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Studies on the synthesis and properties of ploynitro compounds based on esteryl backbones

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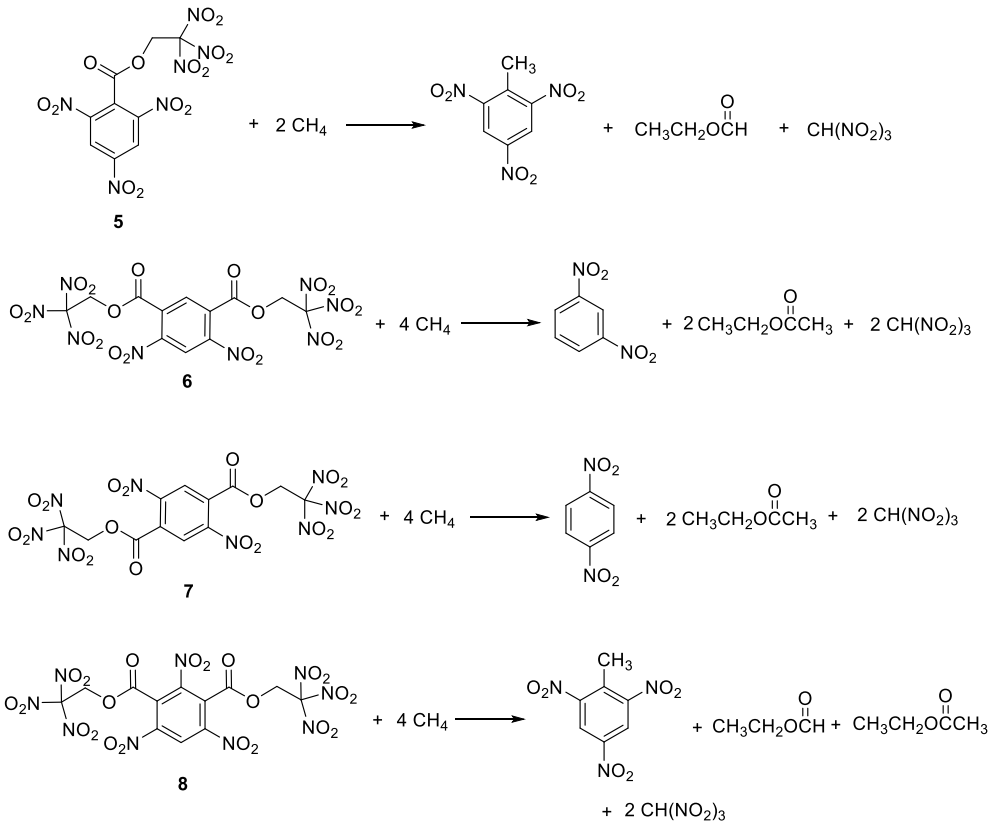
1. Computational Details

Computations were performed by using the Gaussian09 suite of programs.[1] The elementary geometric optimization and the frequency analysis were performed at the level of the Becke three parameter, Lee-Yan-Parr (B3LYP)[2] functional with the 6-311+G** basis set.[3] All of the optimized structures were characterized to be local energy minima on the potential surface without any imaginary frequencies. Atomization energies were calculated by the CBS-4M.[4] All the optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies. The lattice energy of the trinitroethyl derivatives were predicted by using the formula suggested by Jenkins et al.[5]

The predictions of heats of formation (HOF) used the hybrid DFTB3LYP methods with the 6-311+G** basis set through designed isodesmic reactions. The isodesmic reaction processes, that is, the number of each kind of formal bond is conserved, were used with the application of the bond separation reaction (BSR) rules. The molecule was broken down into a set of two heavy-atom molecules containing the same component bonds. The isodesmic reactions used to derive the HOF of compounds **5**- **8** are shown in Scheme S1.



Scheme S1. Isodesmic and tautomeric reactions to compute the HOF.

$$\Delta H_{298} = \Sigma \Delta_f HP - \Sigma \Delta_f HR \qquad (1)$$

$\Delta_f HR$ and $\Delta_f HP$ are the HOF of the reactants and products at 298 K, respectively, and ΔH_{298} can

be calculated from the following expression, see Equation (2).

$$\Delta H_{298} = \Delta E_{298} + \Delta(PV) = \Delta E_0 + \Delta ZPE + \Delta H_T + \Delta nRT \qquad (2)$$

ΔE_0 is the change in total energy between the products and the reactants at 0 K; ΔZPE is the difference between the zero-point energies (ZPE) of the products and the reactants at 0 K; ΔH_T is the thermal correction from 0 to 298 K. The Δ(P*V*) value in Equation [(2)] is the P*V* work term. It equals Δn*RT* for the reactions of an ideal gas. For the isodesmic reactions, $\Delta n = 0$, so Δ(P*V*) = 0. On the left side of Equation [(1)], apart from target compound, all the others are called reference compounds. The HOF of reference compounds are available either from experiments[6-8] or from the the high-level computing such as CBS-4M.

The detonation velocity (*D*) and detonation pressure (*P*) were evaluated by the empirical Kamlet –Jacobs (K-J) equations as shown in Equations (3), (4), (5).

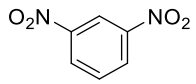
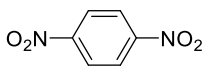
$$P = 1.558\,\rho 2\Phi \qquad (3)$$

$$D = 1.01\Phi 1/2(1 + 1.30\rho_0) \qquad (4)$$

$$\Phi = 0.4889N(MQ)^{1/2} \qquad (5)$$

D is the predicted detonation velocity (km s^{-1}), *P* is the detonation pressure (GPa), and ρ is the compound density (g cm^{-3}). Φ, *N*, *M* and *Q* are characteristic parameters of an explosive; *Q* is the chemical energy of detonation (kJ g^{-1}). The crystal densities and the calculated heats of formation were used to compute the *D* and *P* values.

Table S1. Ab initio computational values of trinitroethyl-substituted furazan derivatives

Compound	E_0[a]	ZPE[b]	H_T[c]	HOF[d]
5	-1726.861343	460.83	71.81	-243.88
6	-2403.203867	649.09	101.28	-504.16
7	-2403.202137	649.21	101.22	-534.93
8	-2607.738754	653.16	108.67	-443.6
CH_4	-40.5339263	112.26	10.04	-74.6
$CH_3COOCH_2CH_3$	-307.8040793	296	22.61	-443.6
$HCOOCH_2CH_3$	-268.4604119	234.41	16.12	-381.88
$CHC(NO_3)_3$	-654.163836	136.82	26.41	-13.4
TNT	-885.3022741	338.5	39.86	21.90
	-641.4316182	263.43	28.13	53.92
	-641.431615	263.43	28.19	18.62

[a] E0 in a.u. ZPE (vibrational zero-point energy)，ΔH_T (thermal correction to enthalpy) and HOF are in kJ mol^{-1}. [b] Data are from Ref. [D. R. Lide, ed., CRC Handbook of Chemistry and Physics, 88th Edition (Internet Version 2008), CRC Press/Taylor and Francis, Boca Raton, FL.]. [c] Data obtained from CBS-4M calculation in combination with the atomization reaction of the corresponding compound. [d] Heat of formation (kJ mol^{-1}).

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2. Selected bond lengths [Å], angles [°] and hydrogen bonds details of esters derivative 5-8

Table S2. Selected bond lengths [Å] and angles [°] for compound **5**

C(1)-C(6)	1.381(3)	C(8)-H(8B)	0.99
C(1)-C(2)	1.479(3)	C(9)-N(2)	1.518(2)
C(1)-N(1)	1.375(3)	C(9)-N(4)	1.521(3)
C(2)-C(3)	0.95	C(9)-N(3)	1.523(2)
C(2)-C(7)	1.374(3)	N(1)-O(2)	1.216(2)
C(3)-C(4)	1.485(3)	N(1)-O(1)	1.221(2)
C(3)-N(5)	0.95	N(2)-O(5)	1.211(2)
C(4)-C(5)	1.196(2)	N(2)-O(6)	1.211(2)
C(4)-H(4)	1.337(2)	N(3)-O(7)	1.213(2)
C(5)-C(6)	1.435(2)	N(3)-O(8)	1.213(2)
C(5)-N(6)	1.507(3)	N(4)-O(9)	1.210(2)
C(6)-H(6)	0.99	N(4)-O(10)	1.214(2)
C(7)-O(4)	1.381(3)	N(5)-O(11)	1.219(2)
C(7)-O(3)	1.479(3)	N(5)-O(12)	1.220(2)
C(8)-O(3)	1.375(3)	N(6)-O(14)	1.215(3)
C(8)-C(9)	0.95	N(6)-O(13)	1.219(2)
C(8)-H(8A)	1.374(3)		
C(6)-C(1)-C(2)	123.58(19)	H(8A)-C(8)-H(8B)	108.5
C(6)-C(1)-N(1)	117.57(19)	C(8)-C(9)-N(2)	113.64(16)
C(2)-C(1)-N(1)	118.86(18)	C(8)-C(9)-N(4)	112.26(16)
C(1)-C(2)-C(3)	115.82(18)	N(2)-C(9)-N(4)	106.81(15)

C(1)-C(2)-C(7)	121.51(17)	C(8)-C(9)-N(3)	110.51(15)
C(3)-C(2)-C(7)	122.58(18)	N(2)-C(9)-N(3)	106.72(14)
C(4)-C(3)-C(2)	122.7(2)	N(4)-C(9)-N(3)	106.49(15)
C(4)-C(3)-N(5)	117.67(17)	O(2)-N(1)-O(1)	125.20(19)
C(2)-C(3)-N(5)	119.64(18)	O(2)-N(1)-C(1)	118.12(18)
C(5)-C(4)-C(3)	117.76(19)	O(1)-N(1)-C(1)	116.68(19)
C(5)-C(4)-H(4)	121.1	O(5)-N(2)-O(6)	127.29(16)
C(3)-C(4)-H(4)	121.1	O(5)-N(2)-C(9)	114.74(16)
C(6)-C(5)-C(4)	123.0(2)	O(6)-N(2)-C(9)	117.96(16)
C(6)-C(5)-N(6)	118.5(2)	O(7)-N(3)-O(8)	127.89(18)
C(4)-C(5)-N(6)	118.54(19)	O(7)-N(3)-C(9)	115.06(16)
C(5)-C(6)-C(1)	117.0(2)	O(8)-N(3)-C(9)	117.04(17)
C(5)-C(6)-H(6)	121.5	O(9)-N(4)-O(10)	128.34(19)
C(1)-C(6)-H(6)	121.5	O(9)-N(4)-C(9)	114.20(16)
O(4)-C(7)-O(3)	125.57(18)	O(10)-N(4)-C(9)	117.46(16)
O(4)-C(7)-C(2)	123.86(18)	O(11)-N(5)-O(12)	124.70(18)
O(3)-C(7)-C(2)	110.56(15)	O(11)-N(5)-C(3)	117.23(17)
O(3)-C(8)-C(9)	107.15(15)	O(12)-N(5)-C(3)	118.07(16)
O(3)-C(8)-H(8A)	110.3	O(14)-N(6)-O(13)	125.3(2)
C(9)-C(8)-H(8A)	110.3	O(14)-N(6)-C(5)	117.6(2)
O(3)-C(8)-H(8B)	110.3	O(13)-N(6)-C(5)	117.1(2)
C(9)-C(8)-H(8B)	110.3	C(7)-O(3)-C(8)	113.67(14)

Table S3. Hydrogen bonds present in compound **5**

D—H•••A	d(D-H)/ Å	d(H...A)/ Å	d(D...A)/ Å	<(DHA)/ °	comment
C(8) —H(8A) •••O(5)^{i}	0.99	2.43	3.3328	151	inter
C(8) —H(8B) •••O(4)^{ii}	0.99	2.42	3.3388	154	inter

i: 1+x,y,z; ii: 1-x,1-y,1-z.

Table S4. Selected bond lengths [Å] and angles [^{o}] for compound **6**

C(1)-C(2)	1.375(3)	C(11)-C(12)	1.502(3)
C(1)-C(6)	1.387(3)	C(11)-H(11A)	0.99
C(1)-N(1)	1.477(2)	C(11)-H(11B)	0.99
C(2)-C(3)	1.376(3)	C(12)-N(8)	1.521(3)
C(2)-H(2)	0.95	C(12)-N(7)	1.523(3)
C(3)-C(4)	1.385(3)	C(12)-N(6)	1.531(2)
C(3)-N(2')	1.477(11)	N(1)-O(2)	1.218(2)
C(3)-N(2)	1.489(8)	N(1)-O(1)	1.222(2)
C(4)-C(5)	1.385(3)	N(3)-O(7)	1.208(2)
C(4)-C(7)	1.507(3)	N(3)-O(8)	1.215(2)

C(5)-C(6)	1.386(3)	N(4)-O(9)	1.207(2)
C(5)-H(5)	0.95	N(4)-O(10)	1.210(2)
C(6)-C(10)	1.491(3)	N(5)-O(12)	1.210(2)
C(7)-O(6)	1.180(2)	N(5)-O(11)	1.210(2)
C(7)-O(5)	1.344(2)	N(6)-O(15)	1.202(2)
C(8)-O(5)	1.437(2)	N(6)-O(16)	1.207(2)
C(8)-C(9)	1.505(3)	N(7)-O(18)	1.210(3)
C(8)-H(8A)	0.99	N(7)-O(17)	1.218(2)
C(8)-H(8B)	0.99	N(8)-O(19)	1.204(2)
C(9)-N(5)	1.518(3)	N(8)-O(20)	1.210(2)
C(9)-N(4)	1.526(2)	N(2)-O(3)	1.179(8)
C(9)-N(3)	1.527(3)	N(2)-O(4)	1.181(8)
C(10)-O(14)	1.194(2)	N(2')-O(4')	1.180(11)
C(10)-O(13)	1.351(2)	N(2')-O(3')	1.197(11)
C(11)-O(13)	1.436(2)		
C(2)-C(1)-C(6)	122.36(17)	O(13)-C(11)-H(11A)	110.3
C(2)-C(1)-N(1)	117.19(16)	C(12)-C(11)-H(11A)	110.3
C(6)-C(1)-N(1)	120.31(17)	O(13)-C(11)-H(11B)	110.3
C(1)-C(2)-C(3)	117.54(17)	C(12)-C(11)-H(11B)	110.3
C(1)-C(2)-H(2)	121.2	H(11A)-C(11)-H(11B)	108.6
C(3)-C(2)-H(2)	121.2	C(11)-C(12)-N(8)	110.35(16)
C(2)-C(3)-C(4)	122.80(19)	C(11)-C(12)-N(7)	110.80(17)
C(2)-C(3)-N(2')	119.6(6)	N(8)-C(12)-N(7)	107.02(17)
C(4)-C(3)-N(2')	117.3(6)	C(11)-C(12)-N(6)	113.91(16)
C(2)-C(3)-N(2)	115.9(5)	N(8)-C(12)-N(6)	106.98(15)
C(4)-C(3)-N(2)	120.6(5)	N(7)-C(12)-N(6)	107.46(15)
N(2')-C(3)-N(2)	14.6(10)	O(2)-N(1)-O(1)	125.49(17)
C(5)-C(4)-C(3)	117.68(18)	O(2)-N(1)-C(1)	117.30(17)
C(5)-C(4)-C(7)	117.04(17)	O(1)-N(1)-C(1)	117.17(16)
C(3)-C(4)-C(7)	125.27(18)	O(7)-N(3)-O(8)	127.21(19)
C(4)-C(5)-C(6)	121.58(18)	O(7)-N(3)-C(9)	116.40(18)
C(4)-C(5)-H(5)	119.2	O(8)-N(3)-C(9)	116.38(19)
C(6)-C(5)-H(5)	119.2	O(9)-N(4)-O(10)	127.3(2)
C(5)-C(6)-C(1)	118.01(18)	O(9)-N(4)-C(9)	115.16(19)
C(5)-C(6)-C(10)	116.69(16)	O(10)-N(4)-C(9)	117.6(2)
C(1)-C(6)-C(10)	125.30(17)	O(12)-N(5)-O(11)	128.1(2)
O(6)-C(7)-O(5)	125.52(19)	O(12)-N(5)-C(9)	117.80(19)
O(6)-C(7)-C(4)	125.5(2)	O(11)-N(5)-C(9)	114.02(19)
O(5)-C(7)-C(4)	108.70(17)	O(15)-N(6)-O(16)	127.15(18)
O(5)-C(8)-C(9)	106.26(15)	O(15)-N(6)-C(12)	116.20(17)

O(5)-C(8)-H(8A)	110.5	O(16)-N(6)-C(12)	116.64(18)
C(9)-C(8)-H(8A)	110.5	O(18)-N(7)-O(17)	127.7(2)
O(5)-C(8)-H(8B)	110.5	O(18)-N(7)-C(12)	117.4(2)
C(9)-C(8)-H(8B)	110.5	O(17)-N(7)-C(12)	114.9(2)
H(8A)-C(8)-H(8B)	108.7	O(19)-N(8)-O(20)	128.0(2)
C(8)-C(9)-N(5)	110.86(17)	O(19)-N(8)-C(12)	114.57(18)
C(8)-C(9)-N(4)	111.28(16)	O(20)-N(8)-C(12)	117.41(18)
N(5)-C(9)-N(4)	106.98(16)	C(7)-O(5)-C(8)	117.16(15)
C(8)-C(9)-N(3)	113.64(17)	C(10)-O(13)-C(11)	114.84(14)
N(5)-C(9)-N(3)	107.92(16)	O(3)-N(2)-O(4)	122.4(8)
N(4)-C(9)-N(3)	105.81(15)	O(3)-N(2)-C(3)	117.9(7)
O(14)-C(10)-O(13)	124.34(18)	O(4)-N(2)-C(3)	119.6(8)
O(14)-C(10)-C(6)	123.78(18)	O(4')-N(2')-O(3')	122.8(12)
O(13)-C(10)-C(6)	111.82(16)	O(4')-N(2')-C(3)	119.6(11)
O(13)-C(11)-C(12)	106.91(15)	O(3')-N(2')-C(3)	117.3(10)

Table S5. Hydrogen bonds present in compound **6**

D—H•••A	d(D-H)/ Å	d(H...A)/ Å	d(D...A)/ Å	<(DHA)/ °	comment
C(2) —H(2) •••O(7)^{i}	0.95	2.53	3.430(2)	158	inter
C(5) —H(5) •••O (17)^{ii}	0.95	2.49	3.401(2)	3.401(2)	inter
C(8) —H(8A••• O(2)^{iii}	0.99	2.41	3.157(2)	131	inter
C(8) —H(8B) •••O(6)	0.99	2.30	2.704(3)	103	intra
C(8) —H(8B) •••O(6)^{iv}	0.99	2.39	3.331(3)	157	inter
C(11) —H(11A)•••O(14)^{ii}	0.99	2.27	3.235(2)	166	inter
C(11) —H(11A) •••O(14)^{v}	0.99	2.52	3.448(3)	156	inter

i: -x,-1/2+y,1/2-z; ii: 1-x,1-y,1-z; iii: x,3/2-y,1/2+z; iv: -x,2-y,1-z; v: 1-x,1-y,1-z.

Table S6. Selected bond lengths [Å] and angles [^{o}] for compound **7**

C(1)-C(3)#1	1.378(3)	C(5)-H(5B)	0.99
C(1)-C(2)	1.392(3)	C(6)-N(4)	1.512(4)
C(1)-N(1)	1.476(3)	C(6)-N(2)	1.520(3)
C(2)-C(3)	1.379(3)	C(6)-N(3)	1.528(3)
C(2)-C(4)	1.498(3)	N(1)-O(2)	1.213(3)
C(3)-C(1)#1	1.378(3)	N(1)-O(1)	1.215(3)
C(3)-H(3)	0.95	N(2)-O(6)	1.211(3)
C(4)-O(4)	1.188(3)	N(2)-O(5)	1.213(3)
C(4)-O(3)	1.333(3)	N(3)-O(7)	1.208(3)
C(5)-O(3)	1.434(3)	N(3)-O(8)	1.220(3)
C(5)-C(6)	1.516(4)	N(4)-O(9)	1.213(3)
C(5)-H(5A)	0.99	N(4)-O(10)	1.214(3)

C(3)#1-C(1)-C(2)	122.9(2)	N(4)-C(6)-N(2)	106.7(2)
C(3)#1-C(1)-N(1)	117.9(2)	C(5)-C(6)-N(2)	109.2(2)
C(2)-C(1)-N(1)	119.2(2)	N(4)-C(6)-N(3)	107.4(2)
C(3)-C(2)-C(1)	118.1(2)	C(5)-C(6)-N(3)	111.6(2)
C(3)-C(2)-C(4)	118.8(2)	N(2)-C(6)-N(3)	107.4(2)
C(1)-C(2)-C(4)	122.9(2)	O(2)-N(1)-O(1)	124.4(2)
C(1)#1-C(3)-C(2)	119.0(2)	O(2)-N(1)-C(1)	117.4(2)
C(1)#1-C(3)-H(3)	120.5	O(1)-N(1)-C(1)	118.2(2)
C(2)-C(3)-H(3)	120.5	O(6)-N(2)-O(5)	127.4(2)
O(4)-C(4)-O(3)	123.5(2)	O(6)-N(2)-C(6)	118.5(2)
O(4)-C(4)-C(2)	124.7(2)	O(5)-N(2)-C(6)	114.1(2)
O(3)-C(4)-C(2)	111.7(2)	O(7)-N(3)-O(8)	128.0(2)
O(3)-C(5)-C(6)	106.1(2)	O(7)-N(3)-C(6)	117.4(2)
O(3)-C(5)-H(5A)	110.5	O(8)-N(3)-C(6)	114.6(2)
C(6)-C(5)-H(5A)	110.5	O(9)-N(4)-O(10)	127.2(3)
O(3)-C(5)-H(5B)	110.5	O(9)-N(4)-C(6)	116.3(2)
C(6)-C(5)-H(5B)	110.5	O(10)-N(4)-C(6)	116.5(2)
H(5A)-C(5)-H(5B)	108.7	C(4)-O(3)-C(5)	113.60(19)
N(4)-C(6)-C(5)	114.3(2)		

Table S7. Hydrogen bonds present in compound **7**

D—H•••A	d(D-H)/ Å	d(H...A)/ Å	d(D...A)/ Å	<(DHA)/ °	comment
C(3) —H(3) •••O(10)^{i}	0.95	2.57	3.235(4)	127	inter
C(3) —H(3) •••O(7)^{ii}	0.95	2.55	3.397(3)	148	inter
C(5) —H(5B) •••O(4)^{iii}	0.99	2.28	3.144(4)	145	inter

i: x,y,1+z; ii: x,3/2-y,1/2+z; iii: x,1/2-y,-1/2+z.

Table S8. Selected bond lengths [Å] and angles [^{o}] for compound **8**

C(1)-C(2)	1.388(3)	C(11)-C(12)	1.513(3)
C(1)-C(6)	1.394(3)	C(11)-H(11A)	0.99
C(1)-N(1)	1.480(3)	C(11)-H(11B)	0.99
C(2)-C(3)	1.390(3)	C(12)-N(8)	1.520(3)
C(2)-C(7)	1.514(3)	C(12)-N(7)	1.523(3)
C(3)-C(4)	1.383(3)	C(12)-N(9)	1.525(3)
C(3)-N(5)	1.474(3)	N(1)-O(2)	1.221(2)
C(4)-C(5)	1.381(3)	N(1)-O(1)	1.222(2)
C(4)-H(4)	0.95	N(2)-O(6)	1.213(2)
C(5)-C(6)	1.391(3)	N(2)-O(5)	1.215(2)
C(5)-N(6)	1.469(3)	N(3)-O(8)	1.208(2)
C(6)-C(10)	1.514(3)	N(3)-O(7)	1.208(2)

C(7)-O(4)	1.191(2)	N(4)-O(9)	1.202(2)
C(7)-O(3)	1.334(2)	N(4)-O(10)	1.214(2)
C(8)-O(3)	1.438(2)	N(5)-O(12)	1.217(2)
C(8)-C(9)	1.513(3)	N(5)-O(11)	1.224(2)
C(8)-H(8A)	0.99	N(6)-O(14)	1.212(2)
C(8)-H(8B)	0.99	N(6)-O(13)	1.228(2)
C(9)-N(2)	1.515(3)	N(7)-O(17)	1.196(2)
C(9)-N(4)	1.522(3)	N(7)-O(18)	1.212(2)
C(9)-N(3)	1.524(3)	N(8)-O(19)	1.208(2)
C(10)-O(16)	1.193(2)	N(8)-O(20)	1.216(2)
C(10)-O(15)	1.335(2)	N(9)-O(21)	1.205(2)
C(11)-O(15)	1.440(2)	N(9)-O(22)	1.214(2)
C(2)-C(1)-C(6)	123.49(18)	O(15)-C(11)-H(11B)	110.7
C(2)-C(1)-N(1)	118.16(18)	C(12)-C(11)-H(11B)	110.7
C(6)-C(1)-N(1)	118.33(18)	H(11A)-C(11)-H(11B)	108.8
C(1)-C(2)-C(3)	116.52(18)	C(11)-C(12)-N(8)	110.60(16)
C(1)-C(2)-C(7)	122.16(18)	C(11)-C(12)-N(7)	109.72(16)
C(3)-C(2)-C(7)	121.29(18)	N(8)-C(12)-N(7)	107.92(17)
C(4)-C(3)-C(2)	122.87(19)	C(11)-C(12)-N(9)	113.78(18)
C(4)-C(3)-N(5)	117.70(18)	N(8)-C(12)-N(9)	108.18(16)
C(2)-C(3)-N(5)	119.35(19)	N(7)-C(12)-N(9)	106.40(16)
C(5)-C(4)-C(3)	117.87(19)	O(2)-N(1)-O(1)	125.50(18)
C(5)-C(4)-H(4)	121.1	O(2)-N(1)-C(1)	117.12(17)
C(3)-C(4)-H(4)	121.1	O(1)-N(1)-C(1)	117.37(18)
C(4)-C(5)-C(6)	122.70(19)	O(6)-N(2)-O(5)	127.57(19)
C(4)-C(5)-N(6)	117.54(19)	O(6)-N(2)-C(9)	114.90(17)
C(6)-C(5)-N(6)	119.70(19)	O(5)-N(2)-C(9)	117.52(18)
C(5)-C(6)-C(1)	116.54(19)	O(8)-N(3)-O(7)	128.48(19)
C(5)-C(6)-C(10)	122.02(19)	O(8)-N(3)-C(9)	114.83(17)
C(1)-C(6)-C(10)	121.44(18)	O(7)-N(3)-C(9)	116.68(17)
O(4)-C(7)-O(3)	125.8(2)	O(9)-N(4)-O(10)	127.0(2)
O(4)-C(7)-C(2)	124.83(18)	O(9)-N(4)-C(9)	117.85(19)
O(3)-C(7)-C(2)	109.38(16)	O(10)-N(4)-C(9)	115.16(18)
O(3)-C(8)-C(9)	106.28(15)	O(12)-N(5)-O(11)	125.80(19)
O(3)-C(8)-H(8A)	110.5	O(12)-N(5)-C(3)	117.42(18)
C(9)-C(8)-H(8A)	110.5	O(11)-N(5)-C(3)	116.75(18)
O(3)-C(8)-H(8B)	110.5	O(14)-N(6)-O(13)	125.3(2)
C(9)-C(8)-H(8B)	110.5	O(14)-N(6)-C(5)	117.9(2)
H(8A)-C(8)-H(8B)	108.7	O(13)-N(6)-C(5)	116.83(19)
C(8)-C(9)-N(2)	112.22(17)	O(17)-N(7)-O(18)	128.2(2)

C(8)-C(9)-N(4)	112.41(17)	O(17)-N(7)-C(12)	118.21(19)
N(2)-C(9)-N(4)	107.90(16)	O(18)-N(7)-C(12)	113.50(18)
C(8)-C(9)-N(3)	110.24(16)	O(19)-N(8)-O(20)	128.0(2)
N(2)-C(9)-N(3)	106.30(15)	O(19)-N(8)-C(12)	117.78(18)
N(4)-C(9)-N(3)	107.48(16)	O(20)-N(8)-C(12)	114.21(18)
O(16)-C(10)-O(15)	125.57(19)	O(21)-N(9)-O(22)	127.79(19)
O(16)-C(10)-C(6)	124.61(19)	O(21)-N(9)-C(12)	116.59(19)
O(15)-C(10)-C(6)	109.81(16)	O(22)-N(9)-C(12)	115.62(17)
O(15)-C(11)-C(12)	105.36(15)	C(7)-O(3)-C(8)	114.42(15)
O(15)-C(11)-H(11A)	110.7	C(10)-O(15)-C(11)	114.13(14)
C(12)-C(11)-H(11A)	110.7	O(15)-C(11)-H(11B)	110.7

Table S9. Hydrogen bonds present in compound **8**

D —H•••A	d(D-H)/ Å	d(H...A)/ Å	d(D...A)/ Å	<(DHA)/ °	comment
C(8) —H(8B) •••O(5)[i]	0.99	2.48	3.384(3)	152	inter
C(11)—H(11B)•••O(19)[ii]	0.99	2.47	3.397(3)	157	inter

i: x,1/2-y,1/2+z; ii: x,1/2-y,-1/2+z.

3. ^{1}H and ^{13}C NMR spectra of compounds 5-8

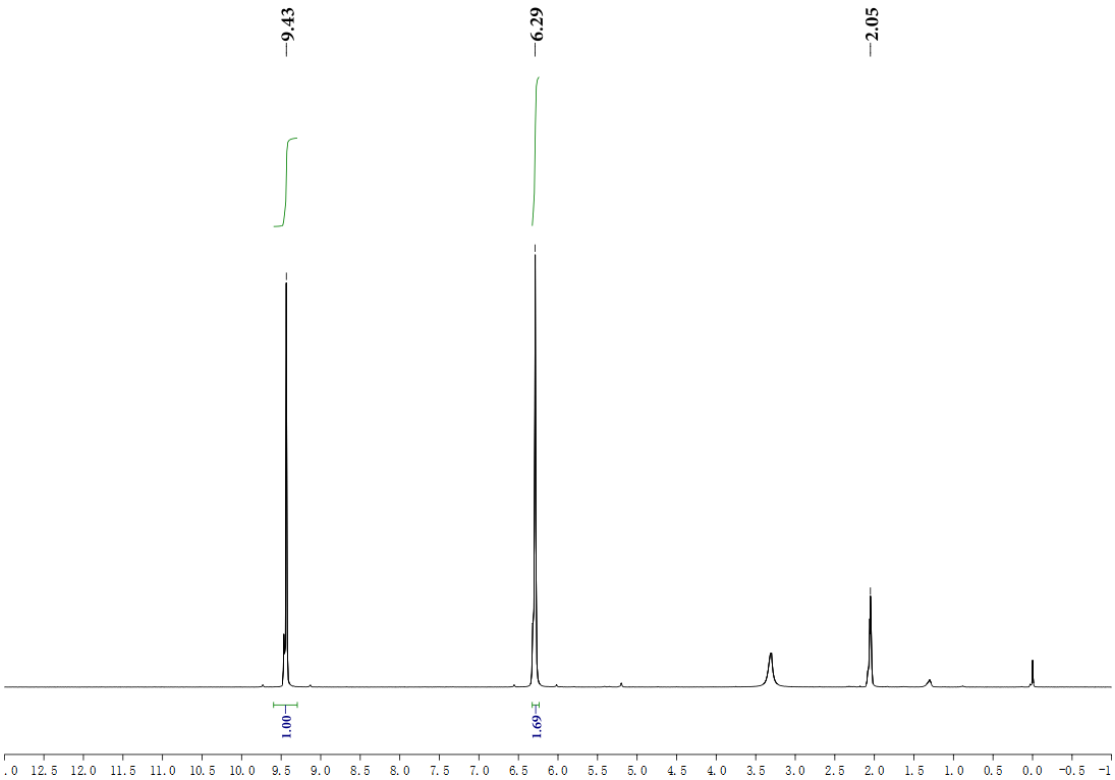

Figure S1 ^{1}H NMR spectra (300 MHz) of **5** in acetone-d_6 at 25 ℃

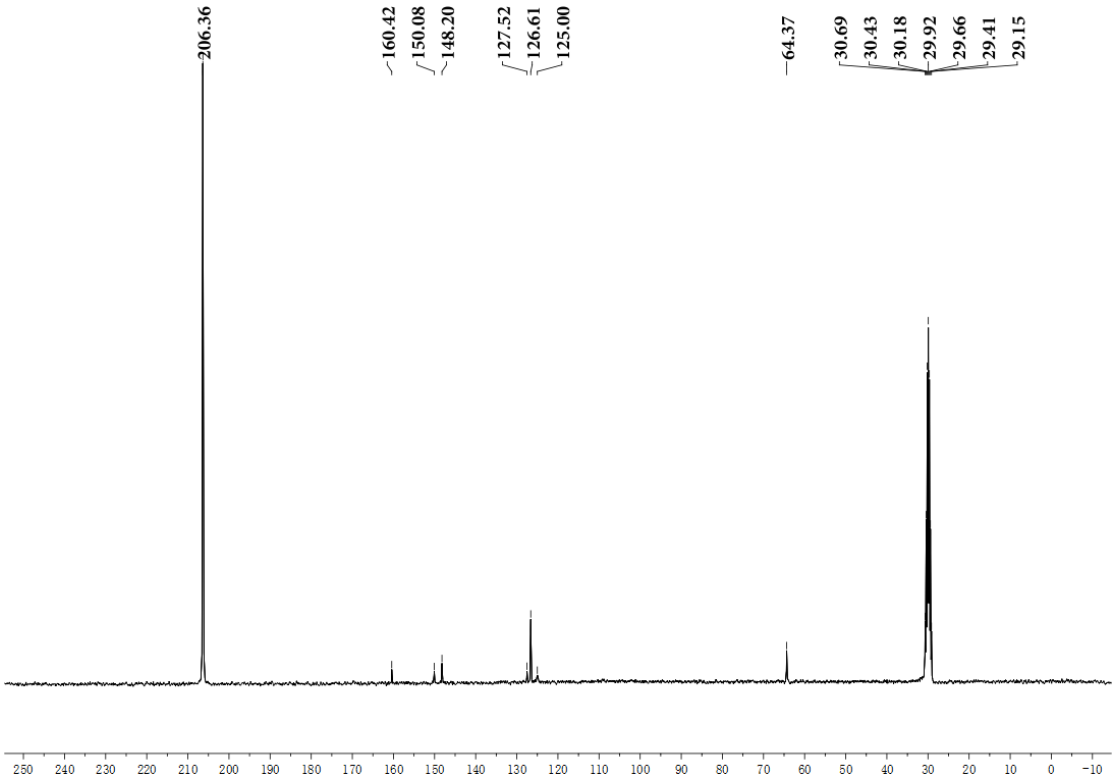

Figure S2 ^{13}C NMR specta (75 MHz) of **5** in acetone-d_6 at 25 ℃

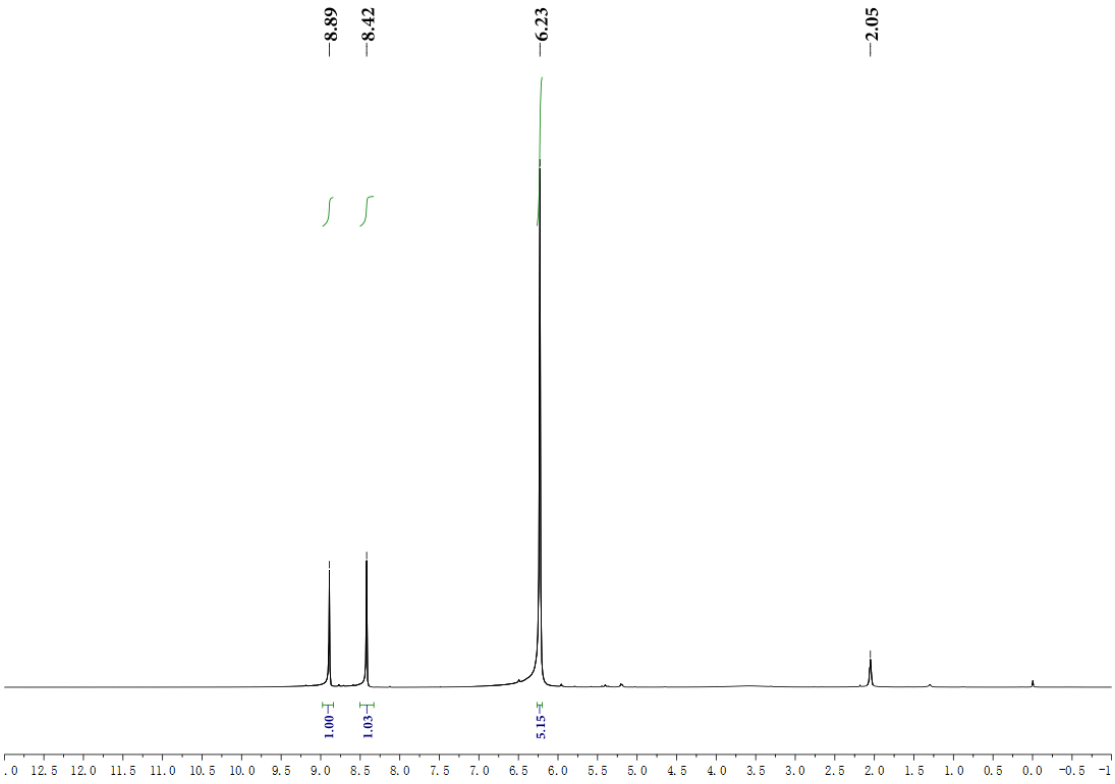

Figure S3 ^{1}H NMR spectra (300 MHz) of **6** in acetone-d_6 at 25 ℃

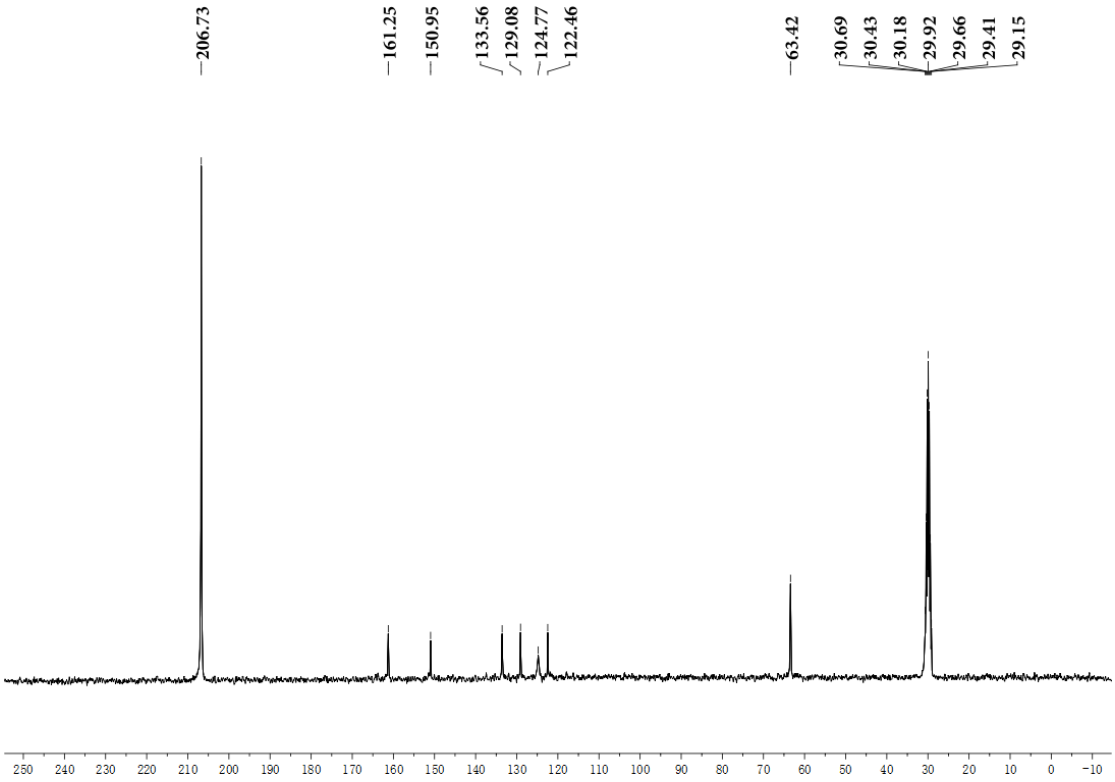

Figure S4 ^{13}C NMR specta (75 MHz) of **6** in acetone-d_6 at 25 ℃

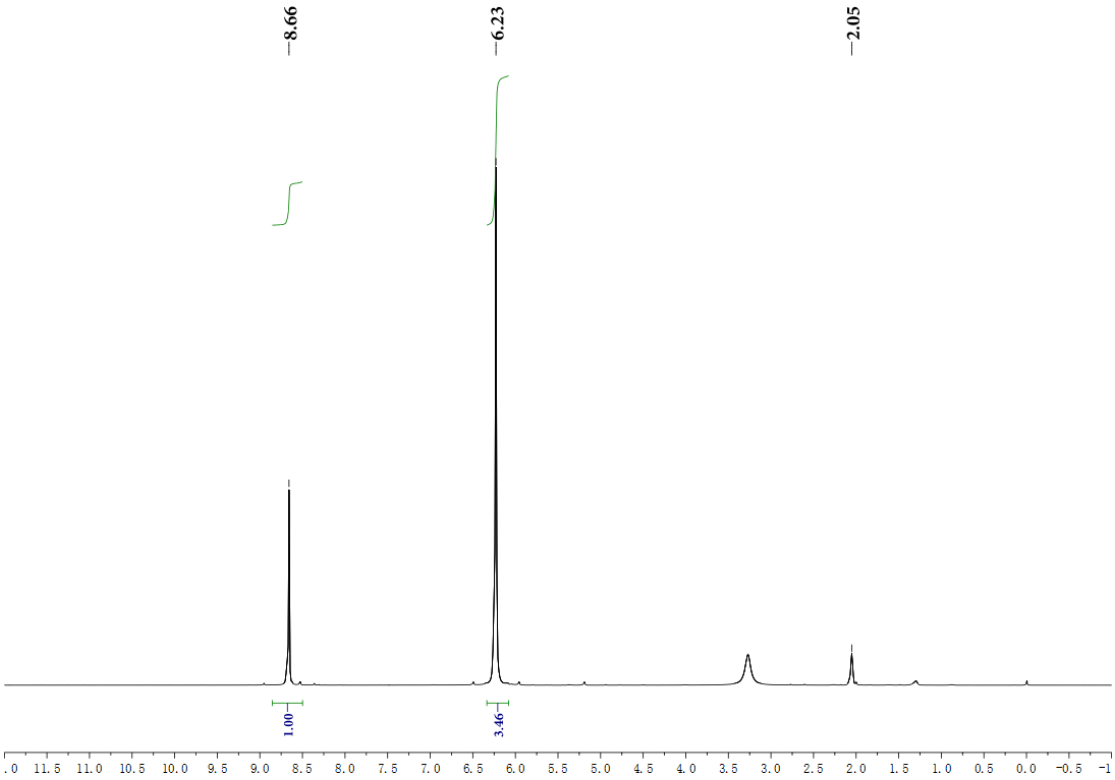

Figure S5 ^{1}H NMR spectra (300 MHz) of **7** in acetone-d_6 at 25 ℃

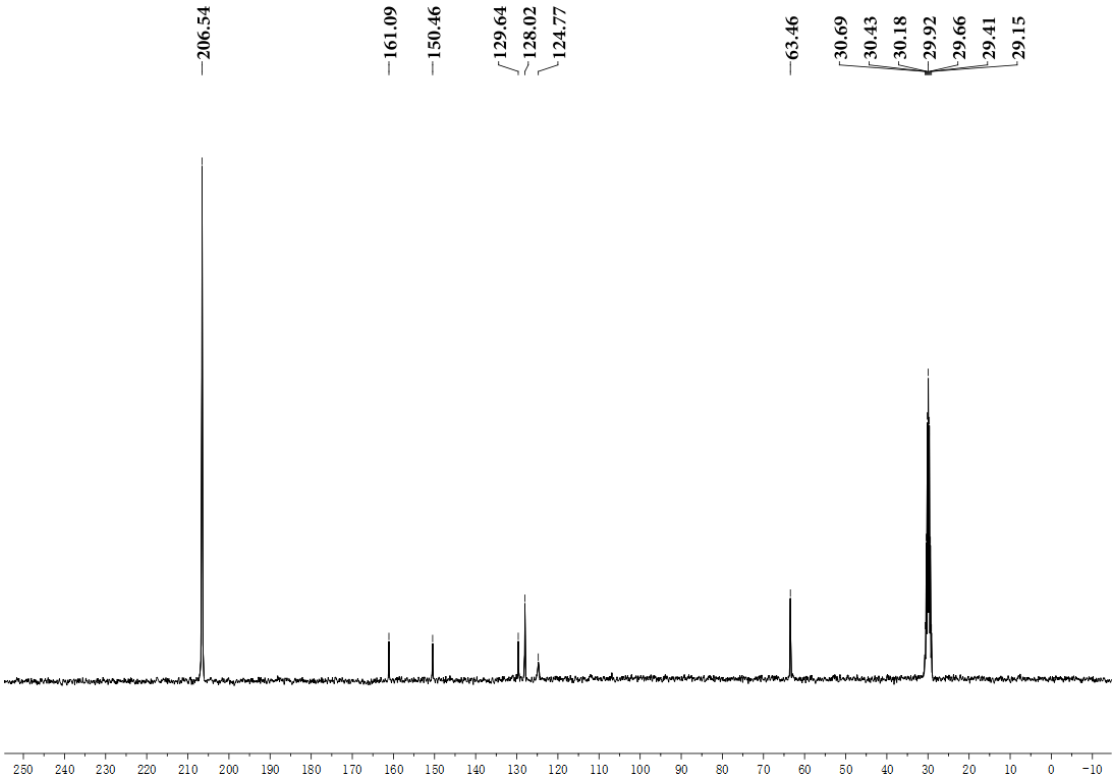

Figure S6 ^{13}C NMR specta (75 MHz) of **7** in acetone-d_6 at 25 ℃

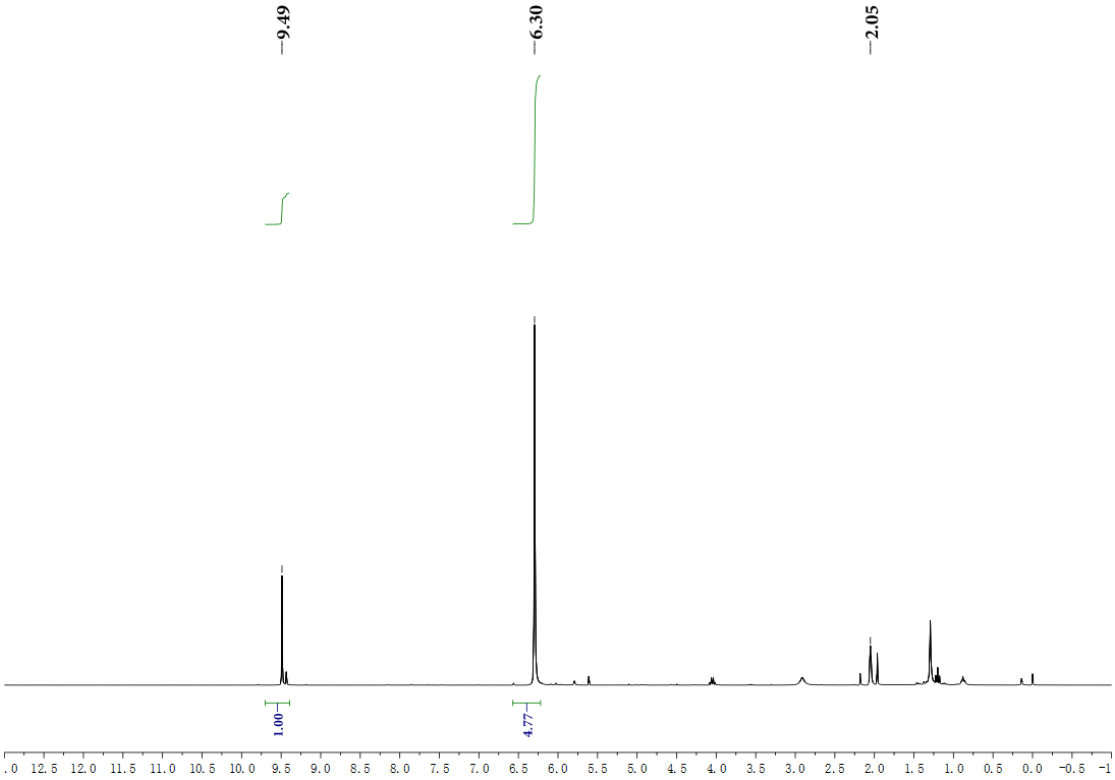

Figure S7 ^{1}H NMR spectra (300 MHz) of **8** in acetone-d_6 at 25 ℃

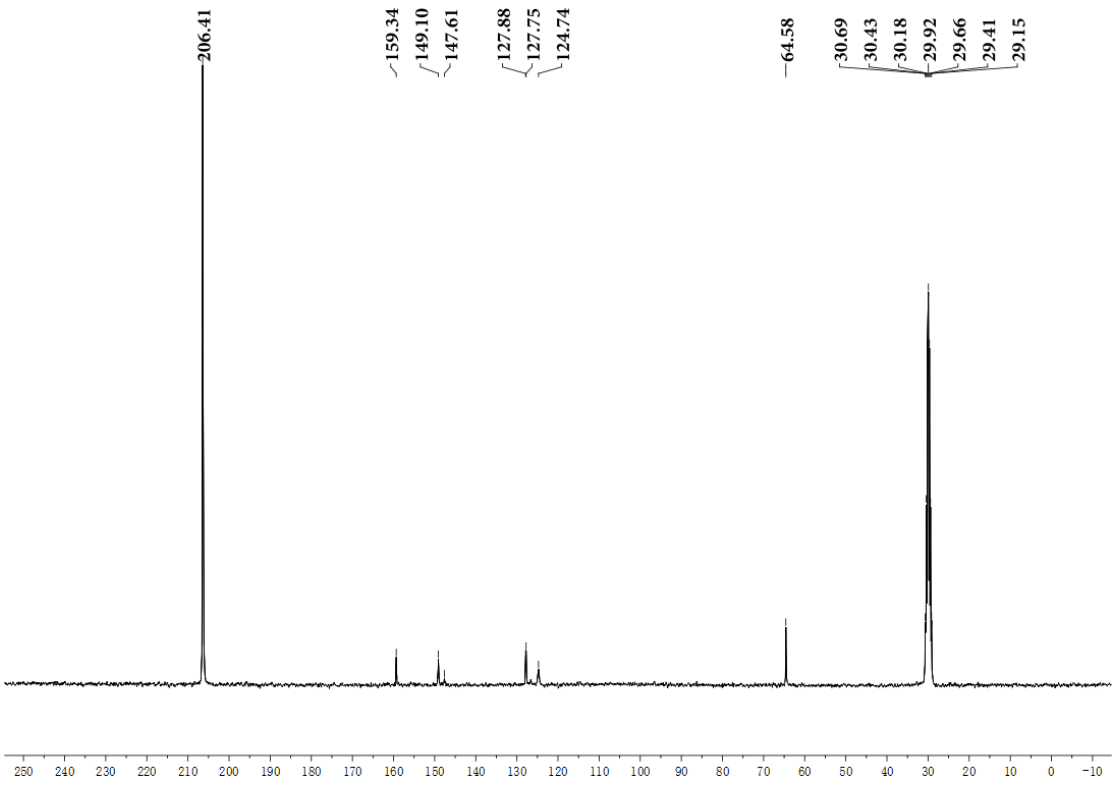

Figure S8 ^{13}C NMR specta (75 MHz) of **8** in acetone-d_6 at 25 ℃

4. DSC curves of compounds 5-8

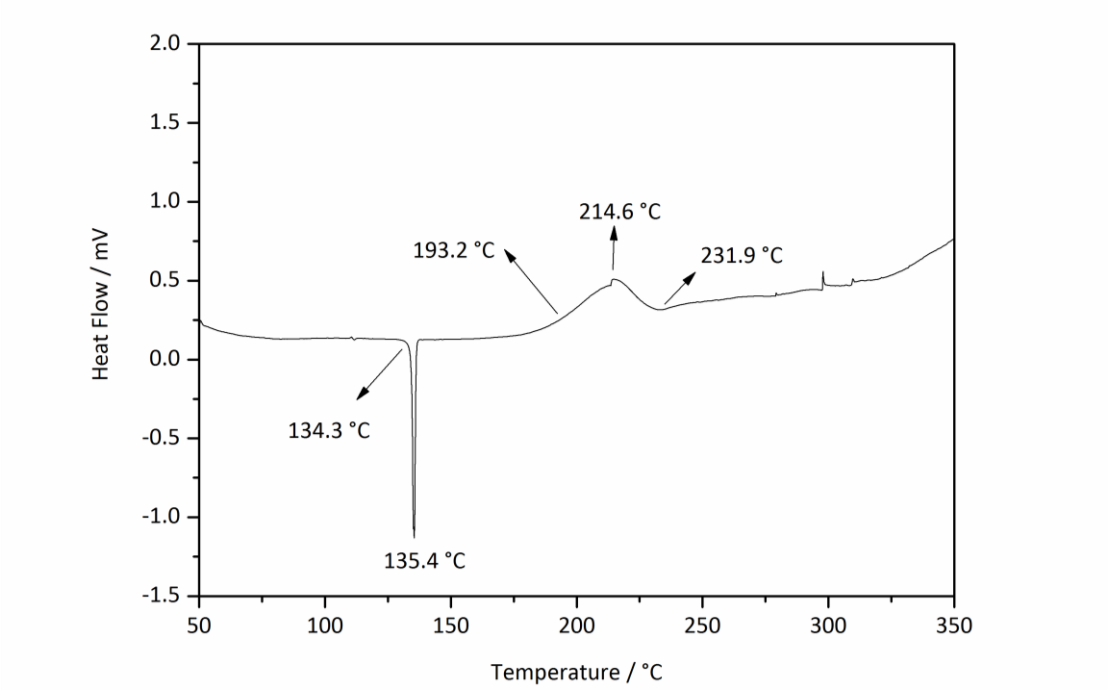

Figure S9 DSC curve of compound **5**

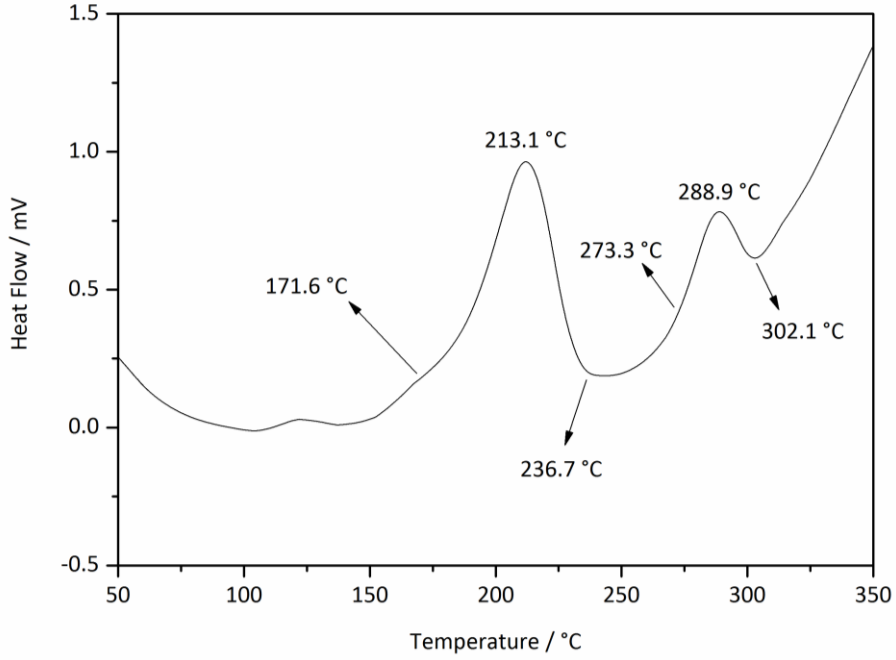

Figure S10 DSC curve of compound **6**

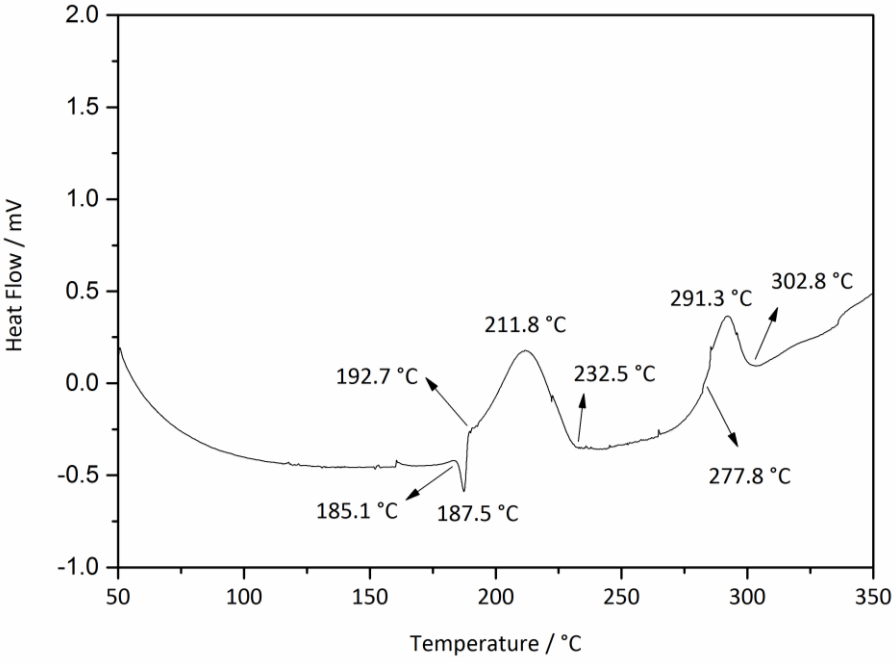

Figure S11 DSC curve of compound **7**

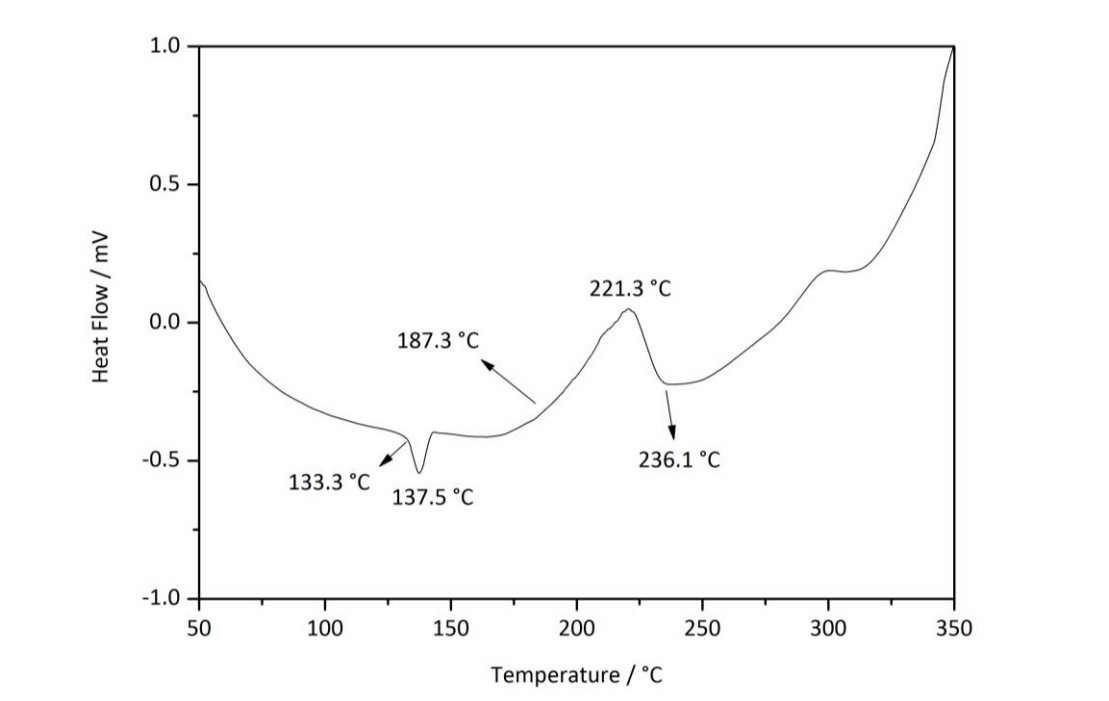

Figure S12 DSC curve of compound **8**