Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

1. NMR Spectrum of the prepared compounds

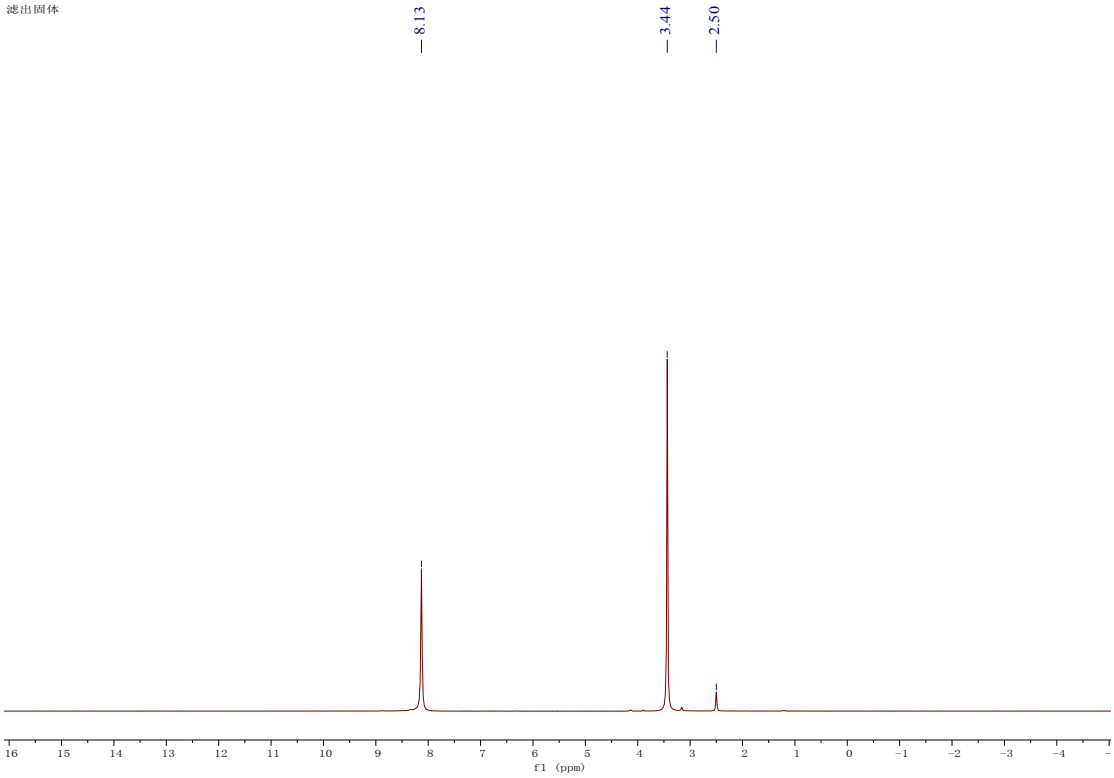


Figure S1 ^{1}H NMR spectrum of compound **2**.

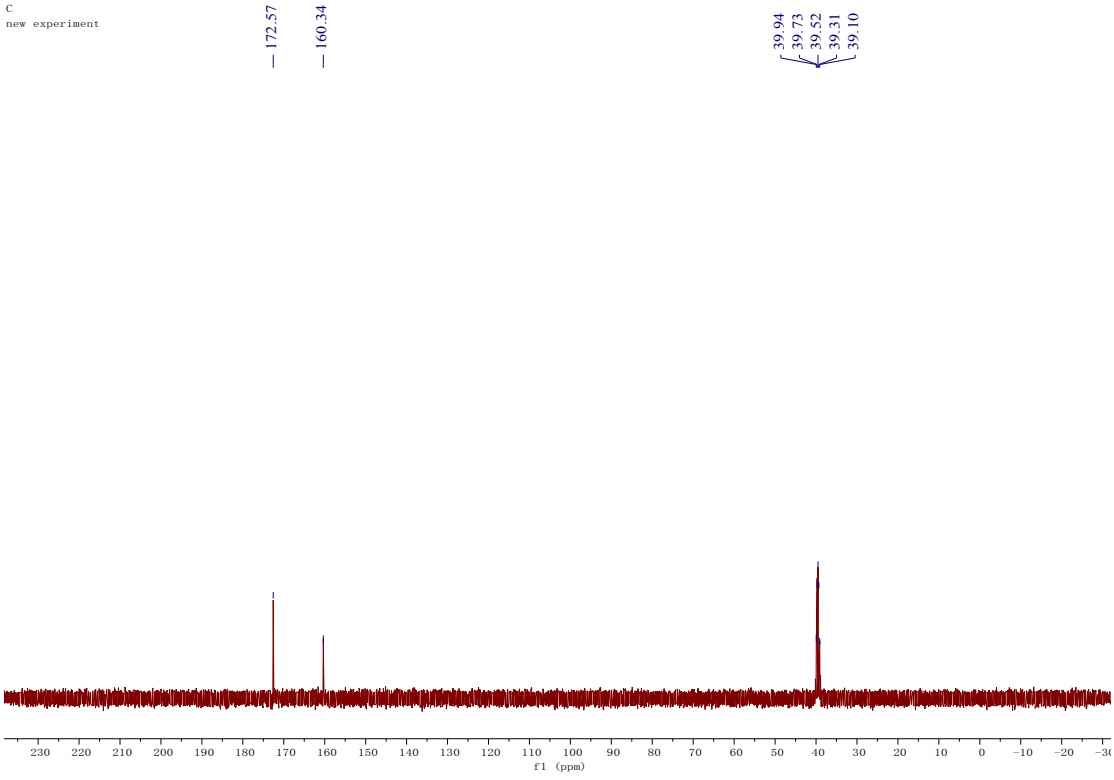


Figure S2 ^{13}C NMR spectrum of compound **2**.

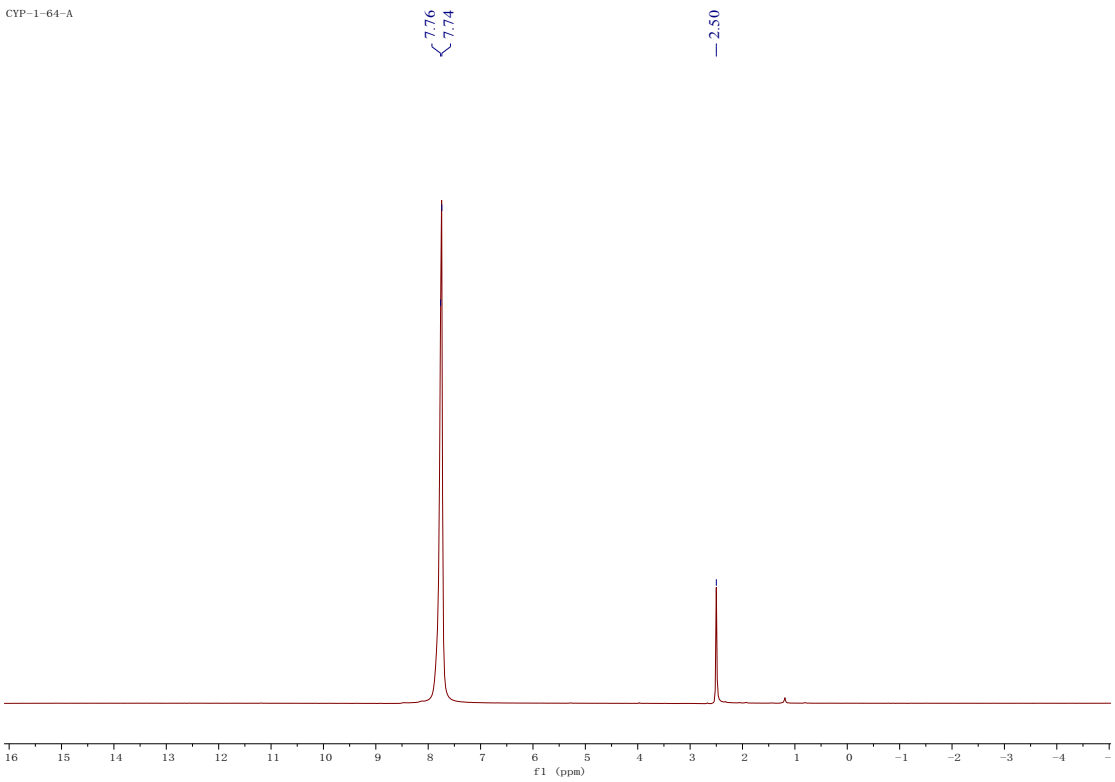


Figure S3 ^{1}H NMR spectrum of compound **3**.

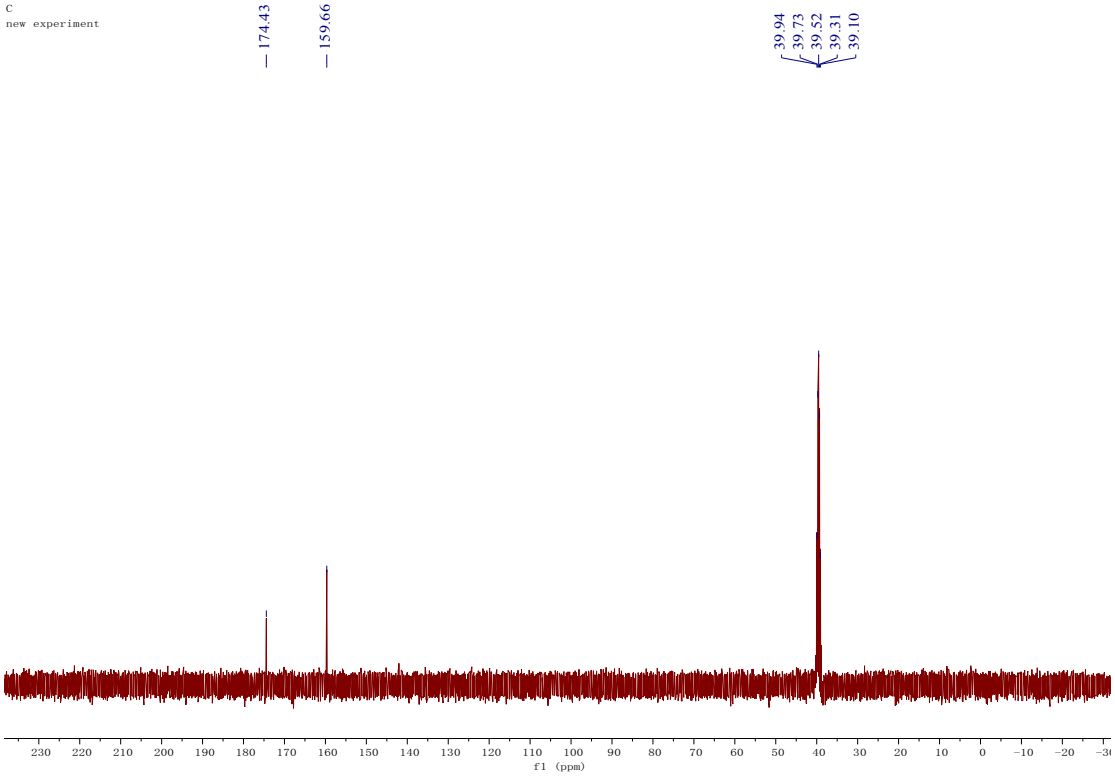


Figure S4 ^{13}C NMR spectrum of compound **3**.

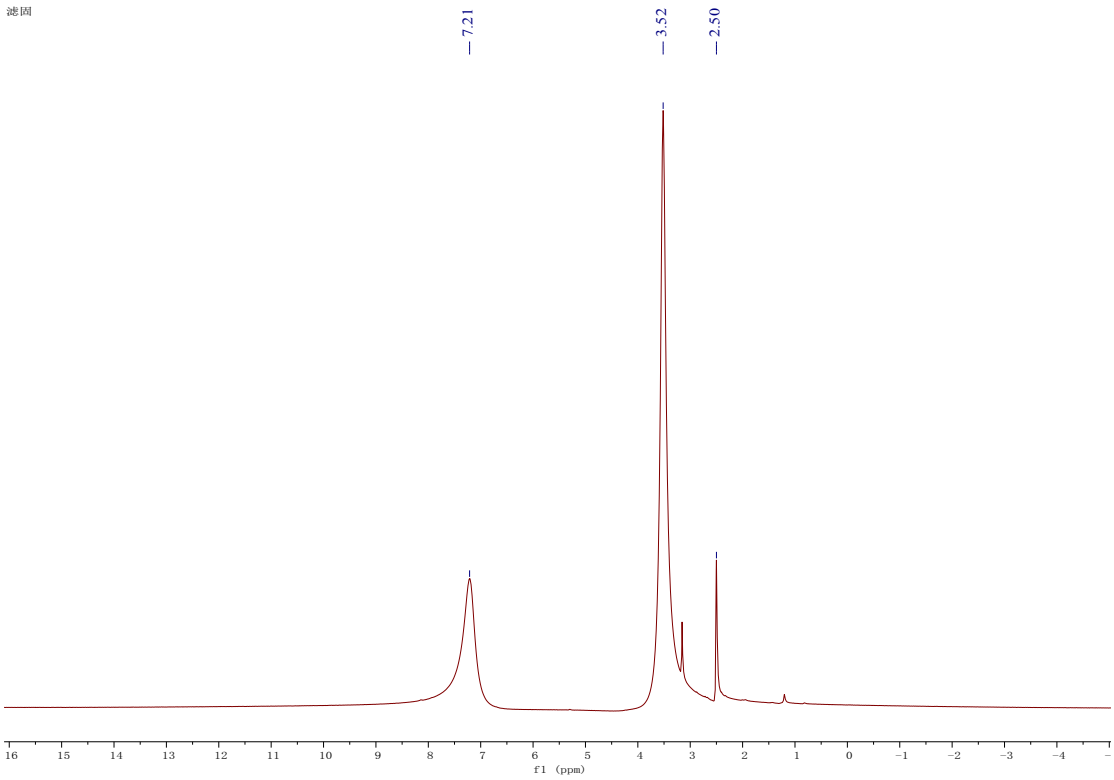


Figure S5 ^{1}H NMR spectrum of compound **4**.

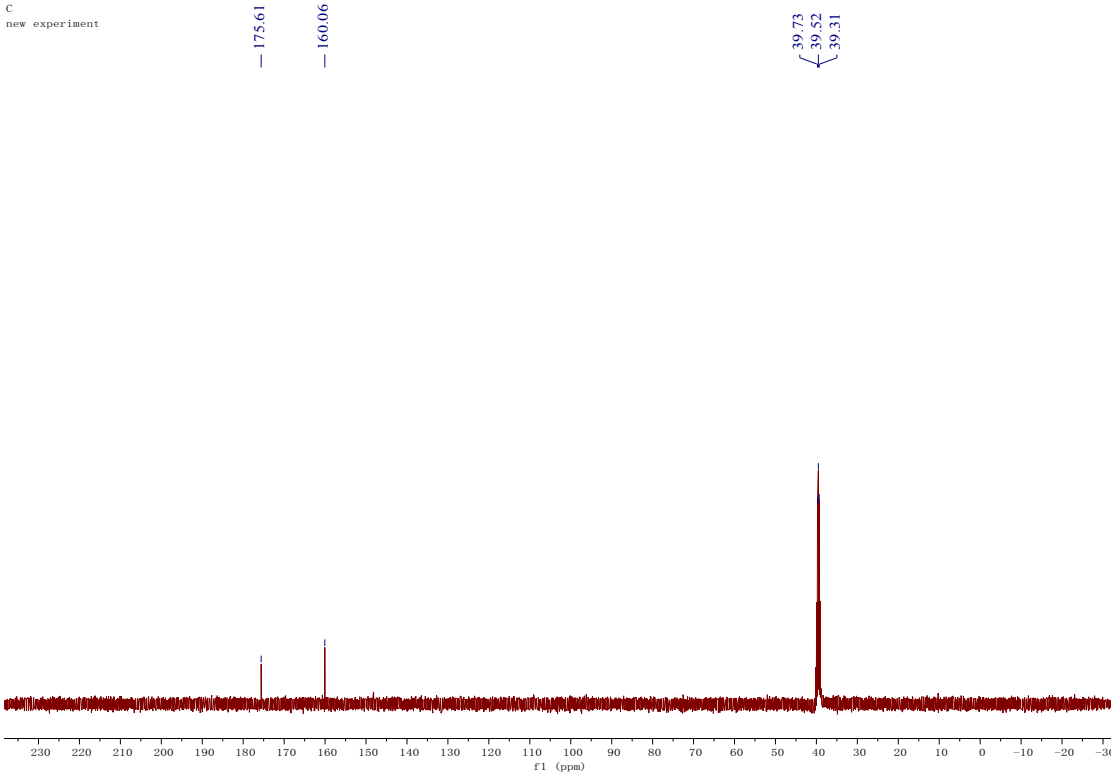


Figure S6 ^{13}C NMR spectrum of compound **4**.

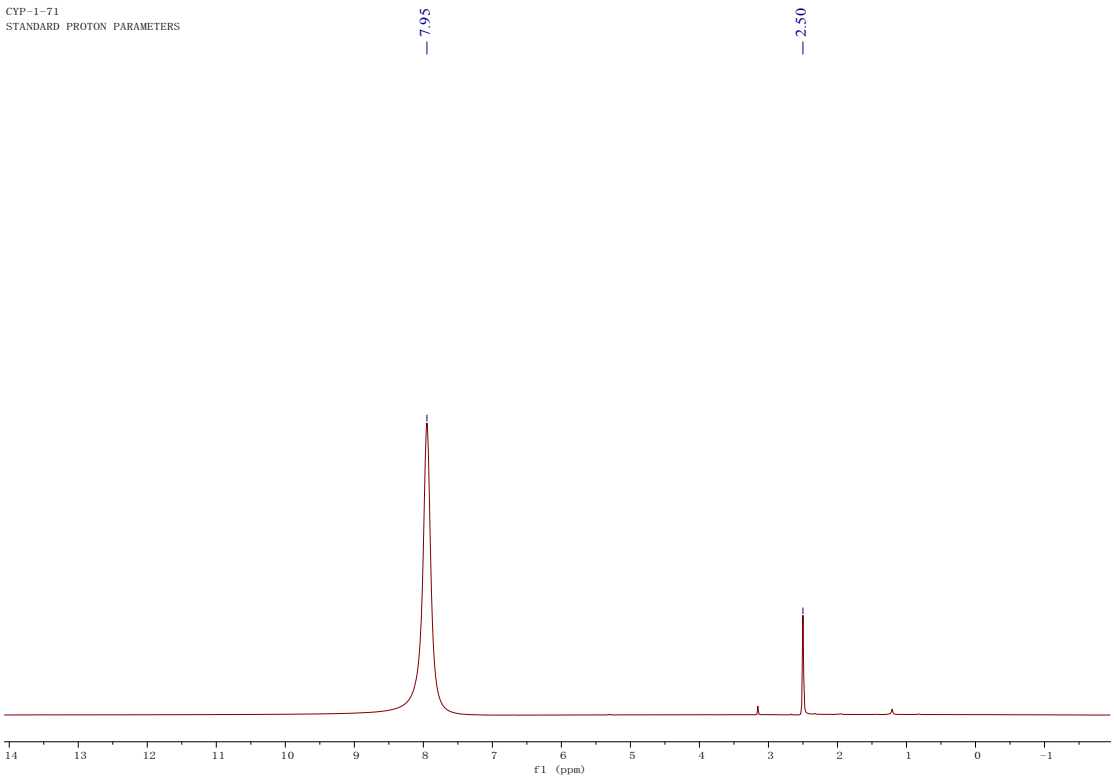


Figure S7 ^{1}H NMR spectrum of compound **5**.

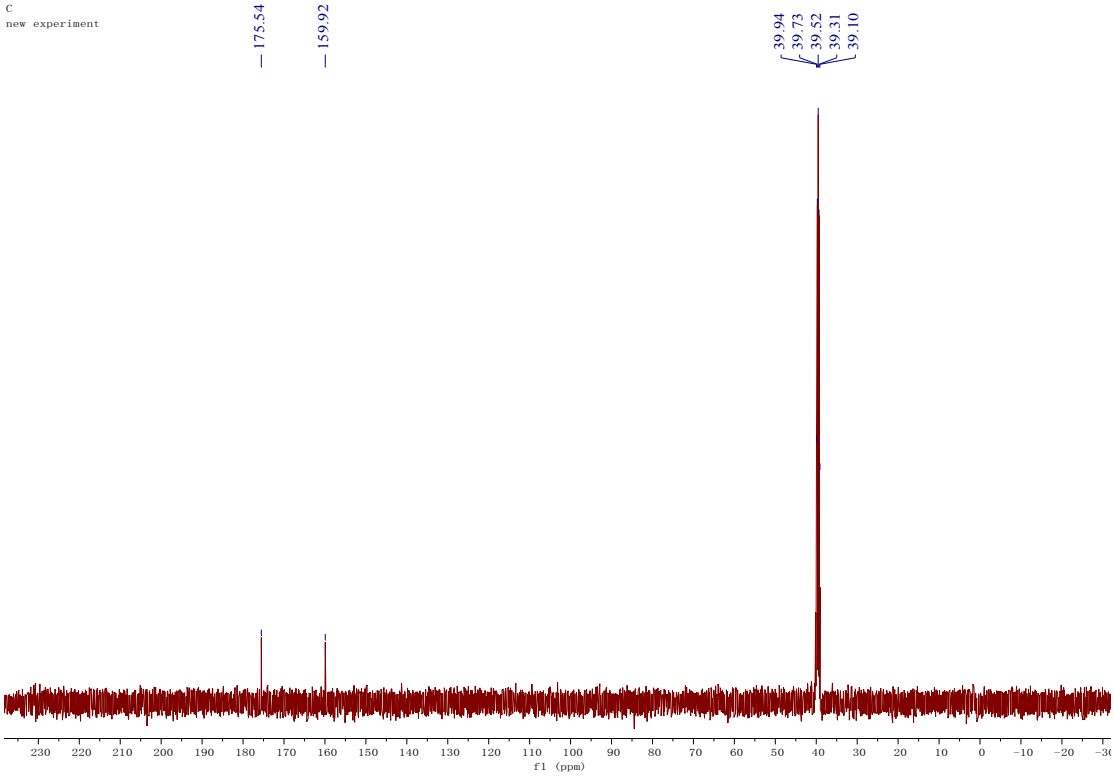


Figure S8 ^{13}C NMR spectrum of compound **5**.

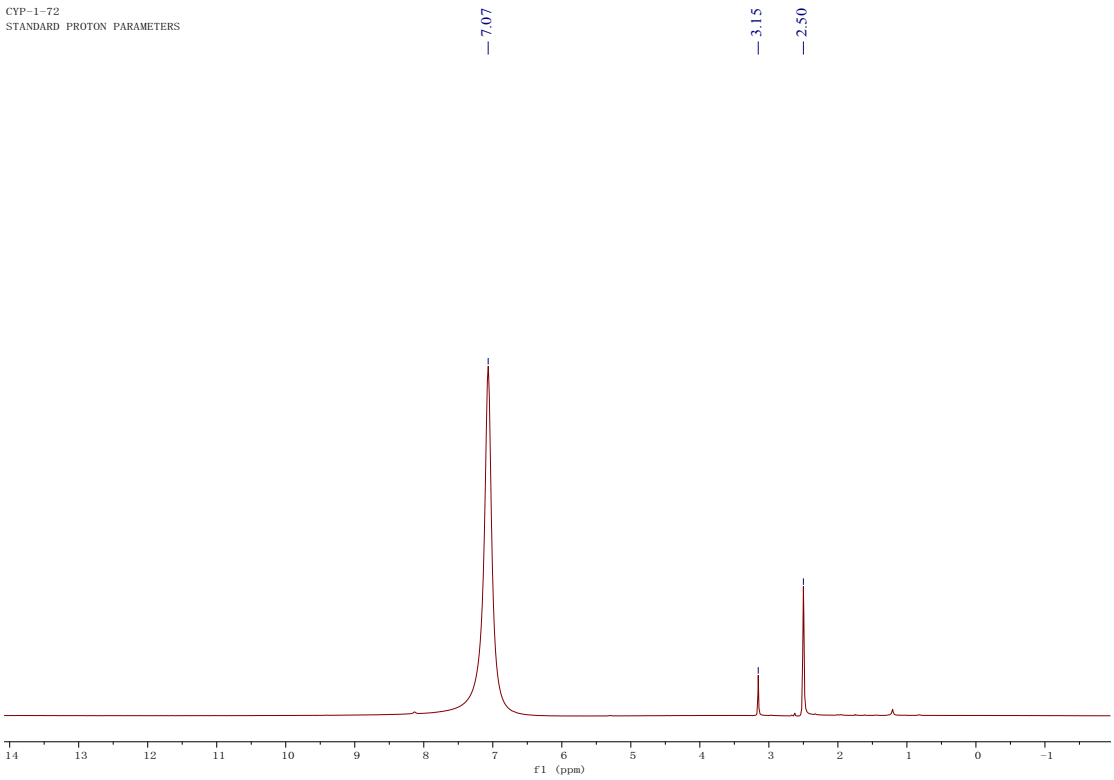


Figure S9 ^{1}H NMR spectrum of compound **6**.

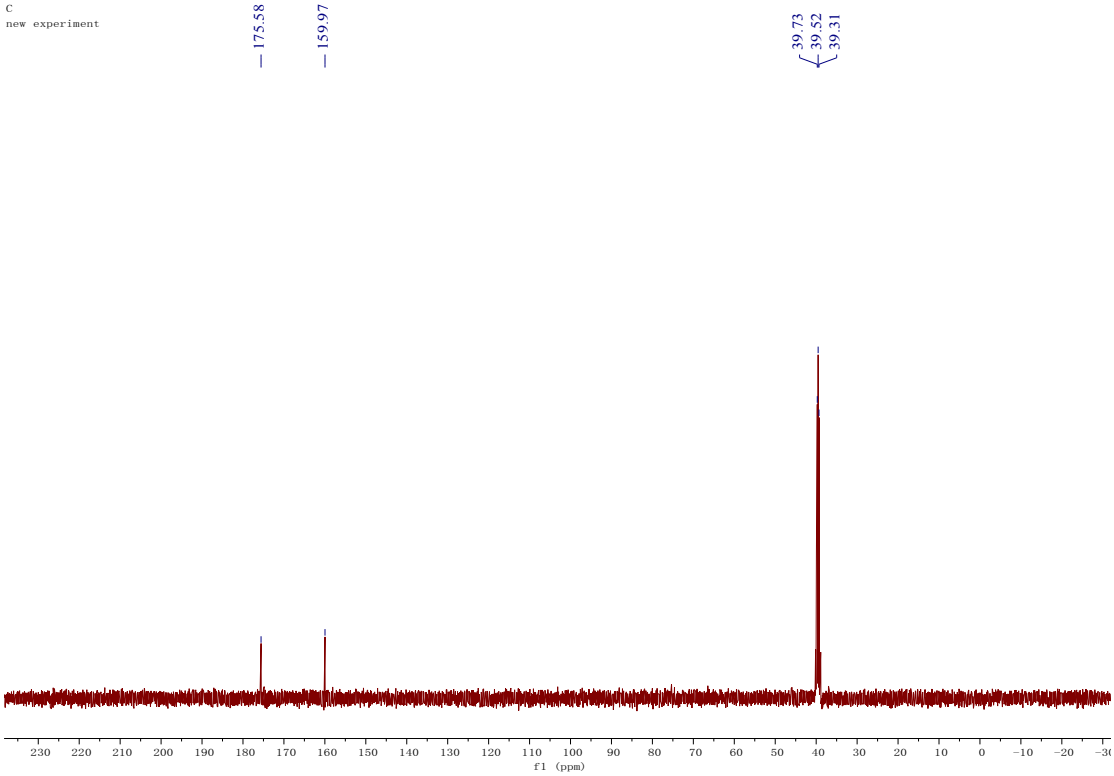


Figure S10 ^{13}C NMR spectrum of compound **6**.

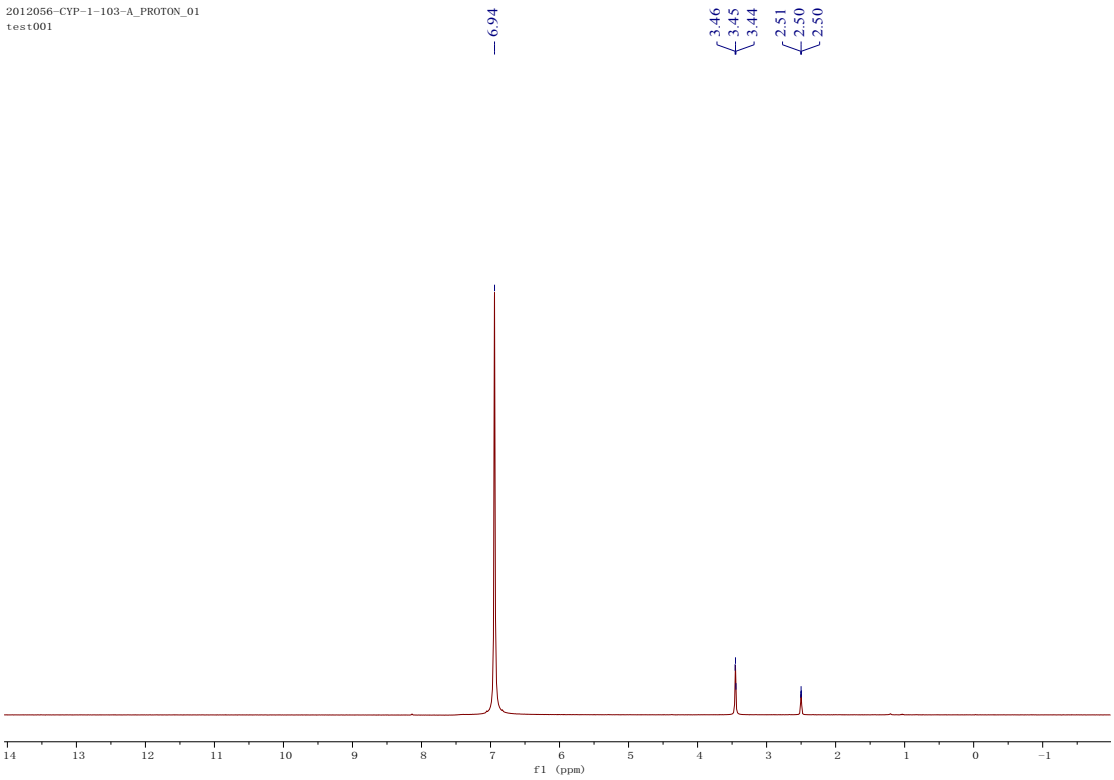


Figure S11 ^{1}H NMR spectrum of compound **7**.

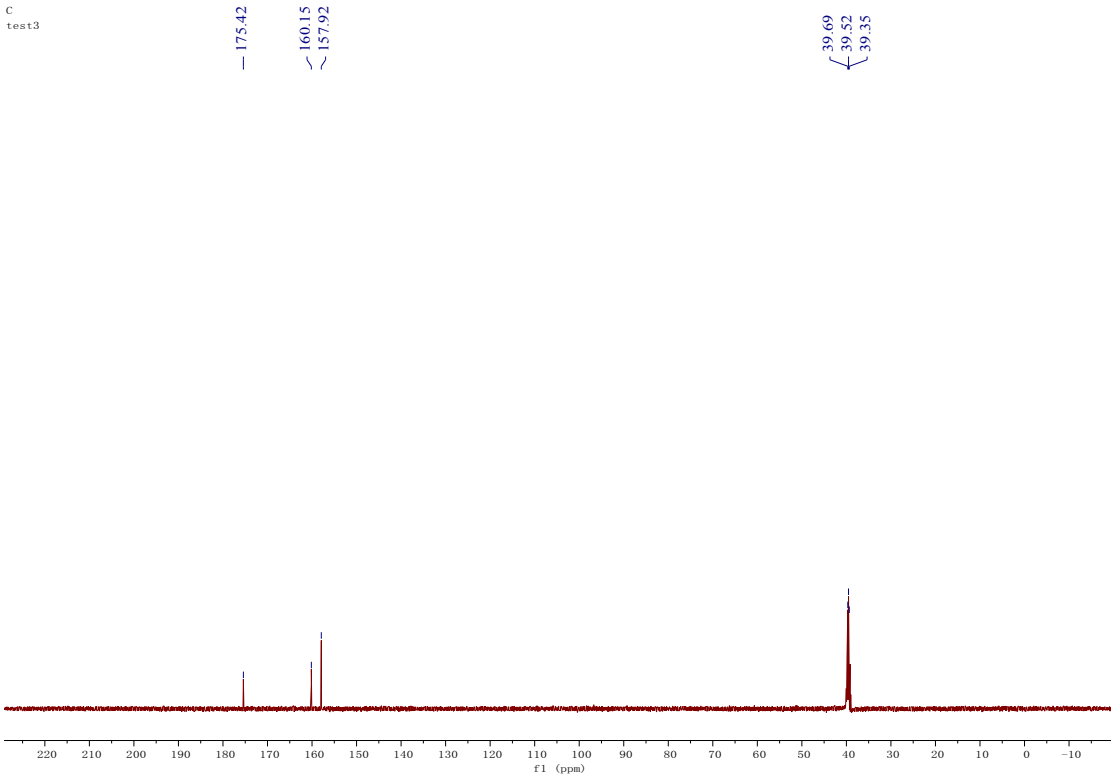


Figure S12 ^{13}C NMR spectrum of compound **7**.

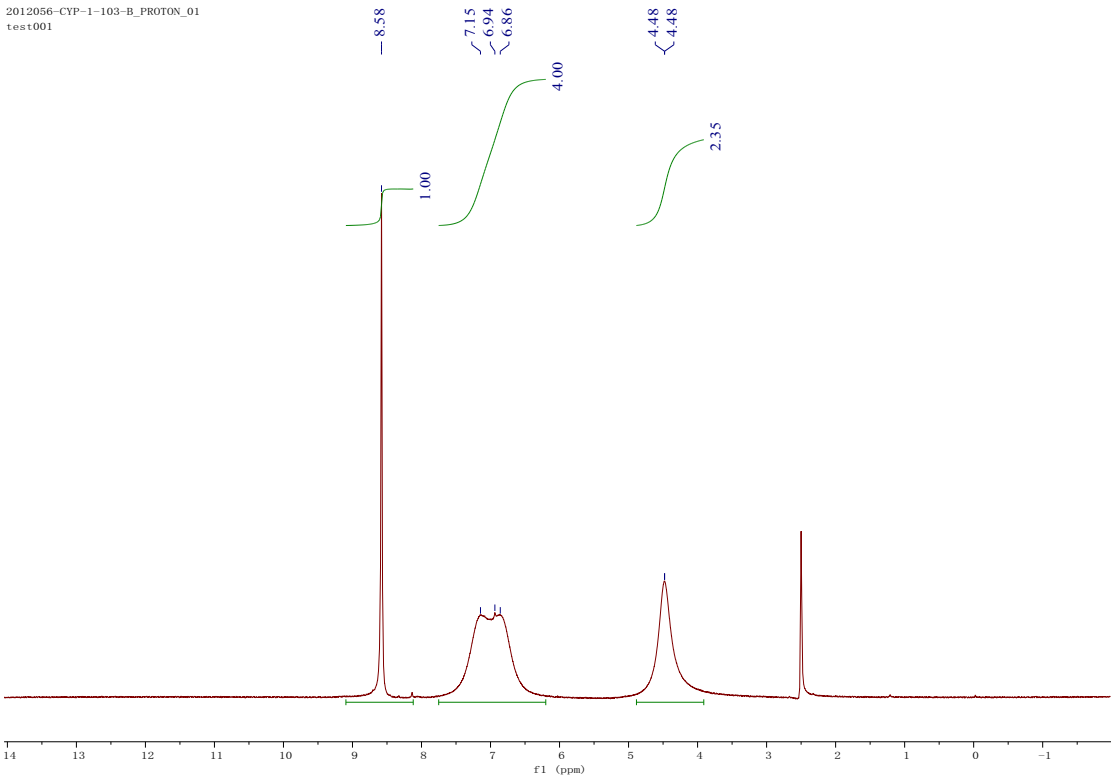


Figure S13 ^{1}H NMR spectrum of compound **8**.

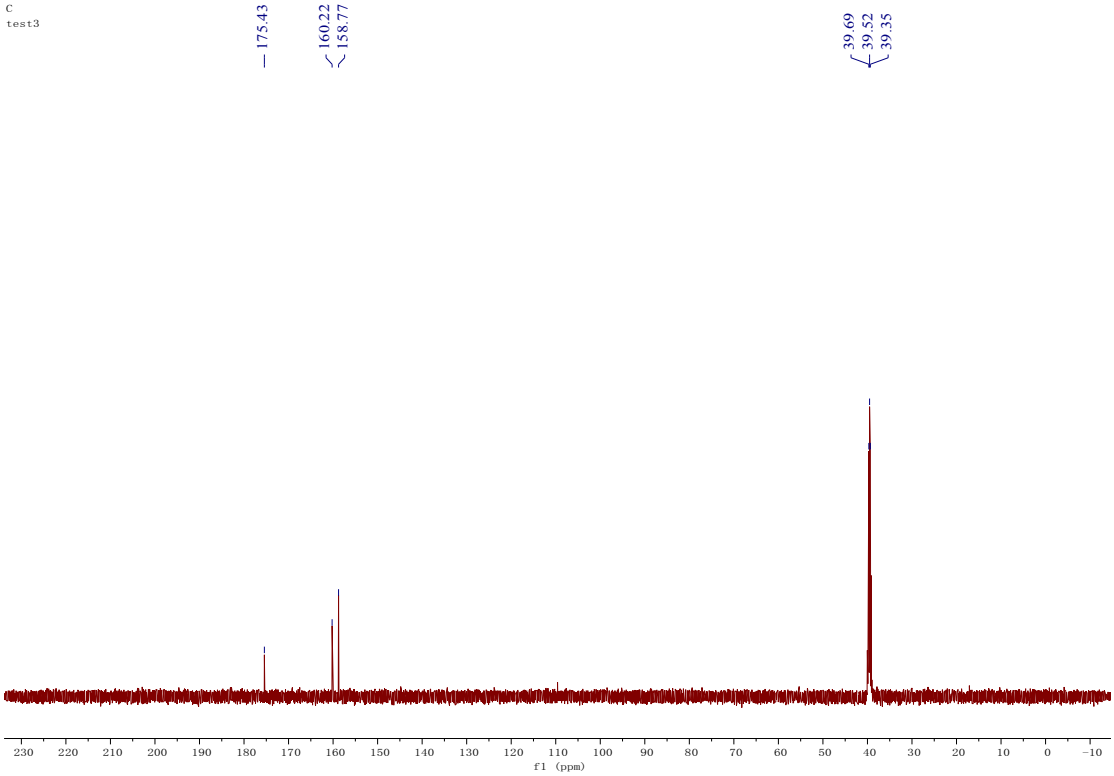


Figure S14 ^{13}C NMR spectrum of compound **8**.

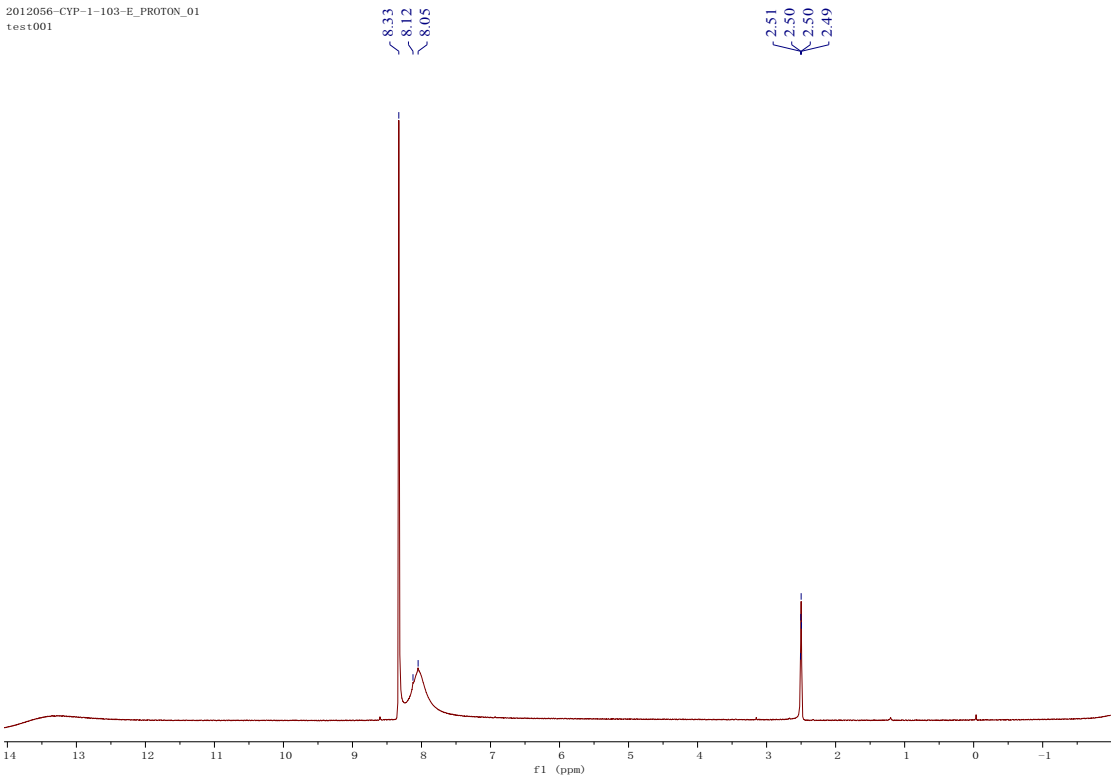


Figure S15 ^{1}H NMR spectrum of compound **9**.

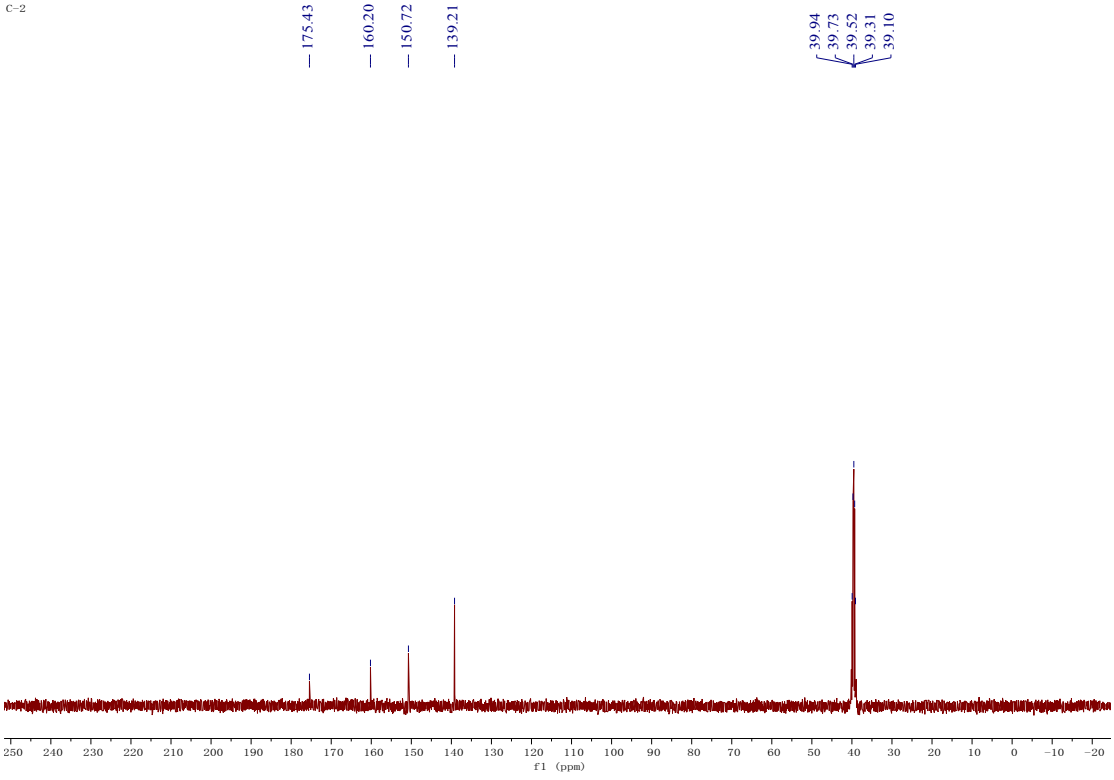


Figure S16 ^{13}C NMR spectrum of compound **9**.

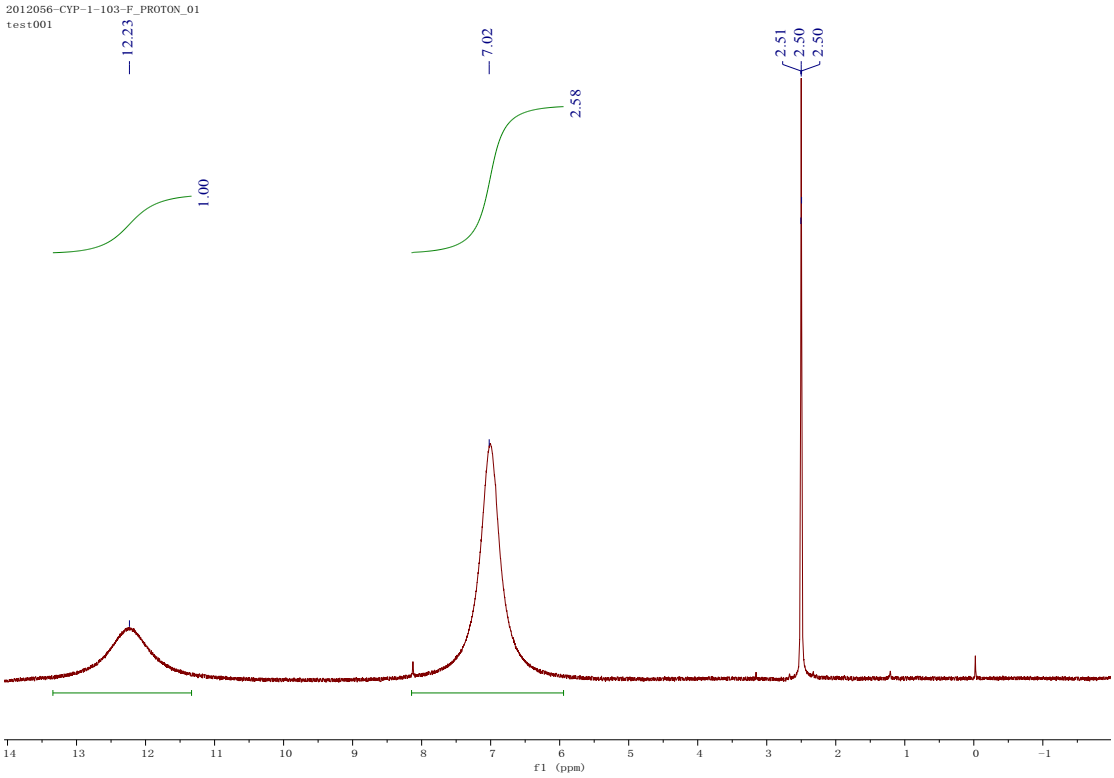


Figure S17 ^{1}H NMR spectrum of compound **10**.

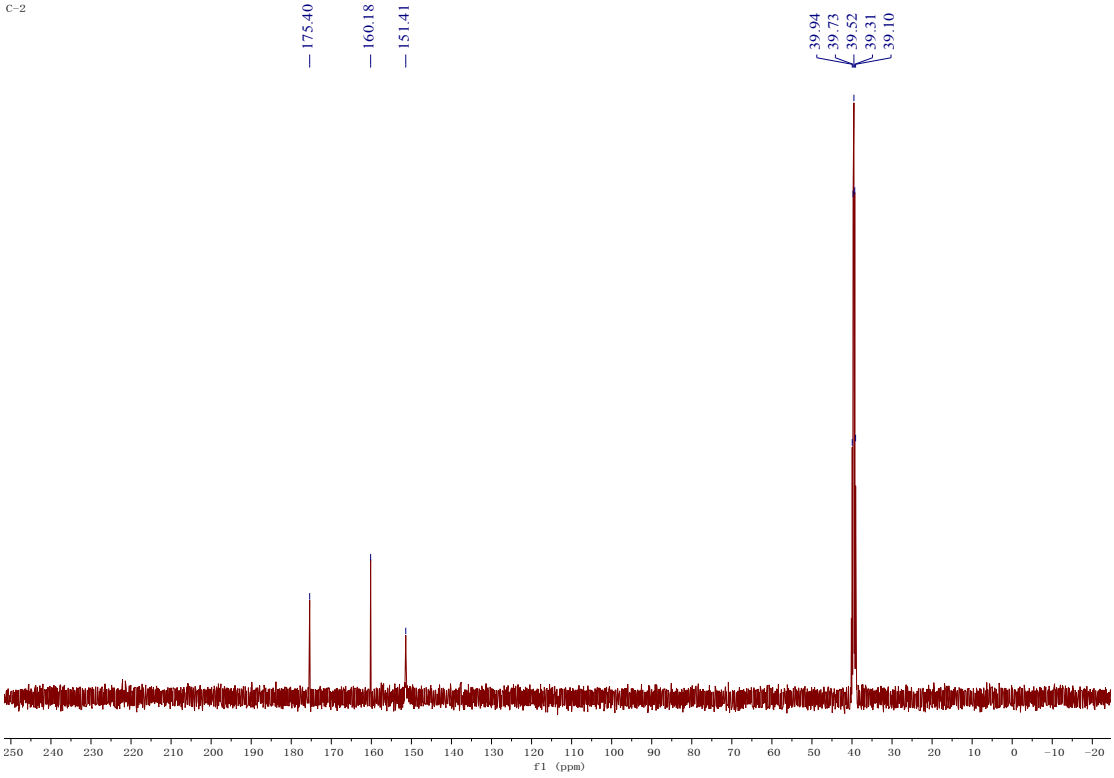
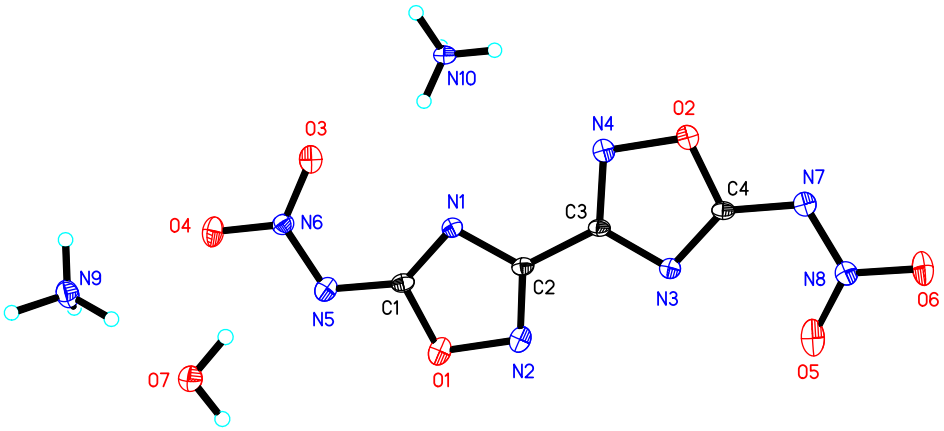
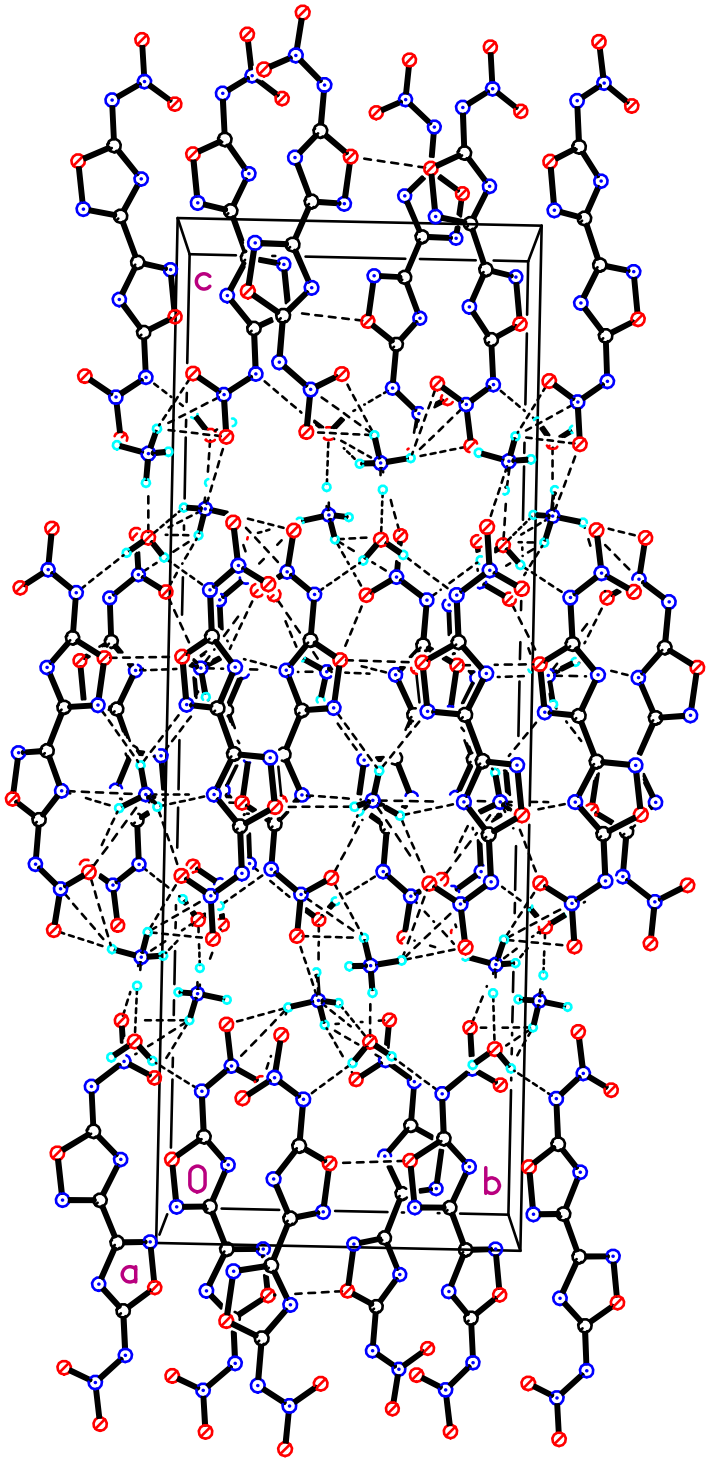


Figure S18 ^{13}C NMR spectrum of compound **10**.

2. Crystallographic data for compound 4



(a)



(b)

Figure S19: (a) Displacement ellipsoid plot (30%) of salt **4**. (b) Ball-and-stick packing diagram of salt **4** viewed down the a-axis. The dashed lines indicate hydrogen bonding.

Table S1. Crystal data and structure refinement for compound **4**.

Identification code	1.4	
Empirical formula	$C_4 H_{10} N_{10} O_7$	
Formula weight	310.22	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c c n	
Unit cell dimensions	a = 7.7918(3) Å	α= 90°.
	b = 10.4242(4) Å	β= 90°.
	c = 29.2890(13) Å	γ = 90°.
Volume	2378.95(17) $Å^3$	
Z	8	
Density (calculated)	1.732 Mg/m^3	
Absorption coefficient	0.160 mm^{-1}	
F(000)	1280	
Crystal size	0.200 x 0.170 x 0.120 mm^3	
Theta range for data collection	2.398 to 25.991°.	
Index ranges	-9<=h<=9, -12<=k<=12, -36<=l<=36	
Reflections collected	20605	
Independent reflections	2334 [R(int) = 0.0366]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6601	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2334 / 0 / 231	
Goodness-of-fit on F^2	1.090	
Final R indices [I>2sigma(I)]	R1 = 0.0319, wR2 = 0.1022	
R indices (all data)	R1 = 0.0379, wR2 = 0.1105	
Largest diff. peak and hole	0.303 and -0.168 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4391(1)	1982(1)	4281(1)	27(1)
O(2)	7405(1)	4707(1)	5737(1)	22(1)
O(3)	7001(1)	4587(1)	3566(1)	28(1)
O(4)	6004(2)	3644(1)	2964(1)	36(1)
O(5)	4486(2)	2294(1)	6444(1)	38(1)
O(6)	5305(2)	3308(1)	7047(1)	37(1)
O(7)	1493(1)	4231(1)	3073(1)	31(1)
N(1)	6032(1)	3703(1)	4382(1)	19(1)
N(2)	4562(2)	2146(1)	4758(1)	26(1)
N(3)	5453(1)	3178(1)	5634(1)	19(1)
N(4)	7226(2)	4552(1)	5261(1)	22(1)
N(5)	5207(2)	2865(1)	3622(1)	25(1)
N(6)	6108(1)	3736(1)	3384(1)	24(1)
N(7)	6385(2)	3942(1)	6394(1)	24(1)
N(8)	5349(2)	3144(1)	6628(1)	24(1)
N(9)	3615(2)	4273(2)	2274(1)	31(1)
N(10)	8667(2)	5694(1)	4354(1)	24(1)
C(1)	5301(2)	2945(1)	4079(1)	20(1)
C(2)	5527(2)	3162(1)	4785(1)	19(1)
C(3)	6072(2)	3653(1)	5231(1)	18(1)
C(4)	6314(2)	3856(1)	5937(1)	19(1)

Table S3. Bond lengths [Å] and angles [°] for compound **4**.

O(1)-C(1)	1.3645(16)
O(1)-N(2)	1.4126(14)
O(2)-C(4)	1.3615(16)
O(2)-N(4)	1.4116(14)
O(3)-N(6)	1.2469(15)
O(4)-N(6)	1.2371(16)
O(5)-N(8)	1.2356(15)
O(6)-N(8)	1.2395(16)
N(1)-C(1)	1.3177(17)
N(1)-C(2)	1.3674(17)
N(2)-C(2)	1.3012(18)
N(3)-C(4)	1.3198(17)
N(3)-C(3)	1.3671(17)
N(4)-C(3)	1.3021(18)
N(5)-N(6)	1.3425(17)
N(5)-C(1)	1.3429(18)
N(7)-C(4)	1.3431(19)
N(7)-N(8)	1.3458(16)
C(2)-C(3)	1.464(2)
C(1)-O(1)-N(2)	106.91(10)
C(4)-O(2)-N(4)	106.84(10)
C(1)-N(1)-C(2)	102.11(11)
C(2)-N(2)-O(1)	102.37(10)
C(4)-N(3)-C(3)	102.05(11)
C(3)-N(4)-O(2)	102.54(10)
N(6)-N(5)-C(1)	116.54(11)
O(4)-N(6)-O(3)	121.16(12)
O(4)-N(6)-N(5)	115.41(11)
O(3)-N(6)-N(5)	123.43(12)
C(4)-N(7)-N(8)	116.17(11)
O(5)-N(8)-O(6)	121.09(12)
O(5)-N(8)-N(7)	123.17(12)
O(6)-N(8)-N(7)	115.74(11)
N(1)-C(1)-N(5)	137.01(13)
N(1)-C(1)-O(1)	111.94(12)

N(5)-C(1)-O(1)	111.04(11)
N(2)-C(2)-N(1)	116.66(12)
N(2)-C(2)-C(3)	120.47(12)
N(1)-C(2)-C(3)	122.84(12)
N(4)-C(3)-N(3)	116.49(12)
N(4)-C(3)-C(2)	120.78(12)
N(3)-C(3)-C(2)	122.70(12)
N(3)-C(4)-N(7)	136.78(12)
N(3)-C(4)-O(2)	112.07(12)
N(7)-C(4)-O(2)	111.14(11)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3) for compound **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	33(1)	22(1)	27(1)	2(1)	-6(1)	-10(1)
O(2)	22(1)	22(1)	23(1)	-1(1)	1(1)	-6(1)
O(3)	29(1)	29(1)	25(1)	-1(1)	-1(1)	-9(1)
O(4)	44(1)	42(1)	20(1)	-1(1)	-5(1)	-3(1)
O(5)	47(1)	40(1)	26(1)	-1(1)	2(1)	-23(1)
O(6)	52(1)	39(1)	21(1)	-1(1)	3(1)	-8(1)
O(7)	34(1)	34(1)	24(1)	1(1)	0(1)	-6(1)
N(1)	19(1)	17(1)	21(1)	0(1)	-1(1)	-1(1)
N(2)	29(1)	24(1)	24(1)	3(1)	-4(1)	-7(1)
N(3)	19(1)	17(1)	22(1)	1(1)	1(1)	-2(1)
N(4)	23(1)	22(1)	23(1)	-1(1)	1(1)	-4(1)
N(5)	29(1)	21(1)	25(1)	0(1)	-5(1)	-3(1)
N(6)	24(1)	24(1)	23(1)	-1(1)	-3(1)	3(1)
N(7)	24(1)	23(1)	25(1)	0(1)	1(1)	-4(1)
N(8)	26(1)	23(1)	24(1)	0(1)	1(1)	-2(1)
N(9)	29(1)	40(1)	24(1)	-1(1)	-2(1)	3(1)
N(10)	25(1)	23(1)	25(1)	0(1)	0(1)	-8(1)
C(1)	18(1)	16(1)	27(1)	0(1)	-3(1)	0(1)
C(2)	16(1)	15(1)	25(1)	2(1)	0(1)	0(1)
C(3)	16(1)	14(1)	24(1)	2(1)	2(1)	1(1)
C(4)	16(1)	15(1)	26(1)	1(1)	1(1)	0(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **4**.

	x	y	z	U(eq)
H(7A)	2070(20)	4708(19)	3274(7)	44(5)
H(9A)	3030(30)	4200(20)	2552(8)	62(7)
H(10A)	8930(30)	6450(20)	4212(7)	49(6)
H(7B)	1080(30)	3610(20)	3223(7)	51(6)
H(9B)	4450(30)	4860(20)	2269(8)	63(7)
H(10B)	7770(30)	5330(20)	4240(8)	59(7)
H(9C)	4110(40)	3420(30)	2208(11)	107(10)
H(10C)	9600(30)	5190(20)	4294(7)	60(7)
H(9D)	2920(40)	4470(30)	2012(10)	91(9)
H(10D)	8580(30)	5860(20)	4648(9)	51(6)

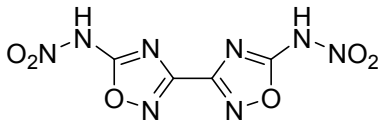
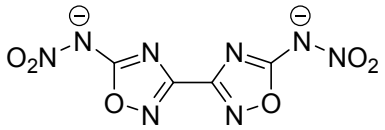
Table S6. Torsion angles [°] for compound **4**.

C(1)-O(1)-N(2)-C(2)	0.06(13)
C(4)-O(2)-N(4)-C(3)	0.25(12)
C(1)-N(5)-N(6)-O(4)	179.94(11)
C(1)-N(5)-N(6)-O(3)	0.11(18)
C(4)-N(7)-N(8)-O(5)	6.37(18)
C(4)-N(7)-N(8)-O(6)	-173.68(12)
C(2)-N(1)-C(1)-N(5)	179.78(15)
C(2)-N(1)-C(1)-O(1)	-0.08(14)
N(6)-N(5)-C(1)-N(1)	2.6(2)
N(6)-N(5)-C(1)-O(1)	-177.57(11)
N(2)-O(1)-C(1)-N(1)	0.02(14)
N(2)-O(1)-C(1)-N(5)	-179.88(11)
O(1)-N(2)-C(2)-N(1)	-0.13(15)
O(1)-N(2)-C(2)-C(3)	-178.13(11)
C(1)-N(1)-C(2)-N(2)	0.14(16)
C(1)-N(1)-C(2)-C(3)	178.09(12)
O(2)-N(4)-C(3)-N(3)	-0.18(15)
O(2)-N(4)-C(3)-C(2)	-178.25(11)
C(4)-N(3)-C(3)-N(4)	0.03(15)
C(4)-N(3)-C(3)-C(2)	178.06(12)
N(2)-C(2)-C(3)-N(4)	170.23(13)
N(1)-C(2)-C(3)-N(4)	-7.7(2)
N(2)-C(2)-C(3)-N(3)	-7.7(2)
N(1)-C(2)-C(3)-N(3)	174.40(11)
C(3)-N(3)-C(4)-N(7)	179.00(15)
C(3)-N(3)-C(4)-O(2)	0.15(14)
N(8)-N(7)-C(4)-N(3)	0.9(2)
N(8)-N(7)-C(4)-O(2)	179.74(11)
N(4)-O(2)-C(4)-N(3)	-0.26(14)
N(4)-O(2)-C(4)-N(7)	-179.42(10)

Symmetry transformations used to generate equivalent atoms:

3 Ab Initio computational data

Table S7. Ab Initio computational data

Species	E_0[a] (Hartree)	H_{corr}[b] (Hartree)	ZPE[c] (Hartree)	HOF[d] (kJ/mol)
	-1040.7285758	0.126615	0.110943	175.8
	-1039.6356204	0.099795	0.085017	69.0
CH_4	-40.3984857	0.048605	0.044793	-74.6[1]
NH_3	-56.4341763	0.038190	0.034372	-45.9[2]
	-261.5728129	0.050912	0.046541	75[2]
NH_2NO_2	-260.5478787	0.042613	0.039257	-6.1[3]
$^{-}NHNO_2$	-260.0119632	0.030444	0.026168	-84.0[4]
CH_3CH_3	-79.6068548	0.079039	0.074609	-84.68[5]
CH_3NH_2	-95.6318759	0.068401	0.064032	-23.0[2]

[a] Total energy (E_0) calculated by B3LYP/6-31+G**/MP2/6-311++G** method (Hartree/Particle); [b] Values of thermal correction (HT) (Hartree/Particle); [c] Zero-point correction (ZPE) (Hartree/Particle); [d] Heat of formation (HOF) (kJ/mol).

Calculations were carried out by using the Gaussian 09 (Revision E.01) suite of programs.[6] The geometric optimization of the structures and frequency analyses were carried out by using the B3LYP functional with the 6-31+G**basis set, and single-point energies were calculated at the MP2(full)/6-311++G**level. All of the optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies.

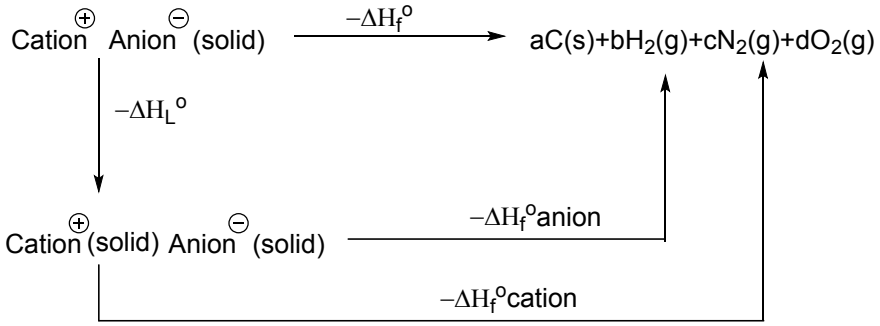


Figure S20. Born-Haber cycle for the formation for energetic salts.

Based on the Born-Haber energy cycle (Figure S20), the heat of formation of a salt can be simplified according to Equation (1), where ΔHL is the lattice energy of the salt.

ΔH_f^o(ionic salt, 298K) = ΔH_f^o (cation, 298K)＋ΔH_f^o (anion, 298K)－ΔH_L (1)

The ΔH_L value could be predicted by the formula suggested by Jenkins et al [Eq. (2)][7], where U_{POT} is the lattice potential energy and nM and nX depend on the nature of the ions $M^{p+}$and X^{q-}, respectively, and are equal to three for monoatomic ions, five for linear polyatomic ions, and six for nonlinear polyatomic ions.

$\Delta H_L = U_{POT} + [p(n_M/2-2) + q(n_X/2-2)]RT$ (2)

The equation for the lattice potential energy, U_{POT}, takes the form of Equation (3), where ρ_m is the density (g cm^{-3}), Mm is the chemical formula mass of the ionic material (g), and the coefficients γ ($kJ^{-1}mol^{-1}cm$) and δ ($kJ^{-1}mol^{-1}$) are assigned literature values[6].

U_{POT} ($kJ^{-1}mol^{-1}$) = γ (ρ_m/Mm)$^{1/3}$ + δ (3)

4 Detonation performances calculation

Detonation pressure (P) and detonation velocity (D) were calculation according to the Kamlet-Jacobs equations[8].

$$D = 1.01\left(N\bar{M}^{1/2}Q^{1/2}\right)^{1/2}(1 + 1.30\rho) \quad (4)$$

$$P = 1.558\rho^2\bar{M}^{1/2}Q^{1/2} \quad (5)$$

where each term in eqs 4 and 5 is defined as follows: D, the detonation velocity (km s^{-1}); P, the detonation pressure (GPa); N, the moles of detonation gases per gram explosive; M , the average molecular weight of these gases (g mol^{-1}); Q, the heat of detonation (J g^{-1}); and ρ, the loaded density of explosives (g cm^{-3}). The measured density was used for the calculation here.

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