@tjnu.edu.cn

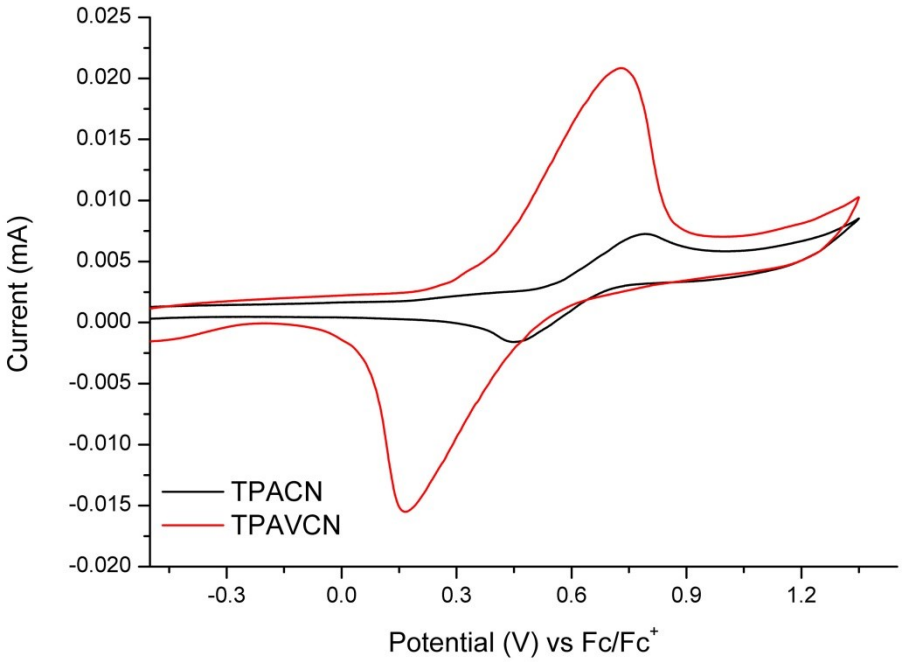

Fig. S1 Cyclic voltammetry curves of two compounds.

Table S1. Photophysical data of TPACN and TPAVCN obtained by quantum chemical calculation.

	Dipole moment (Debye)	Transition	Transition assignment	E (eV)	λ_{abs} (nm)	Oscillator strength
TPAVCN	0.4229	$S_0 \rightarrow S_1$	HOMO→LUMO (96.73 %)	2.7785	446.22	1.3087
		$S_0 \rightarrow S_2$	HOMO→LUMO+1 (96.79%)	2.7829	445.52	1.1527
		$S_0 \rightarrow S_3$	HOMO-1→LUMO+1 (2.07%) HOMO→LUMO+2 (89.48%)	3.2429	382.33	0.0042
TPACN	0.0375	$S_0 \rightarrow S_1$	HOMO→LUMO (97.84 %)	3.2954	376.24	0.7987
		$S_0 \rightarrow S_2$	HOMO→LUMO+1 (97.86%)	3.3153	373.98	0.8283
		$S_0 \rightarrow S_3$	HOMO→LUMO+2 (98.09%)	3.8036	325.96	0.0009

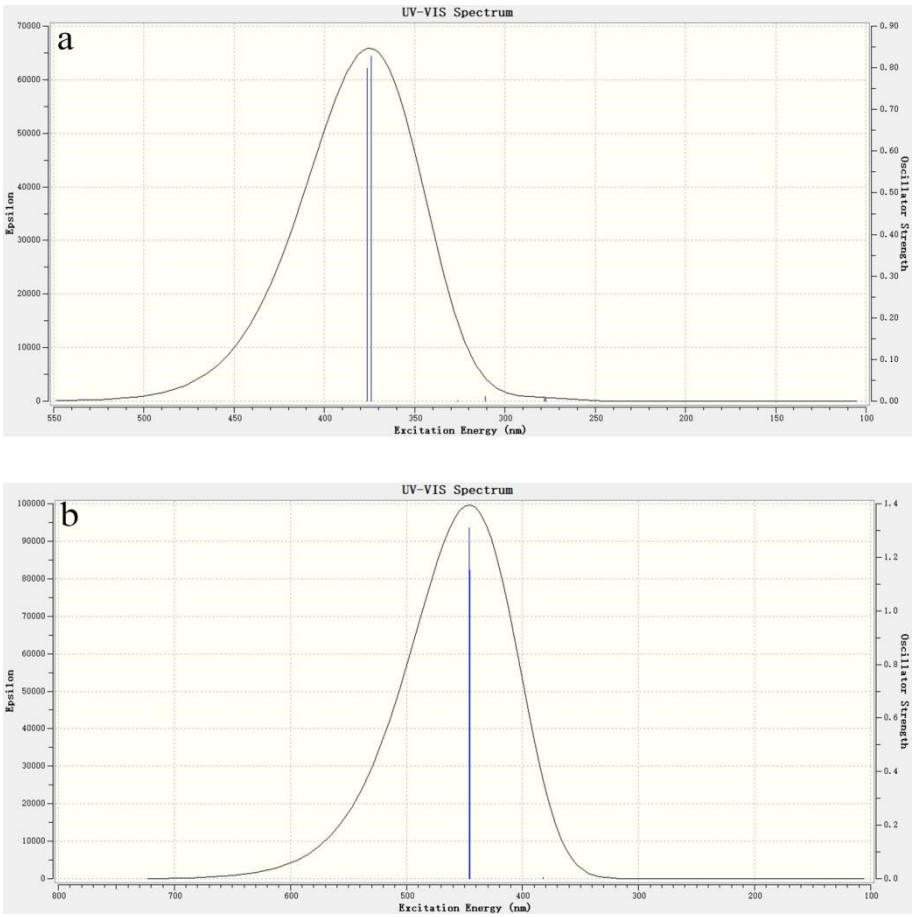

Fig. S2 Simulated UV spectra of (a) TPACN and (b) TPAVCN.

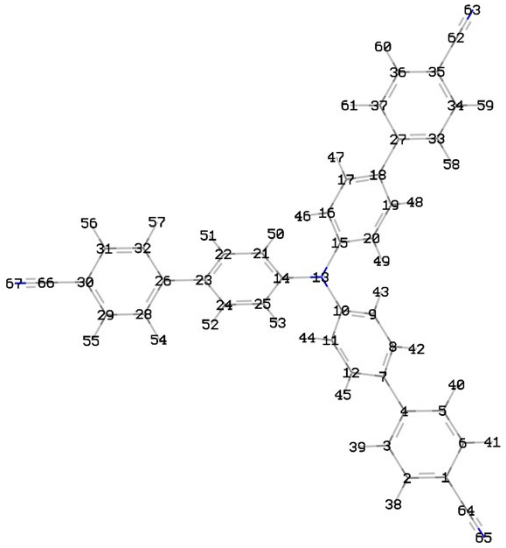

Table S2. Data of orbital composition analysis by natural atomic orbital (NAO) method for TPACN.

HOMO		LUMO		LUMO+1	
1(C)	1.405%	1(C)	9.987%	10(C)	0.539%
3(C)	1.170%	2(C)	3.948%	14(C)	4.602%
5(C)	1.170%	3(C)	3.571%	15(C)	6.111%
7(C)	6.572%	4(C)	10.490%	16(C)	1.165%
9(C)	4.651%	5(C)	3.435%	17(C)	3.064%
10(C)	2.503%	6(C)	4.123%	18(C)	4.362%
11(C)	4.682%	7(C)	5.172%	19(C)	3.011%
13(N)	**25.418%**	8(C)	3.665%	20(C)	1.205%
14(C)	2.636%	9(C)	1.364%	21(C)	0.750%
15(C)	2.655%	10(C)	7.320%	22(C)	2.398%
16(C)	4.909%	11(C)	1.322%	23(C)	3.109%
18(C)	6.944%	12(C)	3.769%	24(C)	2.154%
20(C)	4.901%	14(C)	2.944%	25(C)	0.863%
21(C)	4.848%	15(C)	1.110%	26(C)	6.525%
23(C)	6.916%	18(C)	0.602%	27(C)	8.728%
24(C)	0.509%	21(C)	0.614%	28(C)	2.106%
25(C)	4.857%	22(C)	1.245%	29(C)	2.565%
28(C)	1.237%	23(C)	1.987%	30(C)	6.172%
30(C)	1.489%	24(C)	1.513%	31(C)	2.460%
32(C)	1.231%	26(C)	3.863%	32(C)	2.182%
33(C)	1.207%	27(C)	1.109%	33(C)	2.820%
35(C)	1.450%	28(C)	1.362%	34(C)	3.482%
37(C)	1.212%	29(C)	1.412%	35(C)	8.311%
63(N)	**0.621%**	30(C)	3.690%	36(C)	3.299%
65(N)	**0.601%**	31(C)	1.551%	37(C)	2.958%
67(N)	**0.637%**	32(C)	1.250%	62(C)	1.900%

	35(C)	1.067%	**63(N)**	**5.551%**
	63(N)	**0.708%**	66(C)	1.409%
	64(C)	2.259%	**67(N)**	**4.114%**
	65(N)	**6.637%**		
	66(C)	0.827%		
	67(N)	**2.443%**		

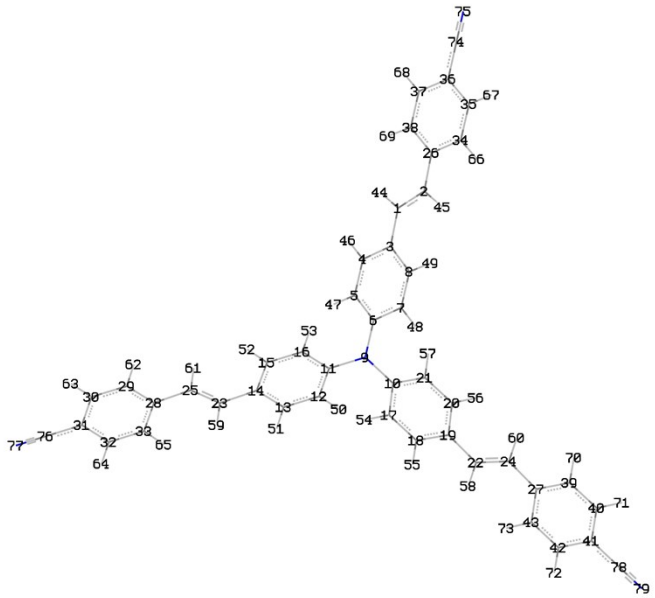

Table S3. Data of orbital composition analysis by natural atomic orbital (NAO) method for TPAVCN.

HOMO		LUMO		LUMO+1	
1(C)	0.904%	6(C)	0.514%	1(C)	9.378%
2(C)	5.050%	10(C)	3.331%	2(C)	7.341%
3(C)	5.733%	11(C)	5.781%	3(C)	3.095%
4(C)	0.721%	12(C)	1.167%	4(C)	2.795%
5(C)	4.011%	13(C)	2.941%	5(C)	1.215%
6(C)	2.475%	14(C)	3.082%	6(C)	5.617%
7(C)	3.558%	15(C)	3.813%	8(C)	3.829%
8(C)	0.683%	17(C)	0.663%	10(C)	3.026%
9(N)	**19.634%**	18(C)	1.654%	11(C)	0.831%
10(C)	2.388%	19(C)	1.743%	17(C)	0.657%
11(C)	2.305%	20(C)	2.046%	18(C)	1.362%
12(C)	3.763%	22(C)	5.245%	19(C)	1.570%
13(C)	0.651%	23(C)	9.602%	20(C)	2.125%
14(C)	5.305%	24(C)	4.115%	22(C)	4.941%
15(C)	0.612%	25(C)	7.435%	23(C)	1.002%
16(C)	3.348%	27(C)	3.080%	24(C)	3.813%
17(C)	3.886%	28(C)	5.640%	25(C)	0.765%
18(C)	0.670%	29(C)	2.799%	26(C)	5.493%
19(C)	5.523%	30(C)	2.612%	27(C)	2.887%
20(C)	0.660%	31(C)	6.823%	28(C)	0.587%
21(C)	3.457%	32(C)	1.323%	31(C)	0.706%
22(C)	0.853%	33(C)	3.903%	34(C)	2.746%
23(C)	0.806%	39(C)	1.542%	35(C)	2.540%
24(C)	4.838%	40(C)	1.423%	36(C)	6.668%
25(C)	4.634%	41(C)	3.740%	37(C)	1.288%
29(C)	1.110%	42(C)	0.723%	38(C)	3.818%

31(C)	1.347%	43(C)	2.145%	39(C)	1.431%
33(C)	1.056%	76(C)	1.058%	40(C)	1.339%
34(C)	1.213%	**77(N)**	**3.937%**	41(C)	3.494%
36(C)	1.476%	78(C)	0.577%	42(C)	0.677%
38(C)	1.154%	**79(N)**	**2.156%**	43(C)	2.000%
39(C)	1.159%			74(C)	1.031%
41(C)	1.409%			**75(N)**	**3.843%**
43(C)	1.104%			78(C)	0.542%
75(N)	0.623%			**79(N)**	**2.017%**
77(N)	0.567%				
79(N)	0.594%				

Table S4. Crystal data of TPAVCN

	TPAVCN
Molecular formula	C39H30N4
Space group	*Cc*
Cell lengths	a=10.4053(2) Å b=32.0280(6) Å c=10.3784(2) Å
Cell angles	α=90° β= 93.2313(18)° γ=90°
Cell volume	3453.20(12)
Z	4
R-factor (%)	6.34

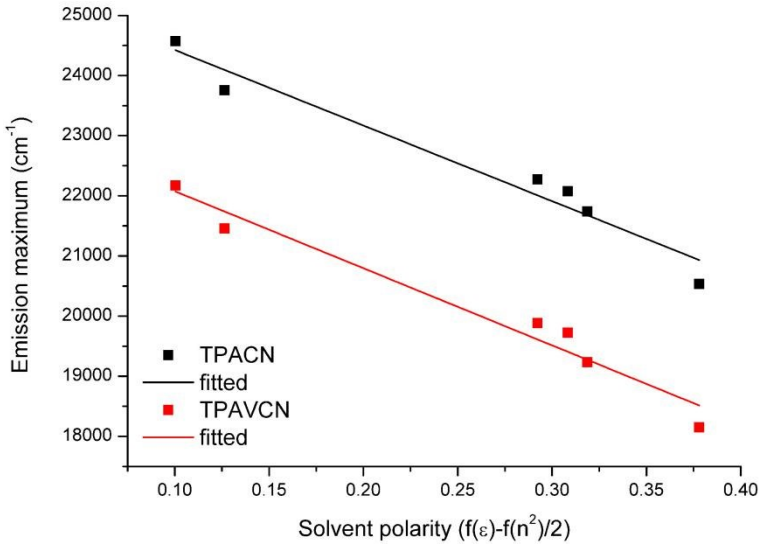

Fig. S3 The plots of $\tilde{\nu}^{max}$ of two compounds against the solvent polarity parameter ($f(\varepsilon) - \frac{1}{2}f(n^2)$).

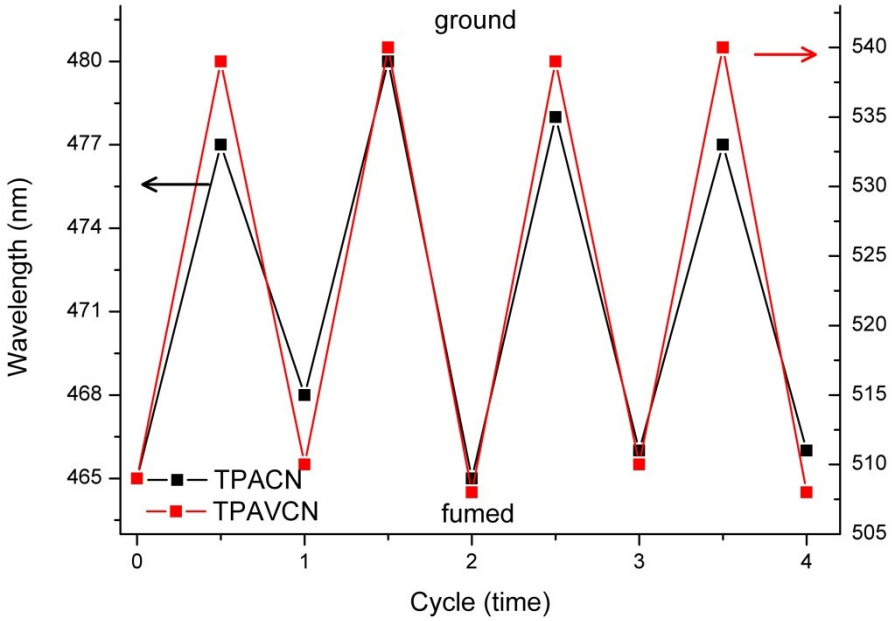

Fig. S4 Reversible curves of fluorescence maxima.

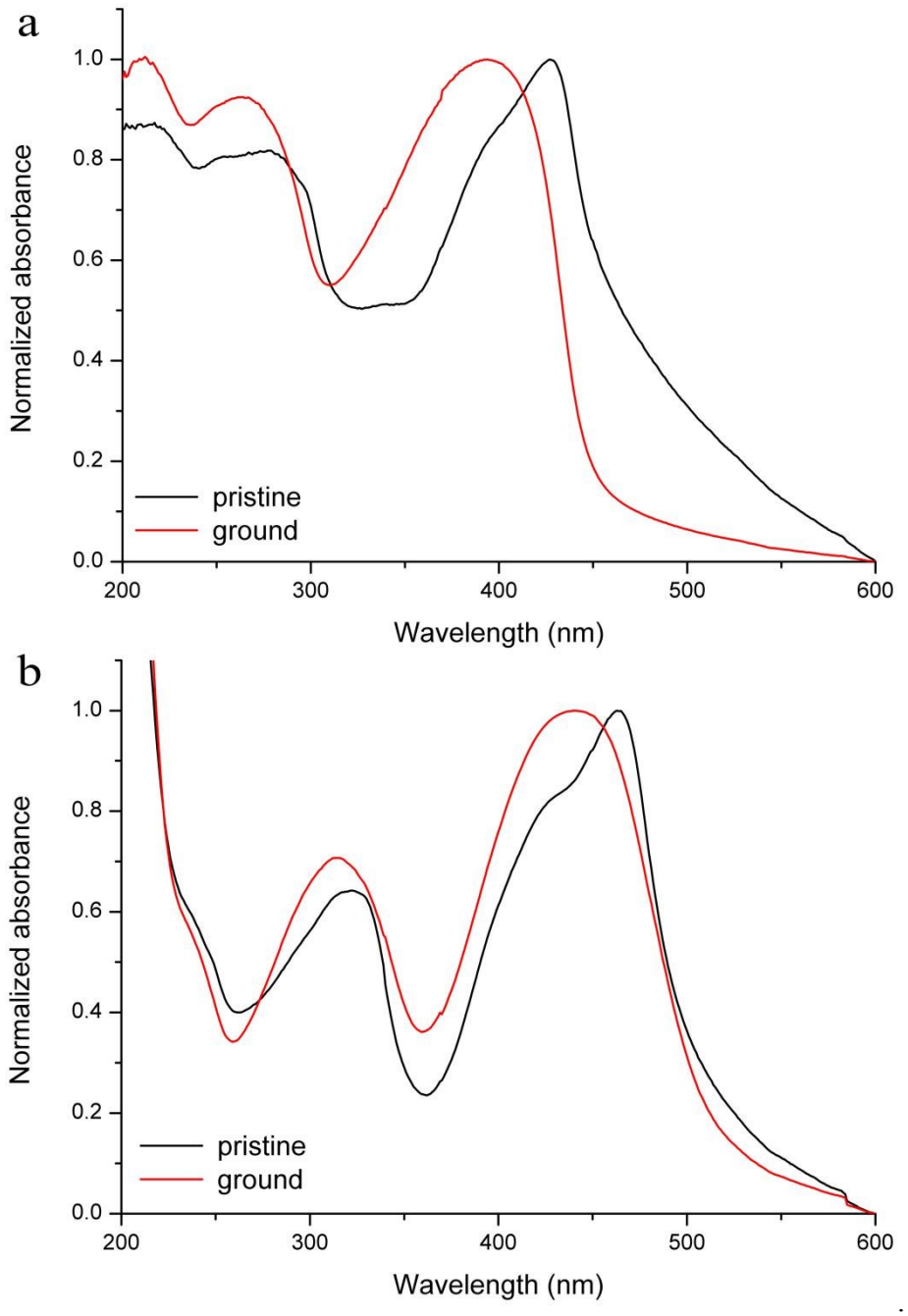

Fig. S5 UV-Vis absorption spectra of (a) TPACN and (b) TPAVCN before and after grinding.

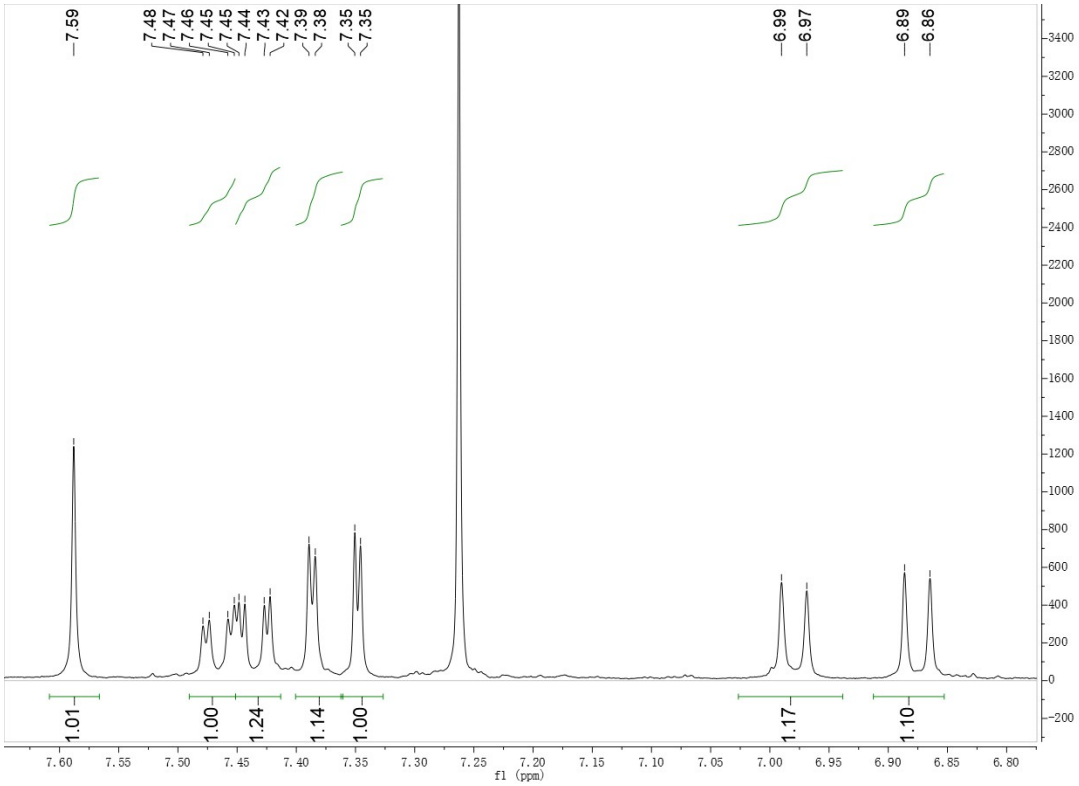

Fig. S6 ^{1}H NMR spectrum of TPACN in $CDCl_3$.

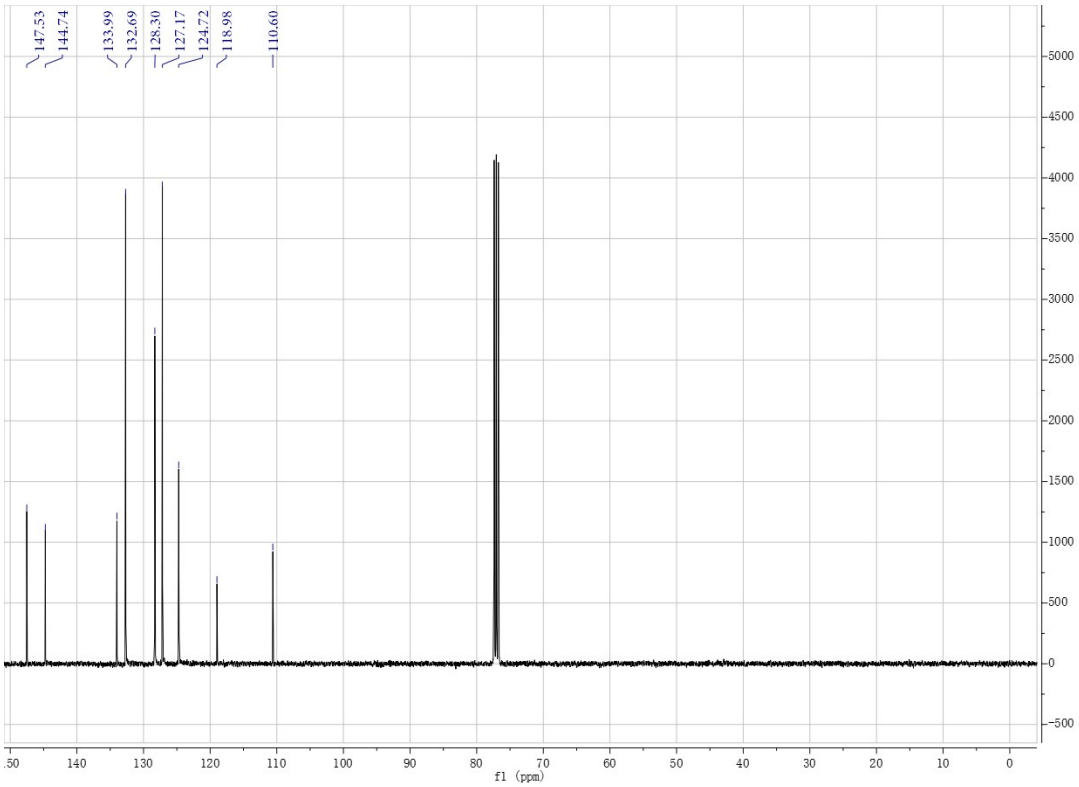

Fig. S7 ^{13}H NMR spectrum of TPACN in $CDCl_3$.

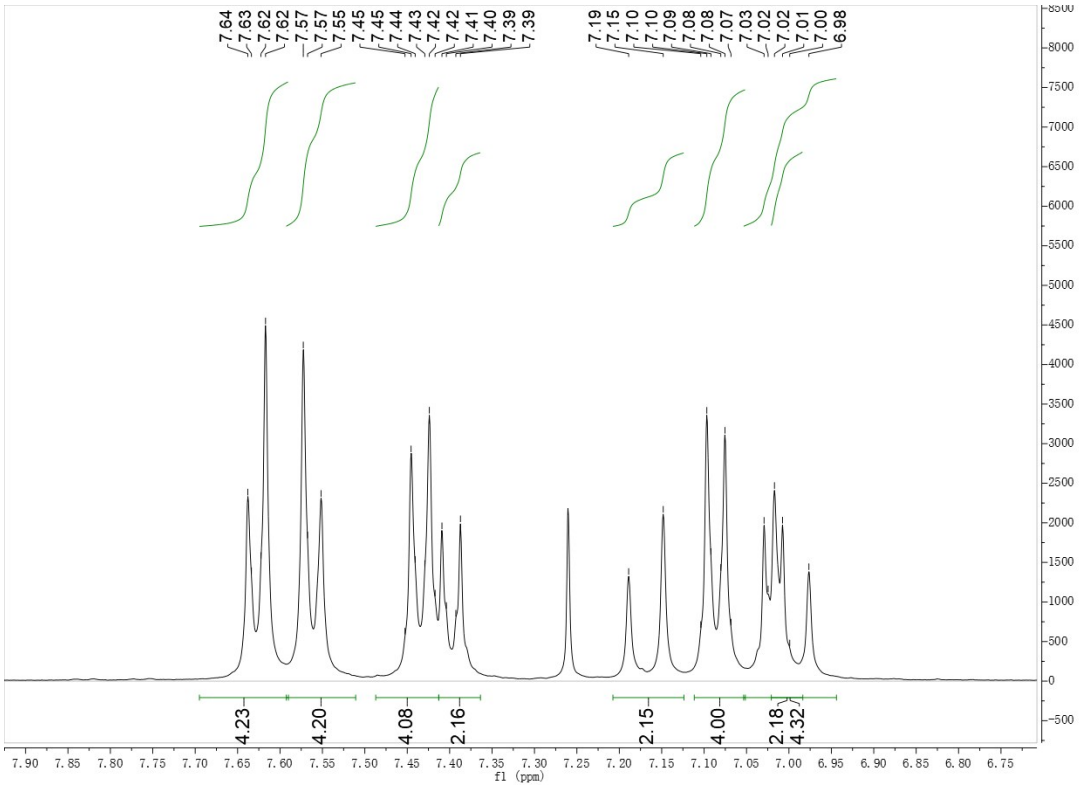

Fig. S8 ^{1}H NMR spectrum of TPAVCN in $CDCl_3$.

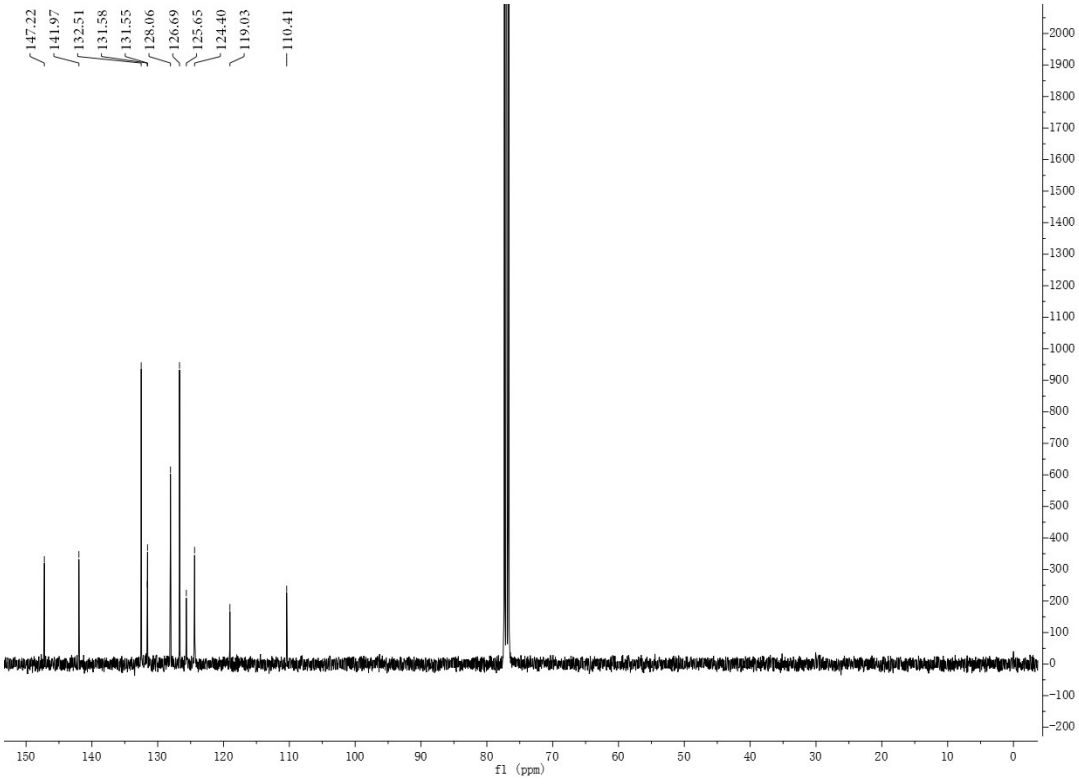

Fig. S9 ^{13}H NMR spectrum of TPAVCN in $CDCl_3$.