Electronic Supplementary Information

TACOT Derived New Nitrogen rich Energetic Compounds: Synthesis, Characterization and Properties

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1. The structure of compound 5

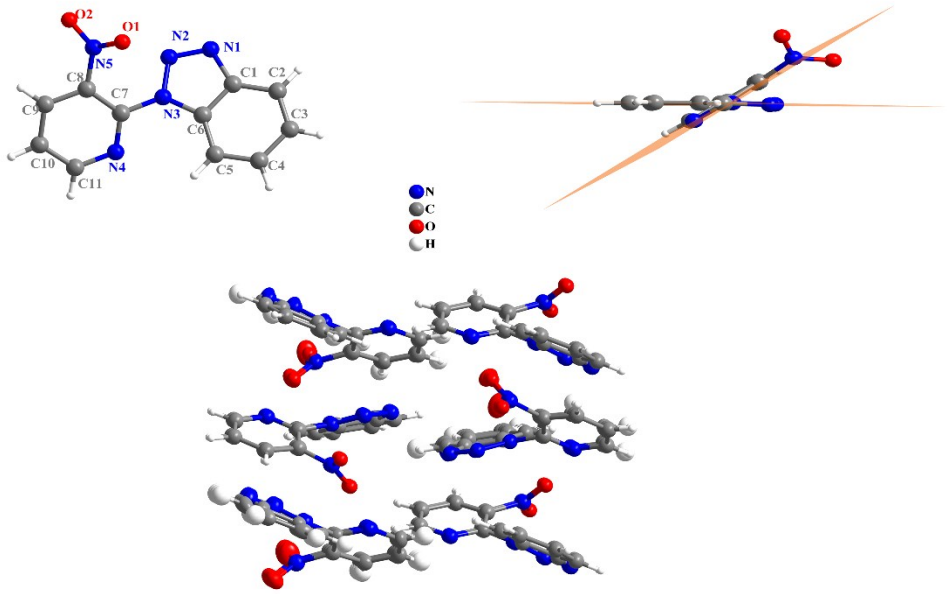

Fig. S1 Molecular structure of compound **5** and its packing diagram viewed down the b-axis.

2. X-ray crystallography determinations

Table S1. Crystal data and structure refinement details of compounds **5, 6** and **8**.

Item	**5**	**6**	**8**
CCDC	1889350	1889351	1889352
Empirical formula	$C_{11}H_7N_5O_2$	$C_{11}H_7N_5$	$C_{14}H_{10}N_{14}O_5$
Formula mass	241.22	209.22	454.36
Temperature/K	153.15	153.15	153.15
Crystal system	orthorhombic	orthorhombic	monoclinic
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_1/c$
a[Å]	7.1519(14)	4.5338(9)	17.868(4)
b[Å]	10.616(2)	12.919(3)	6.8028(14)
c[Å]	13.902(3)	16.167(3)	15.914(3)
β[°]	90.00	90.00	104.01(3)
Volume/Å^3	1055.5(4)	946.9(3)	1876.8(7)
Z	4	4	4
Density/g/cm^3	1.518	1.468	1.608
μ/1/mm	0.111	0.097	0.129
F(000)	496.0	432.0	928.0
Crystal size/mm^3	0.2 × 0.15 × 0.08	0.13 × 0.12 × 0.1	0.23 × 0.2 × 0.14

Radiation/Å	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.86 to 54.98	4.036 to 54.944	5.23 to 54.872
Index ranges	-9 ≤ h ≤ 9, -13 ≤ k ≤ 13, -17 ≤ l ≤ 17	-5 ≤ h ≤ 3, -16 ≤ k ≤ 14, -20 ≤ l ≤ 20	-23 ≤ h ≤ 22, -8 ≤ k ≤ 8, -20 ≤ l ≤ 20
Reflections collected	8386	3835	13443
Independent reflections	2370 [R_{int} = 0.0339, R_{sigma} = 0.0286]	2112 [R_{int} = 0.0303, R_{sigma} = 0.0398]	4232 [R_{int} = 0.0554, R_{sigma} = 0.0532]
Data/restraints/parameters	2370/0/163	2112/0/145	4232/0/300
Goodness-of-fit on F^2	1.183	1.120	1.239
Final R indexes [I>=2σ (I)]	R_1 = 0.0519, wR_2 = 0.1215	R_1 = 0.0480, wR_2 = 0.1095	R_1 = 0.0945, wR_2 = 0.1788
Final R indexes (all data)	R_1 = 0.0551, wR_2 = 0.1388	R_1 = 0.0528, wR_2 = 0.1129	R_1 = 0.1167, wR_2 = 0.1917

3. ^{1}H, ^{13}C NMR for compounds 5, 6, 7 and 8.

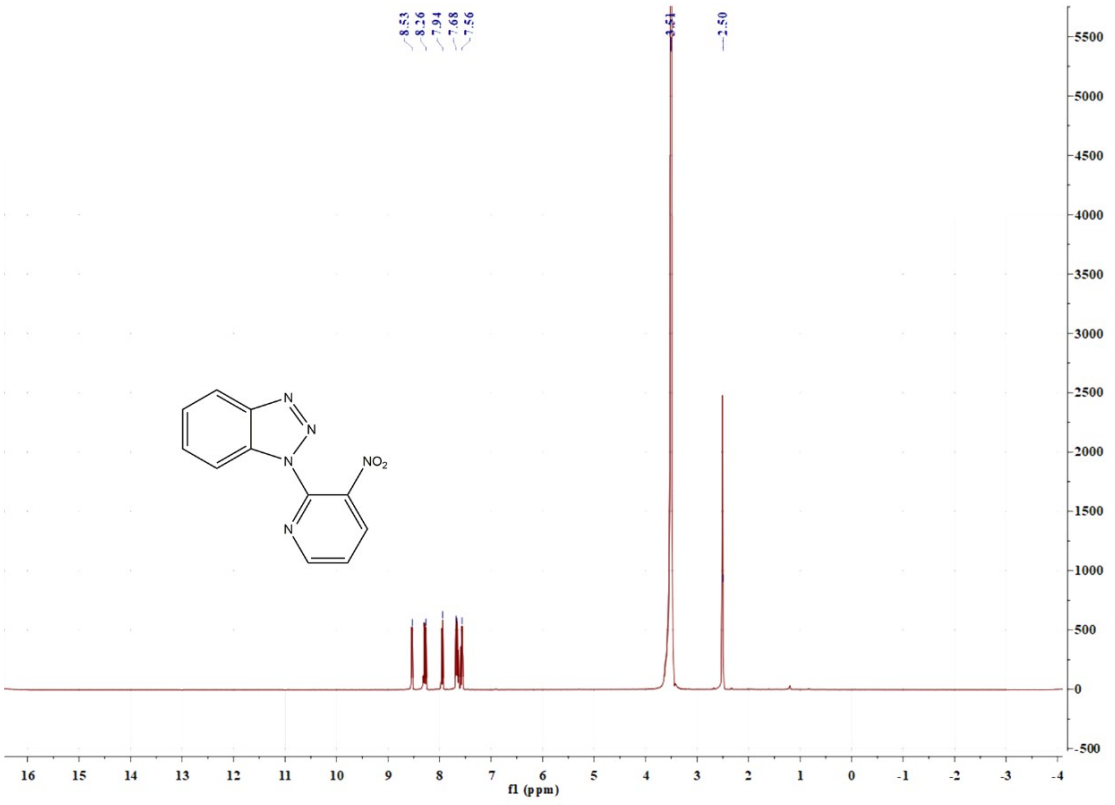

Fig. S2 The ^{1}H NMR of compound **5**.

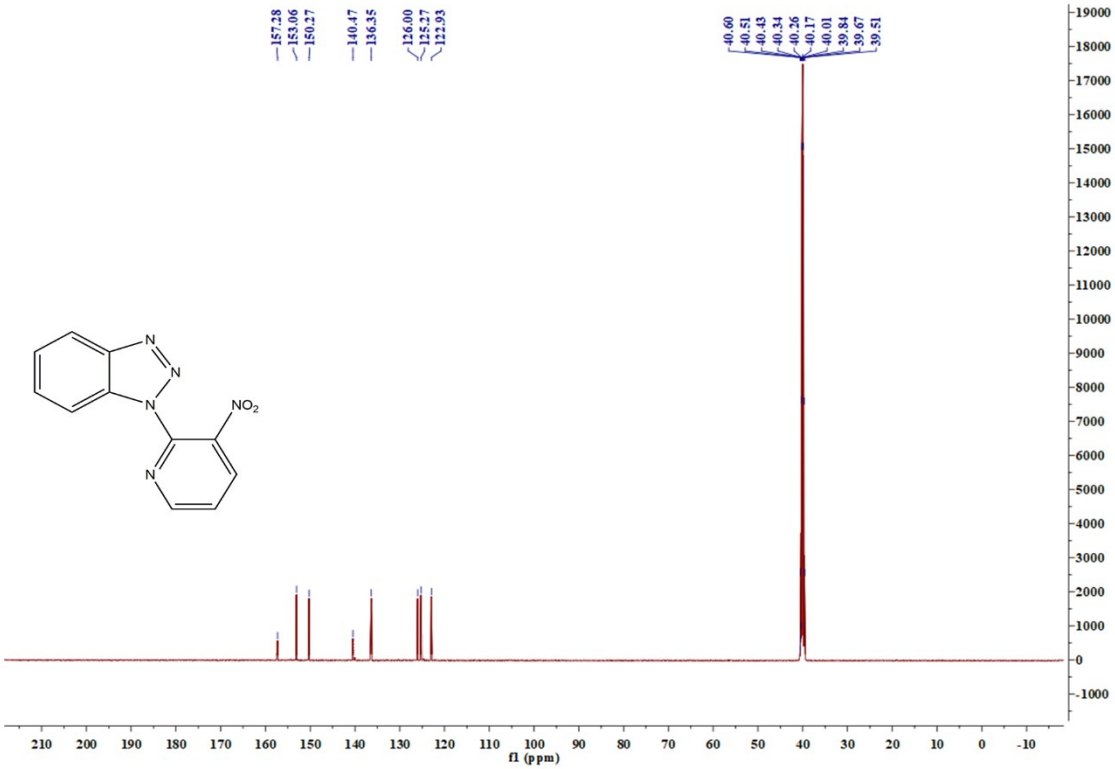

Fig. S3 The ^{13}C NMR of compound **5**.

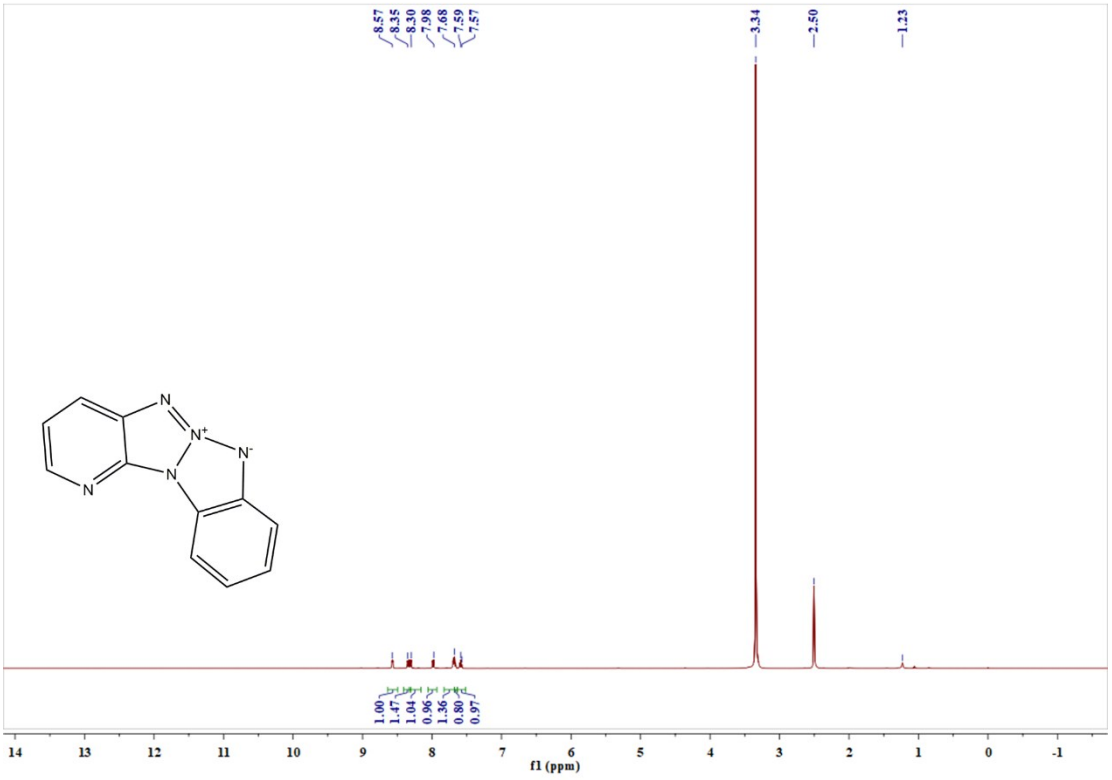

Fig. S4 The ^{1}H NMR of compound **6**

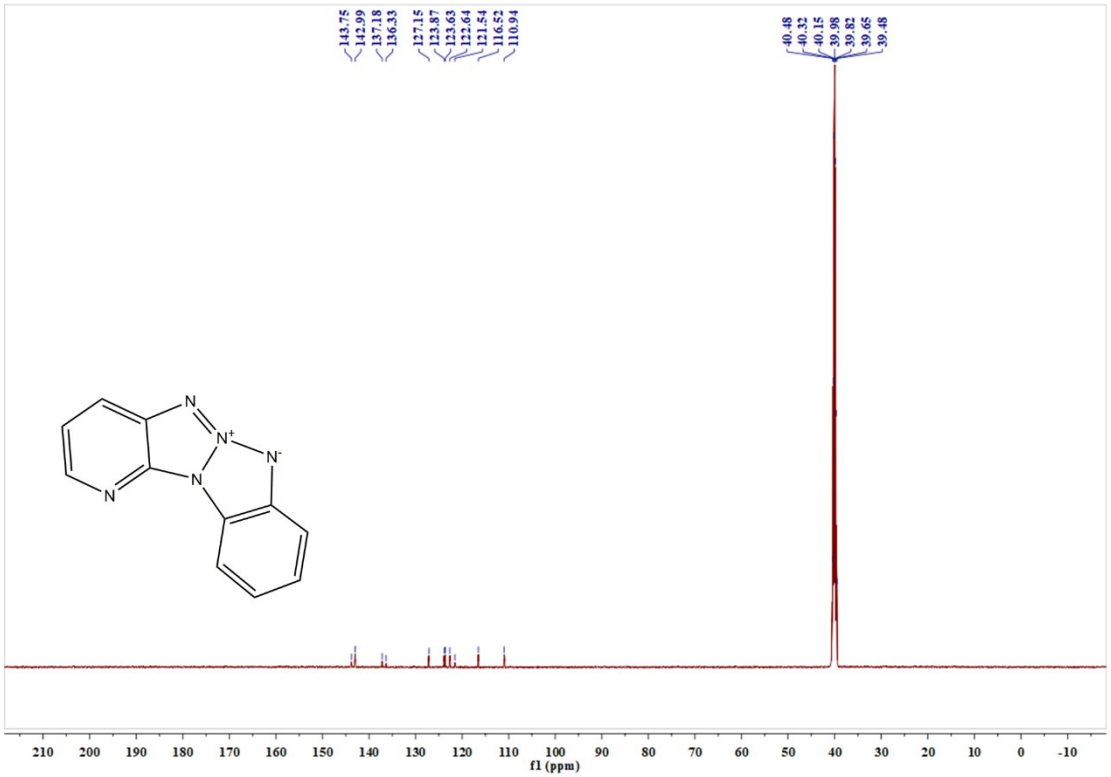

Fig. S5 The ^{13}C NMR of compound **6**.

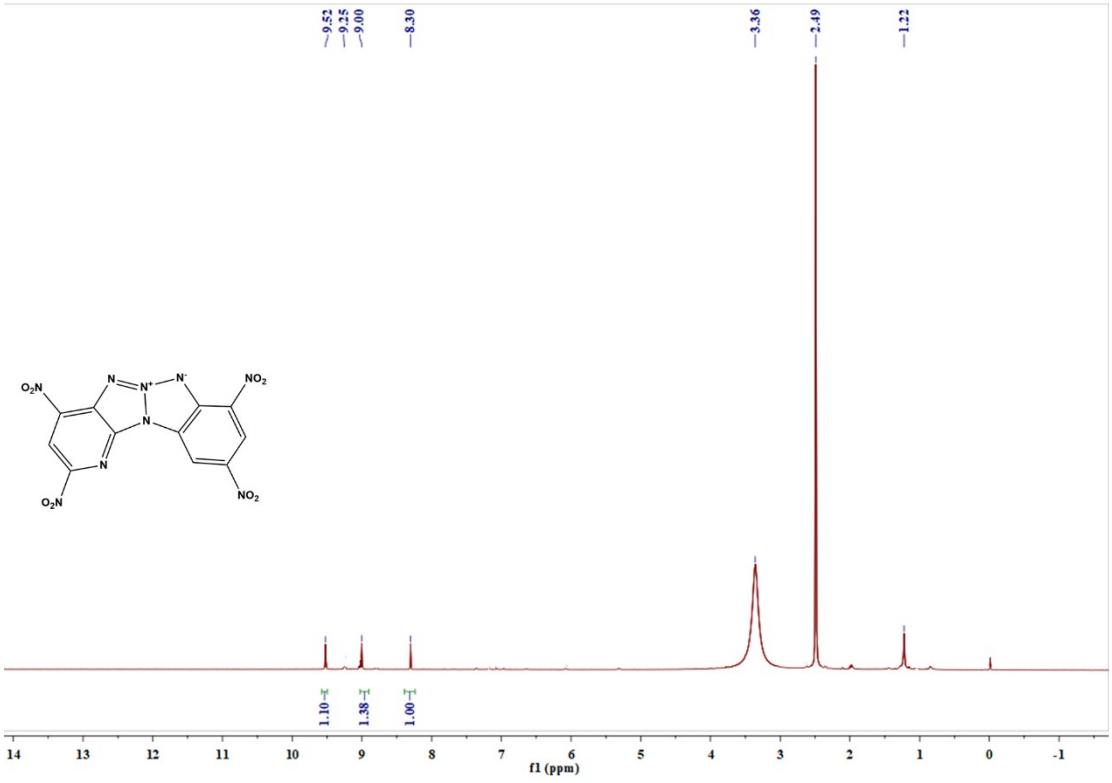

Fig. S6 The ^{1}H NMR of compound **7**.

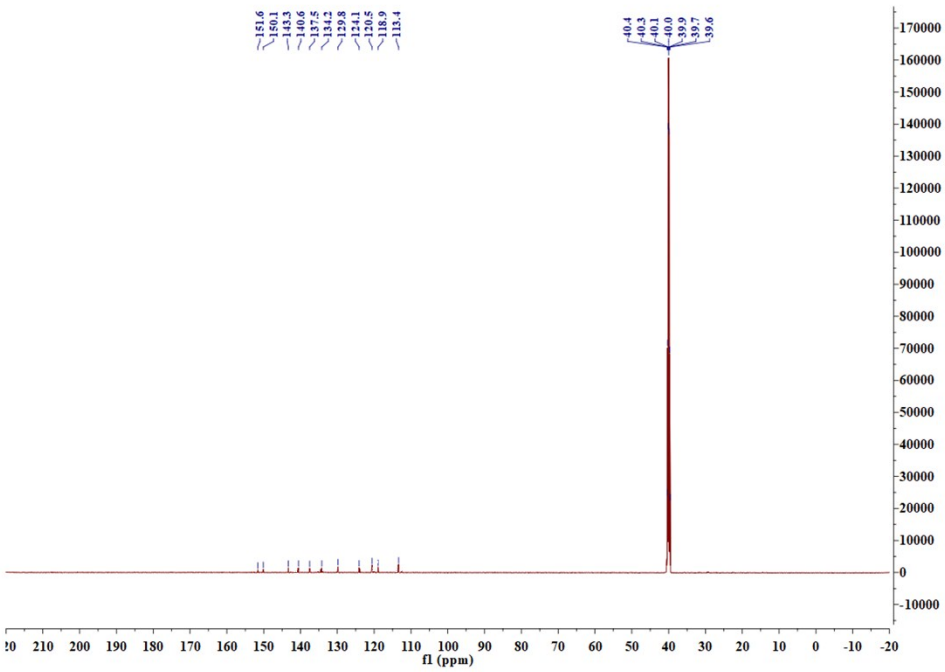

Fig. S7 The ^{13}C NMR of compound **7**.

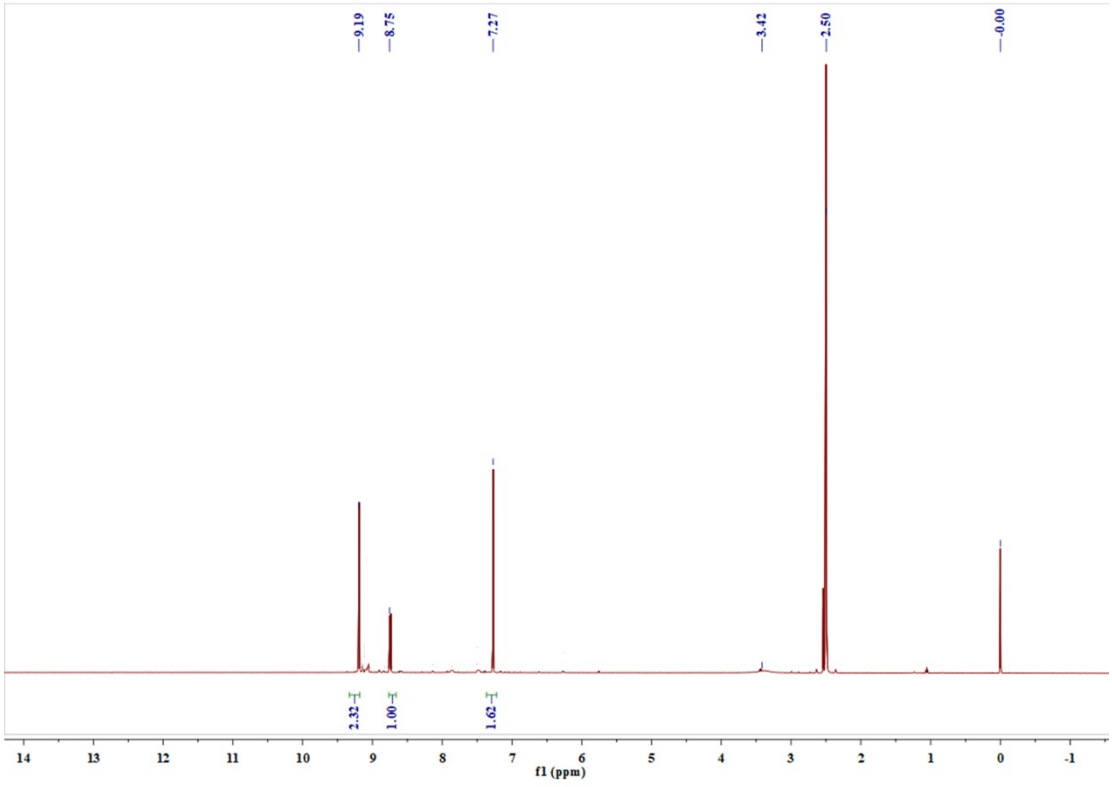

Fig. S8 The ^{1}H NMR of compound **8**.

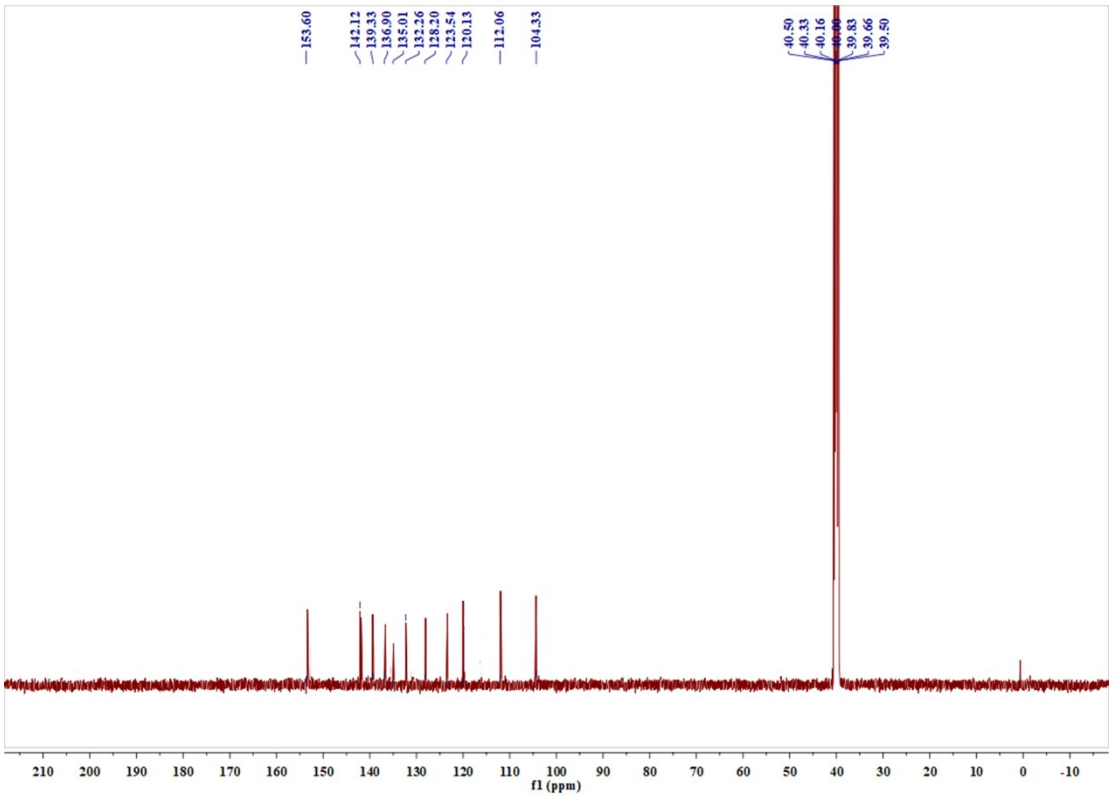

Fig. S9 The ^{13}C NMR of compound **8**.

4. The TG curves of compound 7 and 8

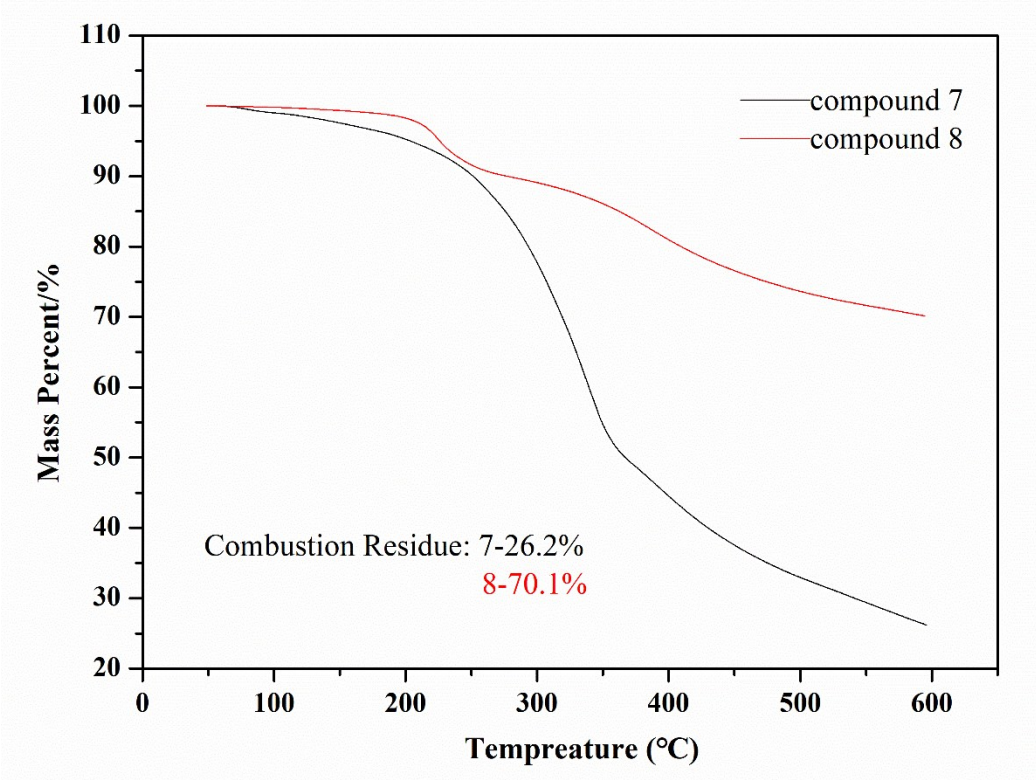

Fig. S10 The TG curves of compound **7** and **8**.

5. The peak temperatures of 7 and 8.

Table S2 The peak temperatures of **7** and **8**.

β (K/min)	Peaks temperatures Tp (K)	
	7	**8**
5	638.85	453.65
10	647.15	457.85
15	648.95	459.95
20	658.05	464.55