Supporting Information (SI)

Synthesis and Characterization of New Energetic Derivatives Containing High Nitrogen Content Moiety and Picryl Group: A New Strategy for Incorporating the Picryl Functionality

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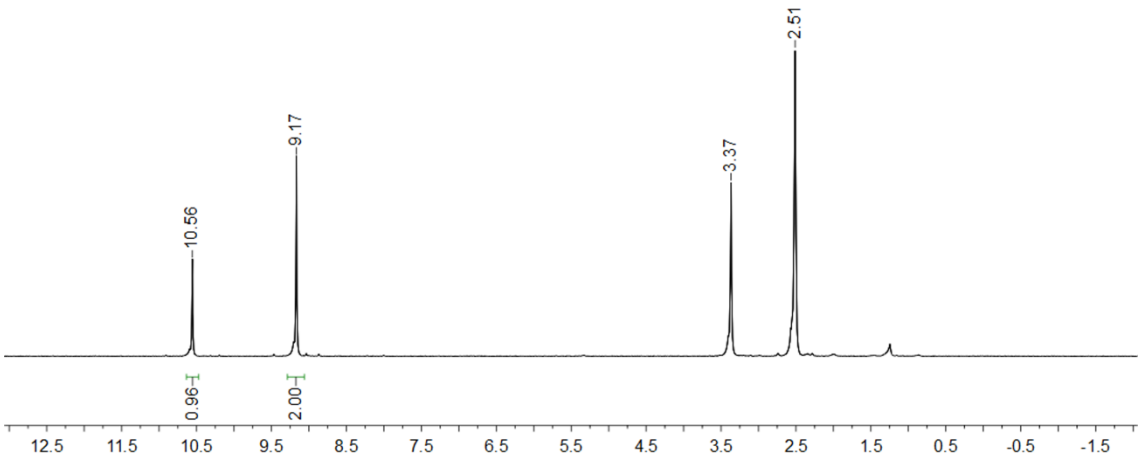


Figure S1 [1]H NMR spectra (500 MHz) of 2,4,6-trinitrobenzaldehyde in [D_6]DMSO at 25 °C

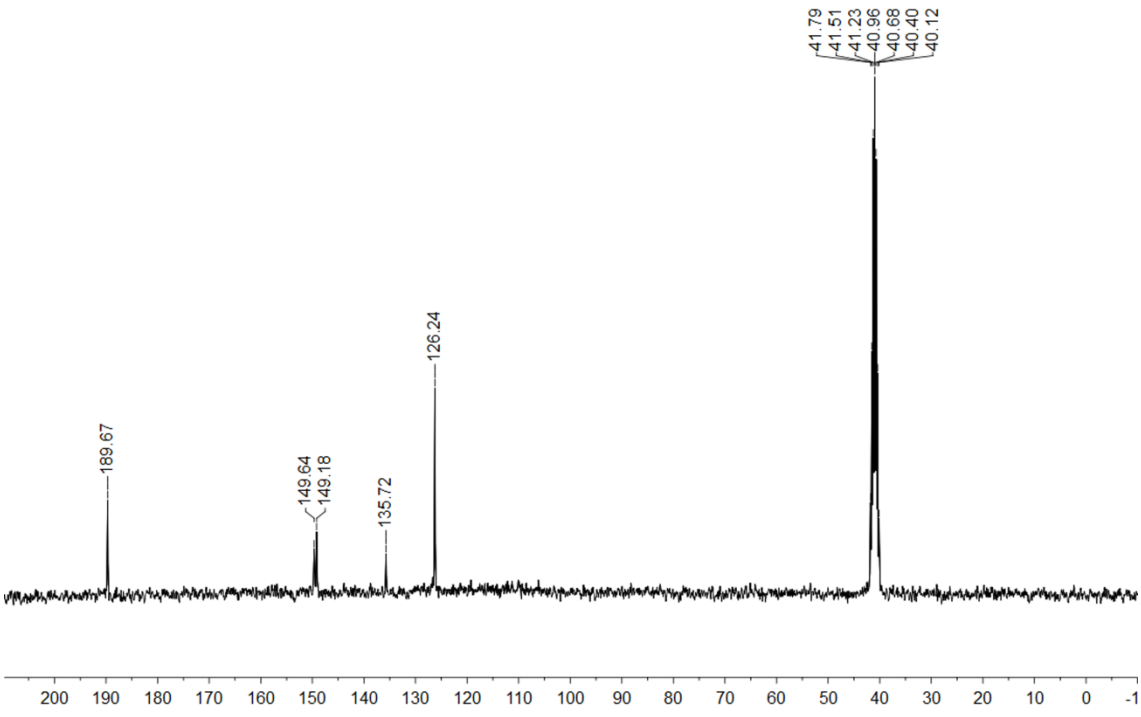


Figure S2 [13]C NMR spectra (75 MHz) of 2,4,6-trinitrobenzaldehyde in [D6]DMSO at 25 °C

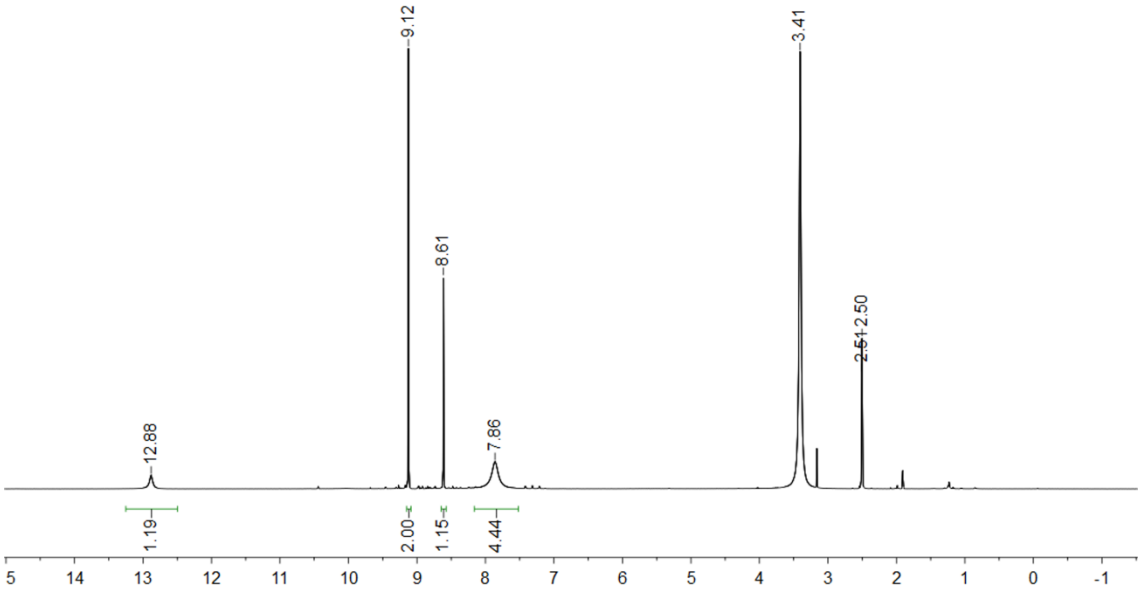


Figure S3 ^{1}H NMR spectra (500 MHz) of **1** in [D6]DMSO at 25 ^{o}C

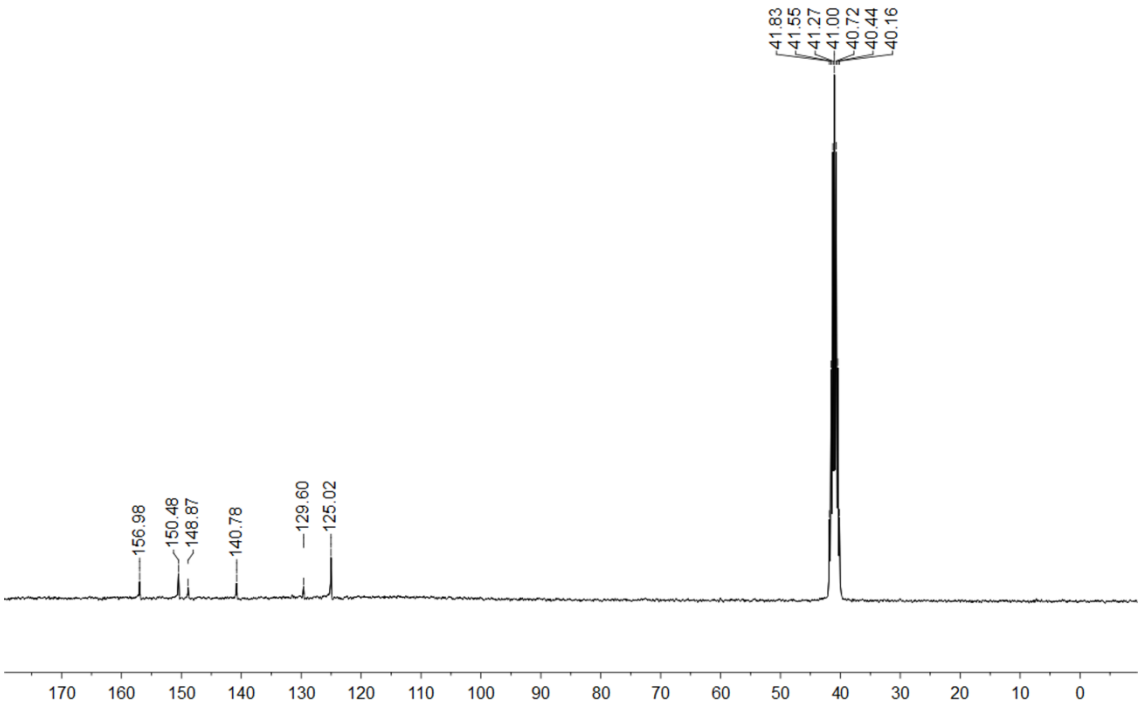


Figure S4 ^{13}C NMR spectra (75 MHz) of **1** in [D6]DMSO at 25 ^{o}C

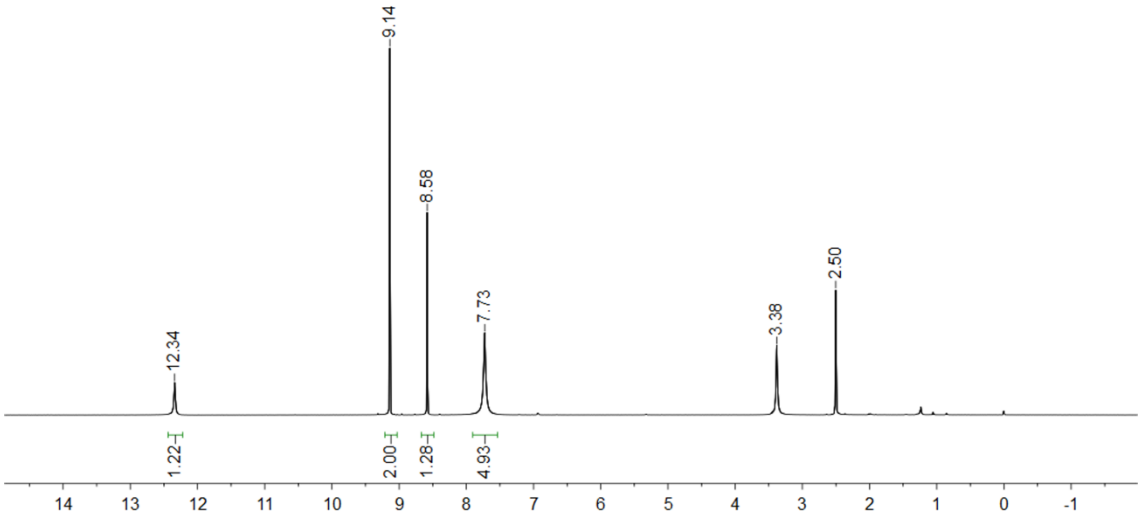


Figure S5 ^{1}H NMR spectra (500 MHz) of **2** in [D6]DMSO at 25 ^{o}C

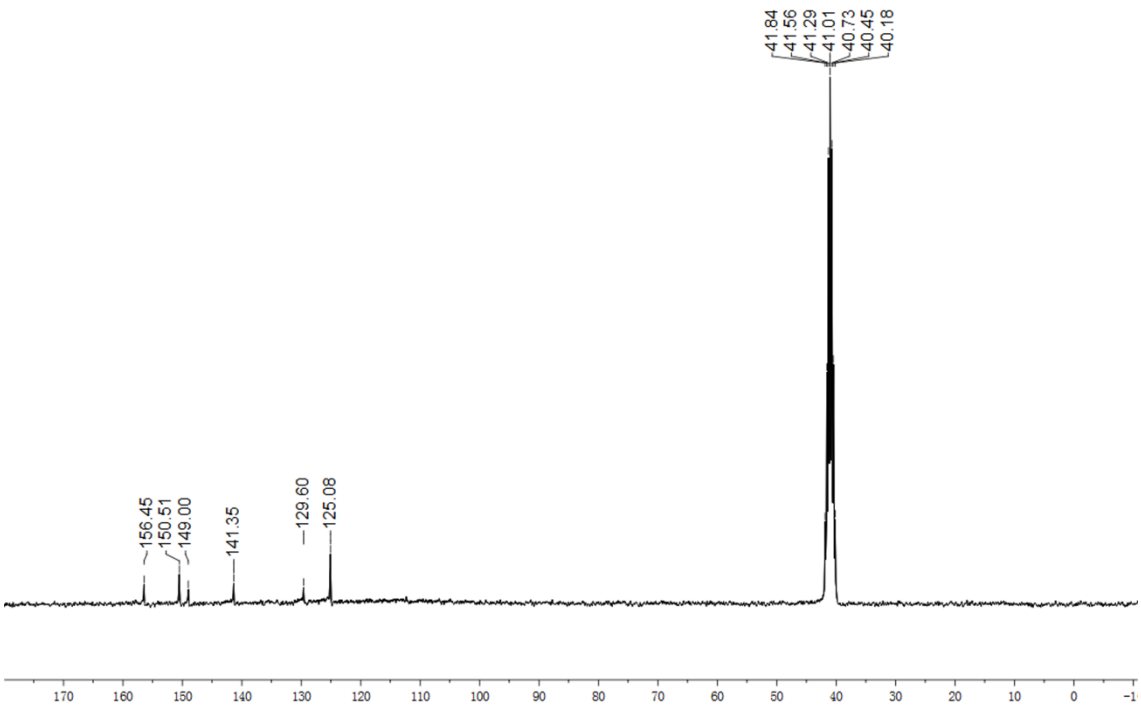


Figure S6 ^{13}C NMR spectra (75 MHz) of **2** in [D6]DMSO at 25 ^{o}C

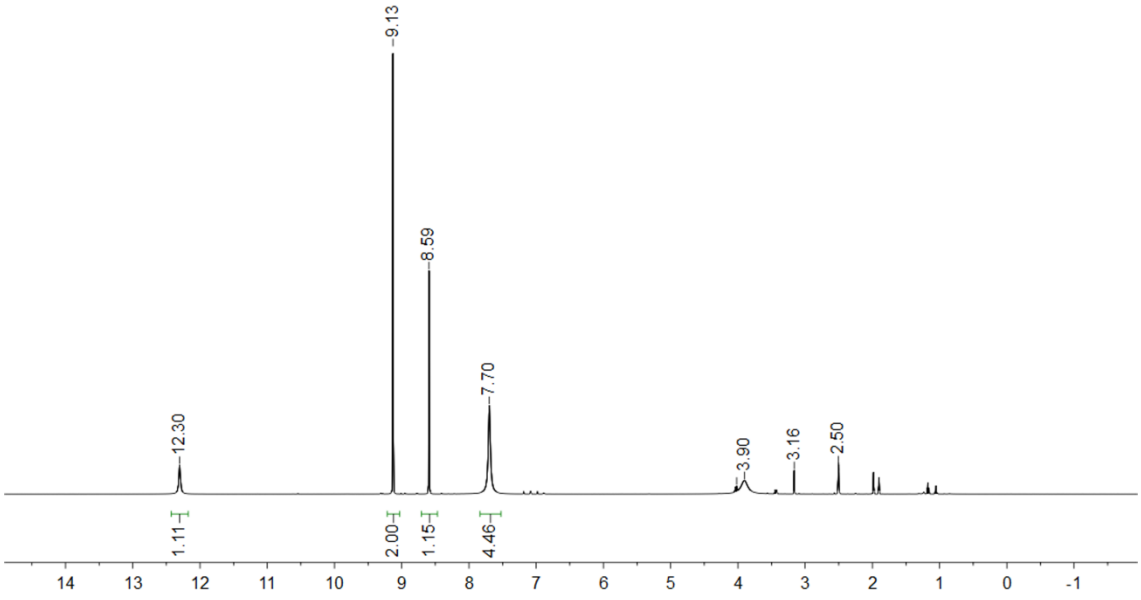


Figure S7 [1]H NMR spectra (500 MHz) of **3** in [D6]DMSO at 25 °C

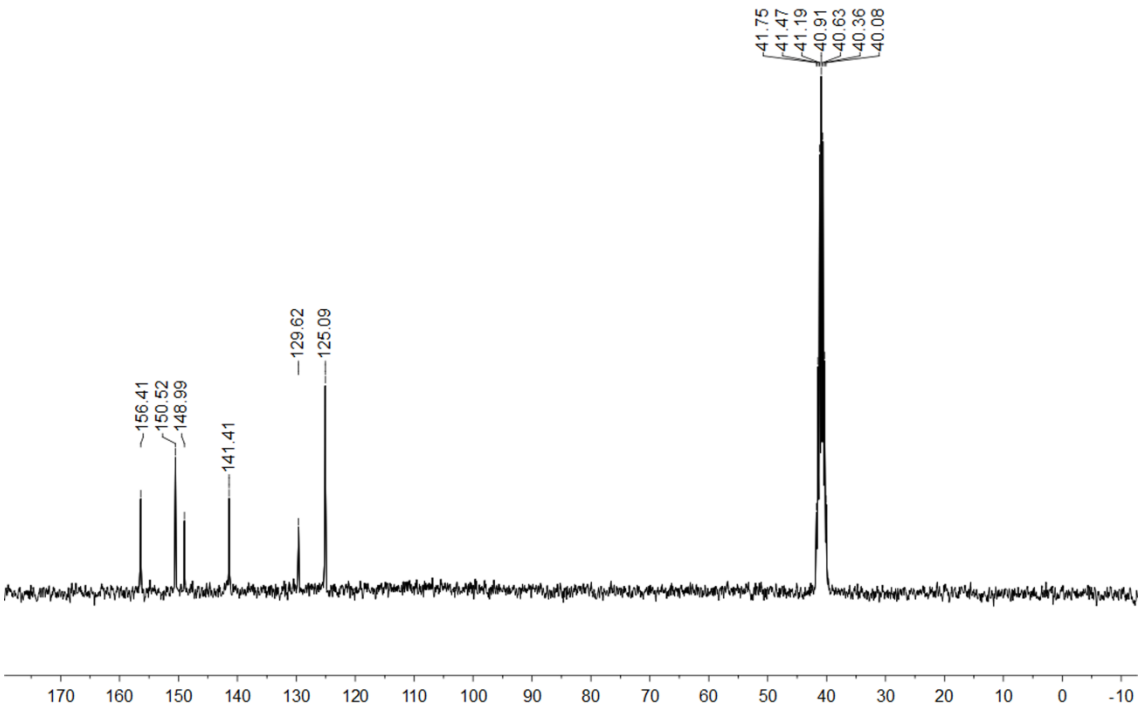


Figure S8 [13]C NMR spectra (75 MHz) of **3** in [D6]DMSO at 25 °C

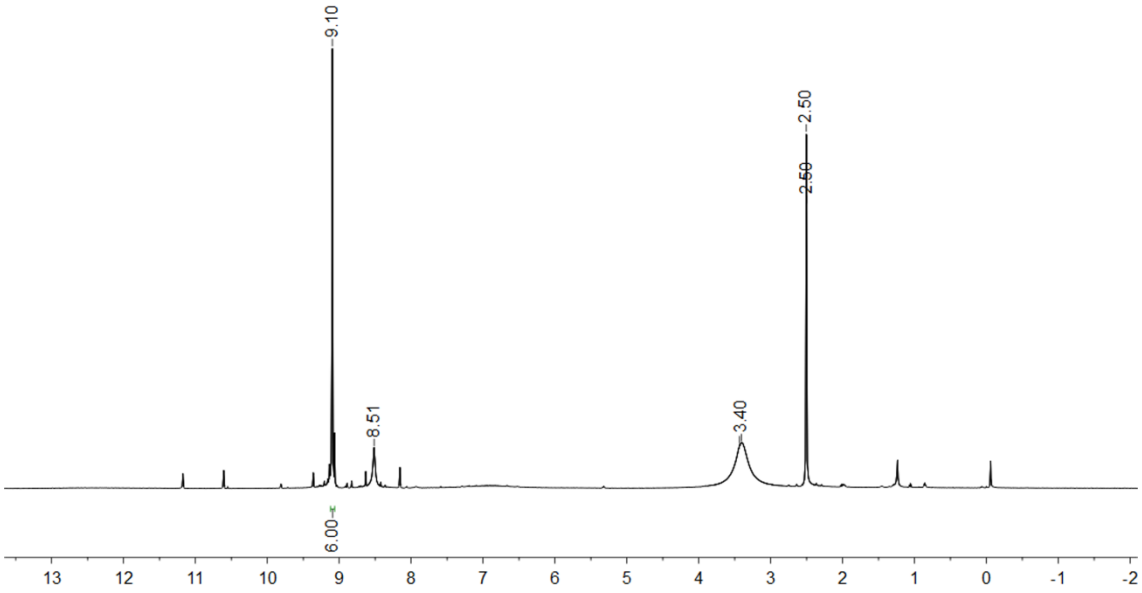


Figure S9 ^{1}H NMR spectra (500 MHz) of **5** in [D6]DMSO at 25 ^{o}C

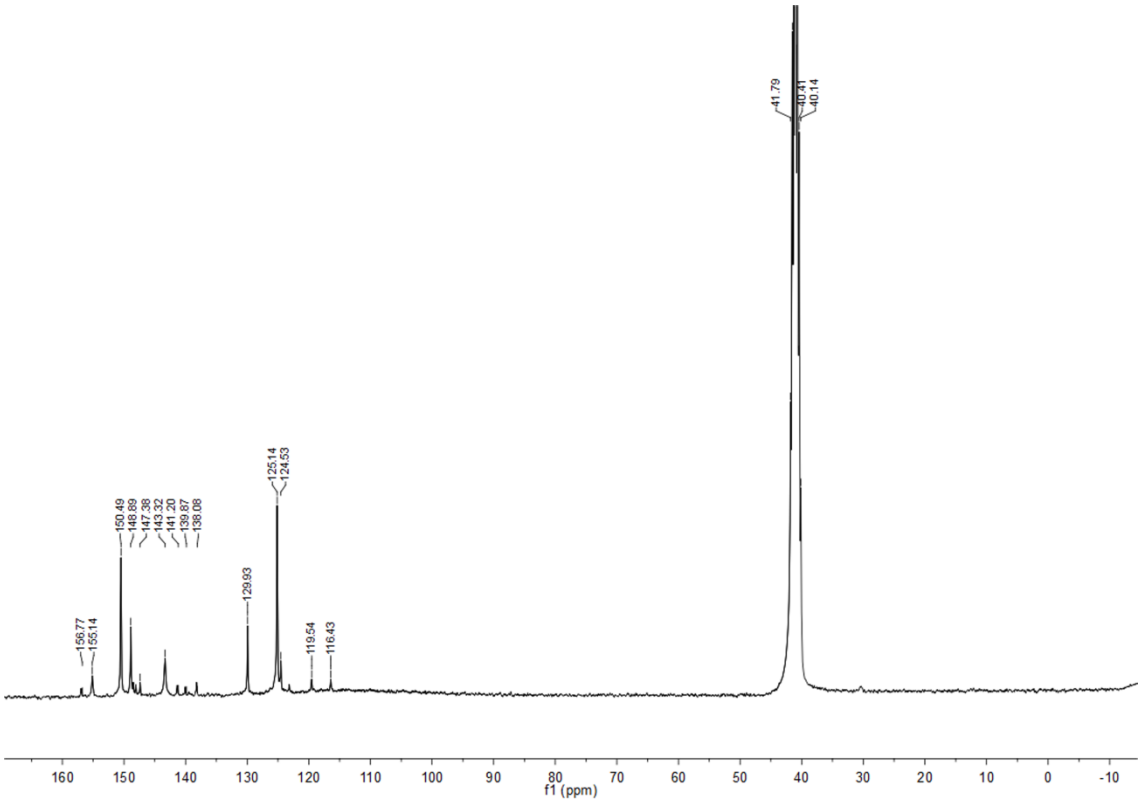


Figure S10 ^{13}C NMR spectra (75 MHz) of **5** in [D6]DMSO at 25 ^{o}C

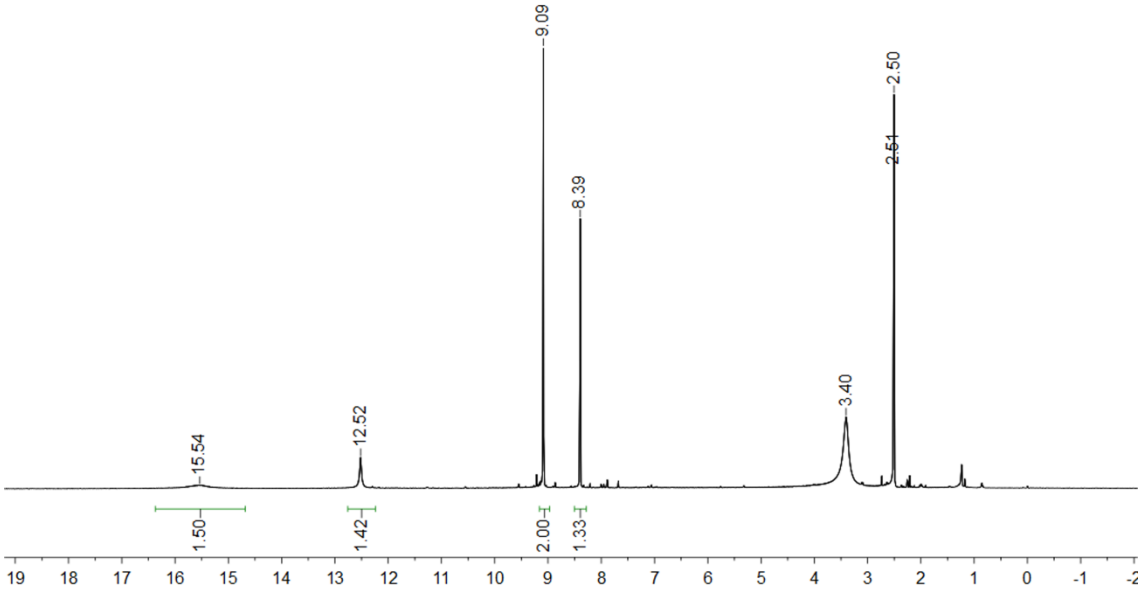


Figure S11 ^{1}H NMR spectra (500 MHz) of **6** in [D6]DMSO at 25 ^{o}C

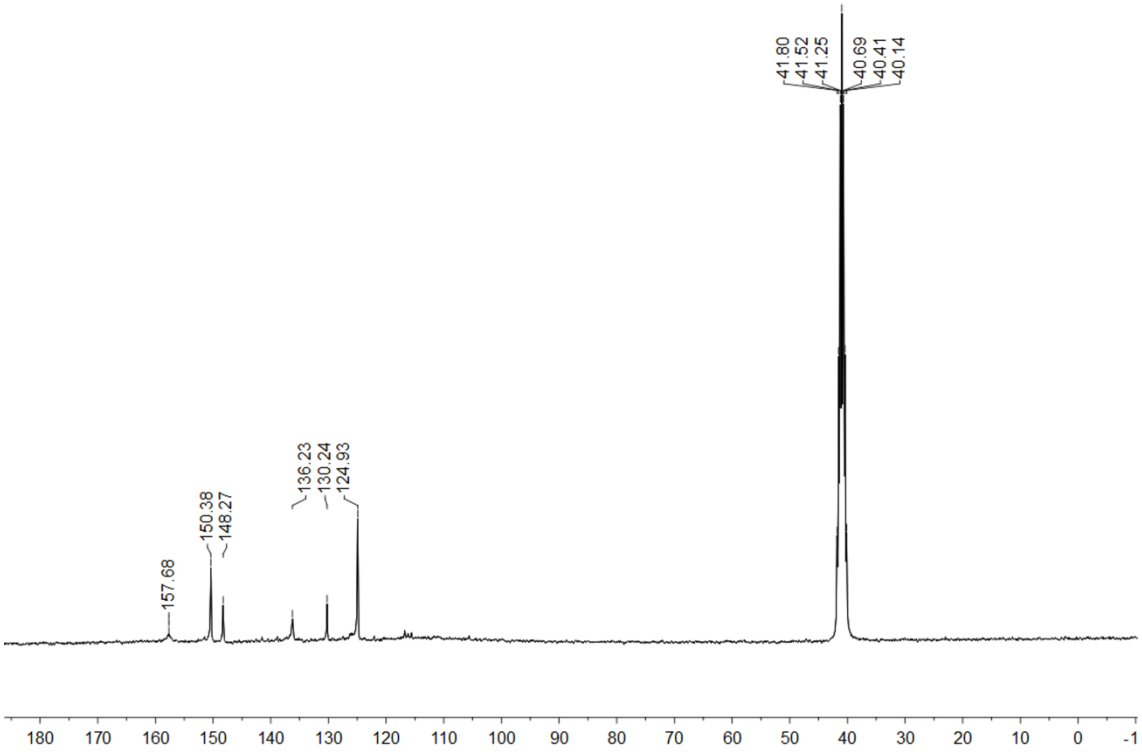


Figure S12 ^{13}C NMR spectra (75 MHz) of **6** in [D6]DMSO at 25 ^{o}C

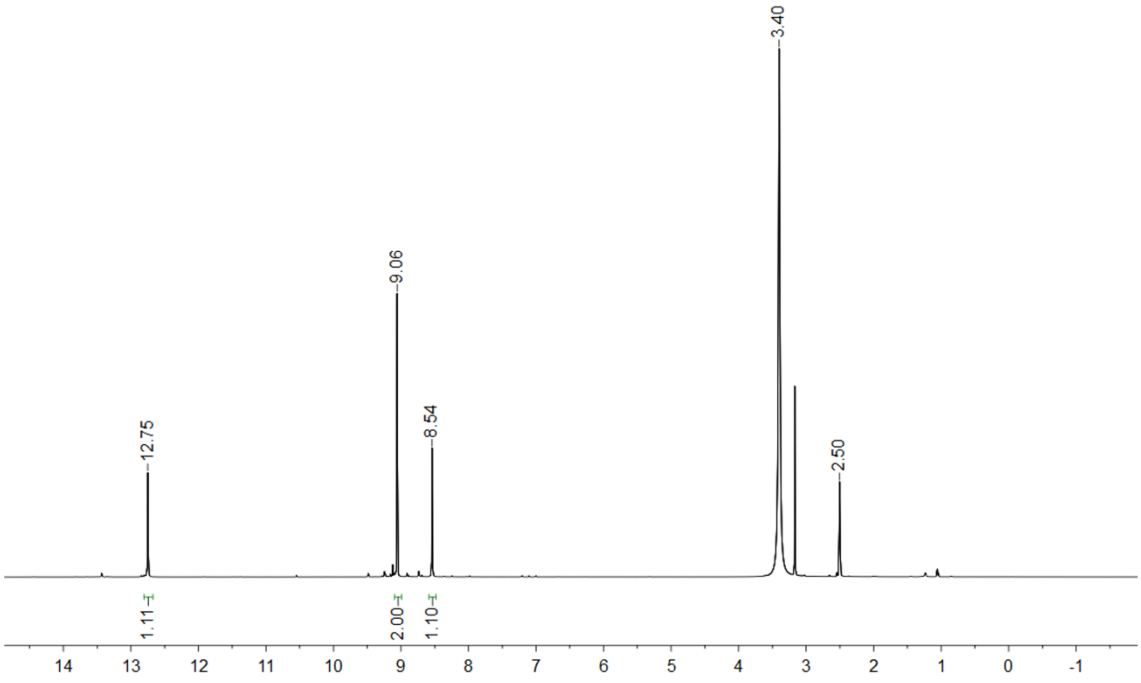


Figure S13 ^{1}H NMR spectra (500 MHz) of **7** in [D6]DMSO at 25 ^{o}C

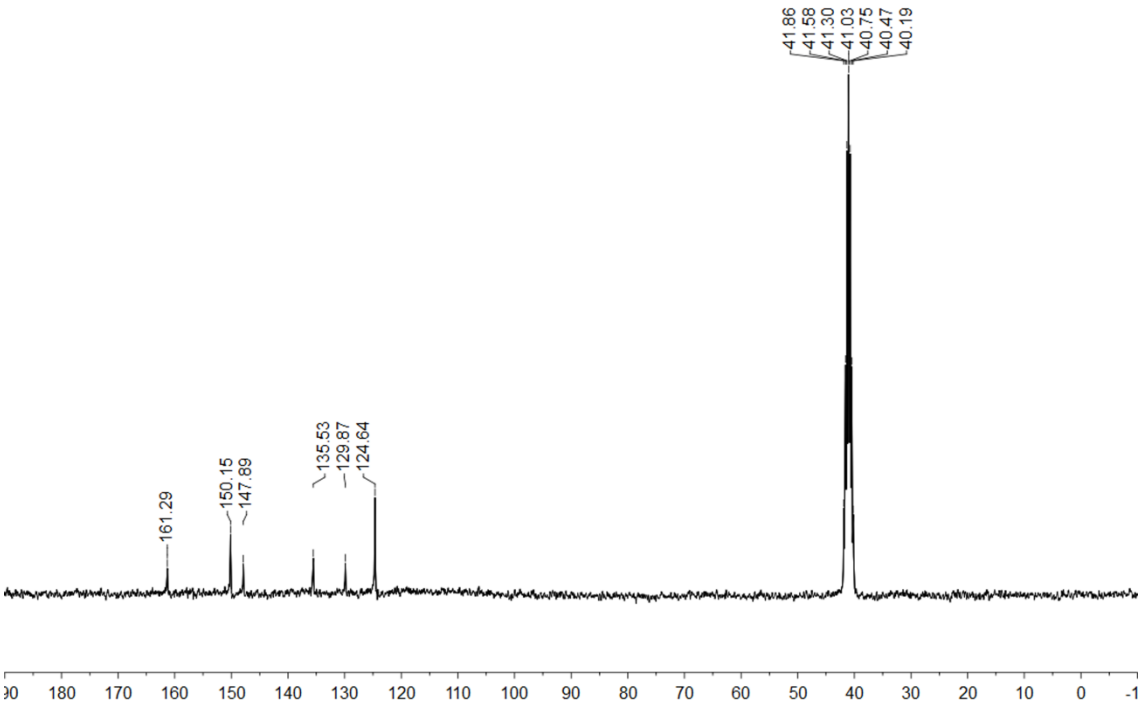


Figure S14 ^{13}C NMR spectra (75 MHz) of **7** in [D6]DMSO at 25 ^{o}C

Table S1. Selected bond distances of **1**

parameter	bond length(Å)	parameter	bond length(Å)
O(1)-N(1)	1.224(3)	N(5)-C(8)	1.346(3)
O(2)-N(1)	1.222(3)	N(6)-C(8)	1.311(3)
O(3)-N(2)	1.210(3)	N(7)-C(8)	1.322(3)
O(4)-N(2)	1.218(3)	C(1)-C(2)	1.378(3)
O(5)-N(3)	1.214(3)	C(1)-C(6)	1.403(3)
O(6)-N(3)	1.220(3)	C(2)-C(3)	1.382(3)
N(1)-C(1)	1.471(3)	C(3)-C(4)	1.375(3)
N(2)-C(3)	1.476(3)	C(4)-C(5)	1.380(3)
N(3)-C(5)	1.477(3)	C(5)-C(6)	1.398(3)
N(4)-C(7)	1.264(3)	C(6)-C(7)	1.487(3)
N(4)-N(5)	1.378(2)		

Table S2. Selected bond angles of **1** (°)

parameter	bond angle (°)	parameter	bond angle (°)
O(2)-N(1)-O(1)	124.7(2)	C(4)-C(3)-C(2)	122.8(2)
O(2)-N(1)-C(1)	117.3(2)	C(4)-C(3)-N(2)	118.7(2)
O(1)-N(1)-C(1)	118.0(2)	C(2)-C(3)-N(2)	118.5(2)
O(3)-N(2)-O(4)	124.0(2)	C(3)-C(4)-C(5)	117.8(2)
O(3)-N(2)-C(3)	118.7(2)	C(4)-C(5)-C(6)	123.4(2)
O(4)-N(2)-C(3)	117.3(2)	C(4)-C(5)-N(3)	116.0(2)
O(5)-N(3)-O(6)	124.2(2)	C(6)-C(5)-N(3)	120.6(2)
O(5)-N(3)-C(5)	118.0(2)	C(5)-C(6)-C(1)	115.1(2)

O(6)-N(3)-C(5)	117.8(2)	C(5)-C(6)-C(7)	123.3(2)
C(7)-N(4)-N(5)	116.1(2)	C(1)-C(6)-C(7)	121.5(2)
C(8)-N(5)-N(4)	118.0(2)	N(4)-C(7)-C(6)	117.2(2)
C(2)-C(1)-C(6)	123.9(2)	N(6)-C(8)-N(7)	121.3(2)
C(2)-C(1)-N(1)	116.3(2)	N(6)-C(8)-N(5)	120.6(2)
C(6)-C(1)-N(1)	119.72(19)	N(7)-C(8)-N(5)	118.1(2)
C(1)-C(2)-C(3)	117.0(2)		

Table S3. Selected bond distances of **2**

parameter	bond length(Å)	parameter	bond length(Å)
C(1)-C(6)	1.384(4)	C(15)-N(9)	1.275(3)
C(1)-C(2)	1.404(4)	C(16)-N(12)	1.308(3)
C(1)-N(1)	1.480(3)	C(16)-N(11)	1.320(3)
C(2)-C(3)	1.397(4)	C(16)-N(10)	1.351(3)
C(2)-C(7)	1.469(4)	N(1)-O(1)	1.220(3)
C(3)-C(4)	1.379(4)	N(1)-O(2)	1.227(3)
C(3)-N(6)	1.476(3)	N(2)-N(3)	1.359(3)
C(4)-C(5)	1.380(3)	N(6)-O(4)	1.217(3)
C(5)-C(6)	1.367(4)	N(6)-O(3)	1.222(3)
C(5)-N(7)	1.475(4)	N(7)-O(5)	1.221(3)
C(7)-N(2)	1.277(3)	N(7)-O(6)	1.228(3)
C(8)-N(4)	1.310(3)	N(8)-O(8)	1.218(3)
C(8)-N(5)	1.314(3)	N(8)-O(7)	1.229(3)

C(8)-N(3)	1.351(3)	N(9)-N(10)	1.363(3)
C(9)-C(14)	1.382(4)	N(13)-O(10)	1.213(3)
C(9)-C(10)	1.404(4)	N(13)-O(9)	1.217(3)
C(9)-N(8)	1.478(3)	N(14)-O(11)	1.217(3)
C(10)-C(11)	1.401(4)	N(14)-O(12)	1.221(3)
C(10)-C(15)	1.467(4)	N(15)-O(14)	1.235(3)
C(11)-C(12)	1.381(4)	N(15)-O(15)	1.243(3)
C(11)-N(13)	1.480(3)	N(15)-O(13)	1.247(3)
C(12)-C(13)	1.371(4)	N(16)-O(18)	1.244(3)
C(13)-C(14)	1.374(4)	N(16)-O(17)	1.246(3)
C(13)-N(14)	1.483(4)	N(16)-O(16)	1.250(3)

Table S4. Selected bond angles of **2** (°)

parameter	bond angle (°)	parameter	bond angle (°)
C(6)-C(1)-C(2)	123.9(3)	N(9)-C(15)-C(10)	118.9(3)
C(6)-C(1)-N(1)	116.0(2)	N(12)-C(16)-N(11)	122.3(3)
C(2)-C(1)-N(1)	119.9(3)	N(12)-C(16)-N(10)	120.1(3)
C(3)-C(2)-C(1)	113.9(2)	N(11)-C(16)-N(10)	117.6(3)
C(3)-C(2)-C(7)	123.2(2)	O(1)-N(1)-O(2)	125.6(3)
C(1)-C(2)-C(7)	122.9(2)	O(1)-N(1)-C(1)	117.5(3)
C(4)-C(3)-C(2)	124.5(3)	O(2)-N(1)-C(1)	116.8(2)
C(4)-C(3)-N(6)	114.3(2)	C(7)-N(2)-N(3)	118.0(2)
C(2)-C(3)-N(6)	121.1(2)	C(8)-N(3)-N(2)	117.5(2)

C(3)-C(4)-C(5)	117.6(3)	O(4)-N(6)-O(3)	125.3(2)
C(6)-C(5)-C(4)	122.1(3)	O(4)-N(6)-C(3)	118.4(2)
C(6)-C(5)-N(7)	119.7(3)	O(3)-N(6)-C(3)	116.3(2)
C(4)-C(5)-N(7)	118.2(3)	O(5)-N(7)-O(6)	125.2(3)
C(5)-C(6)-C(1)	118.0(3)	O(5)-N(7)-C(5)	117.3(3)
N(2)-C(7)-C(2)	117.7(2)	O(6)-N(7)-C(5)	117.5(3)
N(4)-C(8)-N(5)	121.5(3)	O(8)-N(8)-O(7)	125.2(2)
N(4)-C(8)-N(3)	120.5(3)	O(8)-N(8)-C(9)	117.7(3)
N(5)-C(8)-N(3)	118.0(3)	O(7)-N(8)-C(9)	117.1(2)
C(14)-C(9)-C(10)	124.0(3)	C(15)-N(9)-N(10)	116.6(2)
C(14)-C(9)-N(8)	115.6(2)	C(16)-N(10)-N(9)	118.1(2)
C(10)-C(9)-N(8)	120.3(2)	O(10)-N(13)-O(9)	124.7(2)
C(11)-C(10)-C(9)	113.9(3)	O(10)-N(13)-C(11)	116.5(2)
C(11)-C(10)-C(15)	123.3(3)	O(9)-N(13)-C(11)	118.8(2)
C(9)-C(10)-C(15)	122.8(2)	O(11)-N(14)-O(12)	125.4(3)
C(12)-C(11)-C(10)	124.4(3)	O(11)-N(14)-C(13)	117.2(3)
C(12)-C(11)-N(13)	114.5(2)	O(12)-N(14)-C(13)	117.4(3)
C(10)-C(11)-N(13)	121.1(2)	O(14)-N(15)-O(15)	118.8(2)
C(13)-C(12)-C(11)	117.6(3)	O(14)-N(15)-O(13)	121.4(2)
C(12)-C(13)-C(14)	122.3(3)	O(15)-N(15)-O(13)	119.8(2)
C(12)-C(13)-N(14)	118.2(3)	O(18)-N(16)-O(17)	120.5(2)
C(14)-C(13)-N(14)	119.5(3)	O(18)-N(16)-O(16)	119.7(2)
C(13)-C(14)-C(9)	117.8(3)	O(17)-N(16)-O(16)	119.8(2)

Table S5. Selected bond distances of **5**

parameter	bond length(Å)	parameter	bond length(Å)
O(1)-N(3)	1.218(6)	N(7)-C(9)	1.281(7)
O(2)-N(3)	1.226(6)	N(8)-C(11)	1.485(7)
O(3)-N(4)	1.218(7)	N(9)-C(13)	1.476(8)
O(4)-N(4)	1.227(6)	N(10)-C(15)	1.467(7)
O(5)-N(8)	1.223(6)	C(1)-C(2)	1.439(8)
O(6)-N(8)	1.213(6)	C(2)-C(7)	1.401(7)
O(7)-N(9)	1.185(8)	C(2)-C(3)	1.415(7)
O(8)-N(9)	1.202(7)	C(3)-C(4)	1.388(7)
O(9)-N(10)	1.228(7)	C(4)-C(5)	1.374(7)
O(10)-N(10)	1.223(7)	C(5)-C(6)	1.402(8)
N(1)-C(1)	1.311(7)	C(6)-C(7)	1.374(7)
N(1)-N(2)	1.386(6)	C(9)-C(10)	1.466(7)
N(2)-C(3)	1.384(7)	C(10)-C(11)	1.403(7)
N(2)-C(8)	1.419(7)	C(10)-C(15)	1.411(7)
N(3)-C(5)	1.478(7)	C(11)-C(12)	1.371(7)
N(4)-C(7)	1.461(7)	C(12)-C(13)	1.387(8)
N(5)-C(8)	1.337(7)	C(13)-C(14)	1.378(8)
N(6)-C(8)	1.302(7)	C(14)-C(15)	1.383(7)
N(6)-N(7)	1.404(6)		

Table S6. Selected bond angles of **5** (°)

parameter	bond angle (°)	parameter	bond angle (°)
C(1)-N(1)-N(2)	105.7(5)	C(4)-C(3)-C(2)	123.5(5)
C(3)-N(2)-N(1)	112.2(4)	C(5)-C(4)-C(3)	115.2(5)
C(3)-N(2)-C(8)	129.2(4)	C(4)-C(5)-C(6)	124.8(5)
N(1)-N(2)-C(8)	118.3(4)	C(4)-C(5)-N(3)	117.8(5)
O(1)-N(3)-O(2)	123.6(5)	C(6)-C(5)-N(3)	117.4(5)
O(1)-N(3)-C(5)	118.0(5)	C(7)-C(6)-C(5)	117.5(5)
O(2)-N(3)-C(5)	118.4(5)	C(6)-C(7)-C(2)	121.6(5)
O(3)-N(4)-O(4)	122.8(5)	C(6)-C(7)-N(4)	118.4(5)
O(3)-N(4)-C(7)	118.2(5)	C(2)-C(7)-N(4)	120.0(5)
O(4)-N(4)-C(7)	119.0(5)	N(6)-C(8)-N(5)	129.2(5)
C(8)-N(6)-N(7)	109.9(4)	N(6)-C(8)-N(2)	114.6(5)
C(9)-N(7)-N(6)	111.5(4)	N(5)-C(8)-N(2)	116.2(5)
O(6)-N(8)-O(5)	125.4(5)	N(7)-C(9)-C(10)	118.8(5)
O(6)-N(8)-C(11)	117.7(5)	C(11)-C(10)-C(15)	113.6(5)
O(5)-N(8)-C(11)	116.9(4)	C(11)-C(10)-C(9)	123.2(5)
O(7)-N(9)-O(8)	123.3(6)	C(15)-C(10)-C(9)	123.2(5)
O(7)-N(9)-C(13)	118.0(6)	C(12)-C(11)-C(10)	125.1(5)
O(8)-N(9)-C(13)	118.2(6)	C(12)-C(11)-N(8)	115.3(5)
O(10)-N(10)-O(9)	123.0(5)	C(10)-C(11)-N(8)	119.4(4)
O(10)-N(10)-C(15)	119.9(5)	C(11)-C(12)-C(13)	117.1(5)
O(9)-N(10)-C(15)	117.0(5)	C(14)-C(13)-C(12)	122.5(5)
N(1)-C(1)-C(2)	111.9(5)	C(14)-C(13)-N(9)	118.4(5)

C(7)-C(2)-C(3)	117.2(5)	C(12)-C(13)-N(9)	119.1(5)
C(7)-C(2)-C(1)	137.9(5)	C(13)-C(14)-C(15)	117.4(5)
C(3)-C(2)-C(1)	104.9(5)	C(14)-C(15)-C(10)	124.2(5)
N(2)-C(3)-C(4)	131.3(5)	C(14)-C(15)-N(10)	116.3(5)
N(2)-C(3)-C(2)	105.2(4)	C(10)-C(15)-N(10)	119.5(5)

Table S7. Hydrogen bonds present in compound **1**

D—H•••A	d(D-H)/ Å	d(H...A)/ Å	d(D...A)/ Å	<(DHA)/ °	comment
N(6) —H(6B) •••Cl^{i}	0.885(9)	2.436(15)	3.215(2)	147(2)	inter
N(7) —H(7A) •••Cl ^{i}	0.895(9)	2.447(14)	3.242(3)	148(2)	inter
N(7) —H(7B) •••Cl^{ii}	0.892(10)	2.470(15)	3.253(3)	147(2)	inter
N(6) —H(6A) •••N(4)	0.888(16)	2.33(2)	2.663(3)	102.2(17)	intra
N(6) —H(6A) •••O(4)^{iii}	0.888(16)	2.194(15)	3.014(3)	153(2)	inter
N(7) —H(7A) •••O(2)^{iv}	0.895(17)	2.48(2)	3.022(3)	119.5(16)	inter
N(5) —H(5) •••Cl^{ii}	0.902(10)	2.351(15)	3.196(2)	156(2)	inter

[i] 1-x, -y, 1-z; [ii] -0.5+x, 0.5-y, 1-z; [iii] 1-x,-1/2+y,3/2-z; [iv] 1/2-x,-y,-1/2+z

Table S8. Hydrogen bonds present in compound **2**

D—H•••A	D•••H (Å)	H•••A (Å)	D•••A (Å)	D—H•••A (Å)	comment
N(3) —H(3) •••O(16)^{i}	0.88	2.02	2.844(3)	156	inter
N(3) —H(3) •••O(17) ^{i}	0.88	2.47	3.144(3)	134	inter
N(4) —H(4A) •••O(17) ^{ii}	0.88	2.06	2.930(3)	170	inter
N(4) —H(4B) •••O(4)	0.88	2.59	3.417(3)	157	intra
N(4) —H(4B) •••N(2)	0.88	2.32	2.646(3)	102	intra
N(5) —H(5A) •••O(18) ^{ii}	0.88	2.03	2.888(3)	165	inter
N(5) —H(5A) •••O(14) ^{i}	0.88	2.38	2.925(3)	120	inter
N(5) —H(5B) •••O(13) ^{i}	0.88	2.30	2.984(4)	135	inter
N(5) —H(5B) •••O(16) ^{i}	0.88	2.42	3.154(3)	141	inter
N(10) —H(10) •••O(13) ^{iii}	0.88	2.26	3.035(3)	146	inter

N(10) —H(10) •••O(15) [iii]	0.88	2.15	2.976(3)	155	inter
N(11) —H(11A) •••O(18) [iii]	0.88	2.35	2.974(3)	128	inter
N(11) —H(11A) •••O(14) [iv]	0.88	2.18	3.000(3)	156	inter
N(11) —H(11B) •••O(13) [iii]	0.88	2.24	3.027(3)	149	inter
N(12) —H(12A) •••O(14) [iv]	0.88	2.56	3.288(3)	140	inter
N(12) —H(12A) •••O(15) [iv]	0.88	2.07	2.932(3)	165	inter
N(12) —H(12B) •••N(9)	0.88	2.32	2.650(3)	102	intra
C(7) —H(7) •••O(2)	0.95	2.28	2.807(3)	114	intra
C(7) —H(7) •••O(17)[i]	0.95	2.51	3.230(4)	132	inter
C(12) —H(12) •••O(4) [i]	0.95	2.51	3.349(4)	147	inter
C(15) —H(15) •••O(7)	0.95	2.31	2.786(3)	110	intra
C(15) —H(15) •••O(15) [iii]	0.95	2.42	3.205(4)	140	inter

[i] 1-x,1-y,1-z; [ii] 1-x,1/2+y,3/2-z; [iii] 1+x,y,z; [iv] 1+x,1/2-y,1/2+z

Table S9. Hydrogen bonds present in compound **5**

D—H•••A	D•••H (Å)	H•••A (Å)	D•••A (Å)	D—H•••A (Å)	comment
N(5) —H(5A) •••O(9)[i]	0.83(8)	2.58(8)	3.117(8)	124(6)	inter
N(5) —H(5B) •••N(1)	0.91(8)	2.26(7)	2.671(8)	107(6)	intra
C(1) —H(1) •••O(3)	0.95	2.47	2.900(7)	107	intra
C(4) —H(4) •••N(6)	0.95	2.40	2.904(7)	113	intra
C(6) —H(6) •••O(3)[ii]	0.95	2.47	3.347(7)	154	inter
C(9) —H(9) •••O(10)	0.95	2.40	2.778(7)	103	intra
C(9) —H(9) •••O(5)[iii]	0.95	2.56	3.491(7)	165	inter
C(12) —H(12) •••O(8)[iv]	0.95	2.48	3.321(8)	147	inter

[i] x,y,1+z; [ii] 1/2-x,y,-1/2+z; [iii] 1-x,1/2-y,-1/2+z; [iv] 3/2-x,y,1/2+z

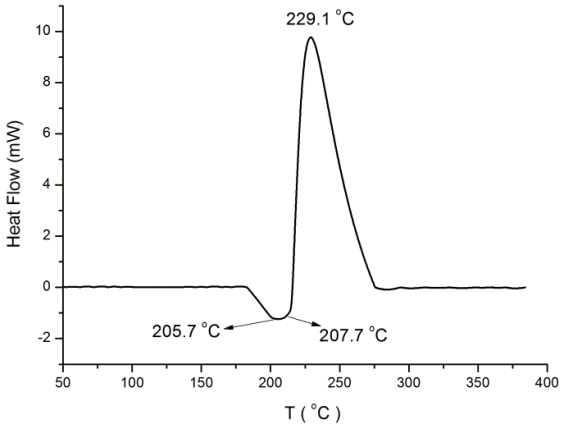


Figure S15 The DSC plots of **1**

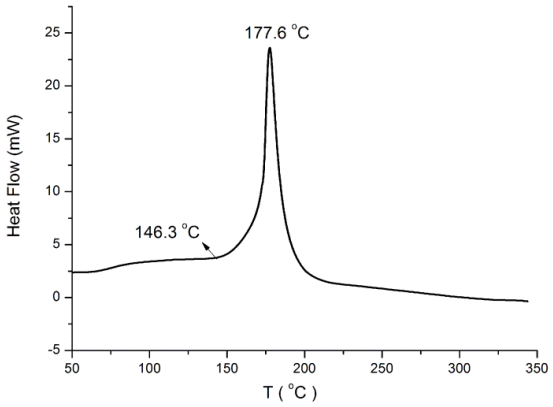


Figure S16 The DSC plots of **2**

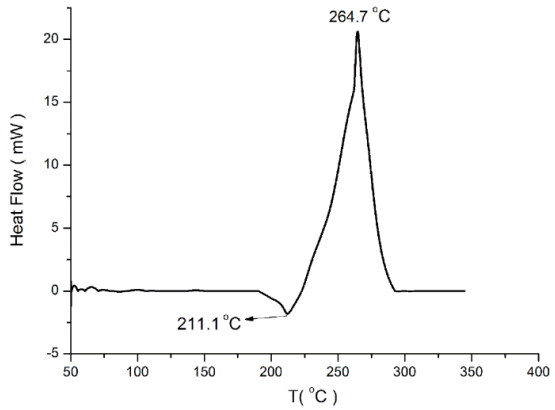


Figure S 17 The DSC plots of **3**

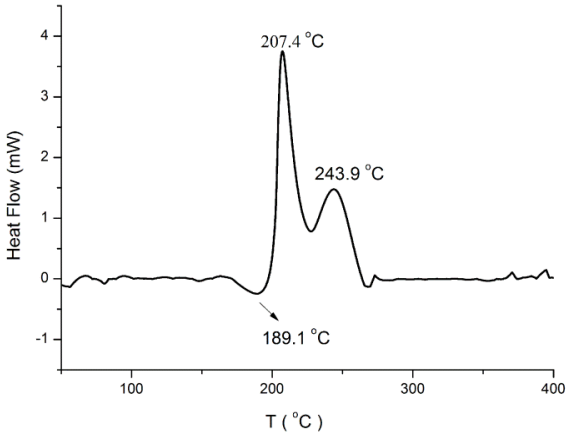


Figure S18 The DSC plots of **5**

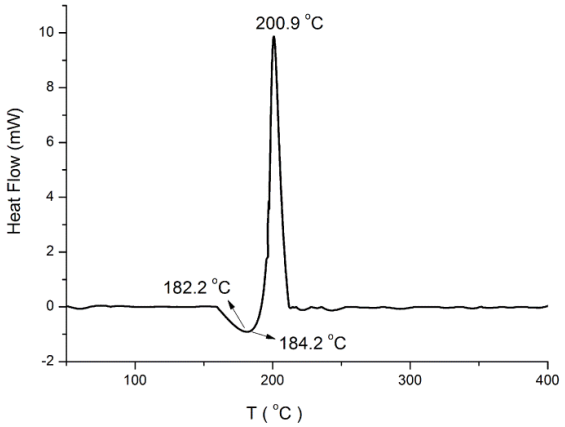


Figure S19 The DSC plots of **6**

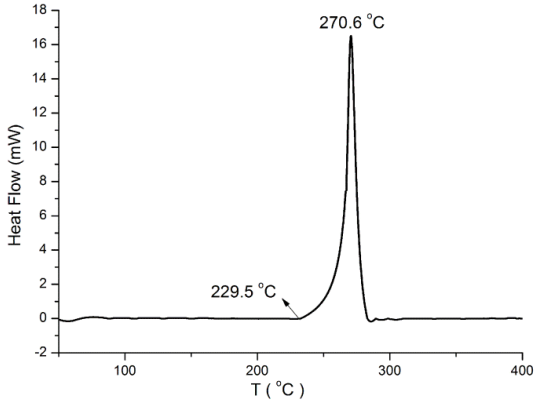


Figure S20 The DSC plots of **7**

Computation details

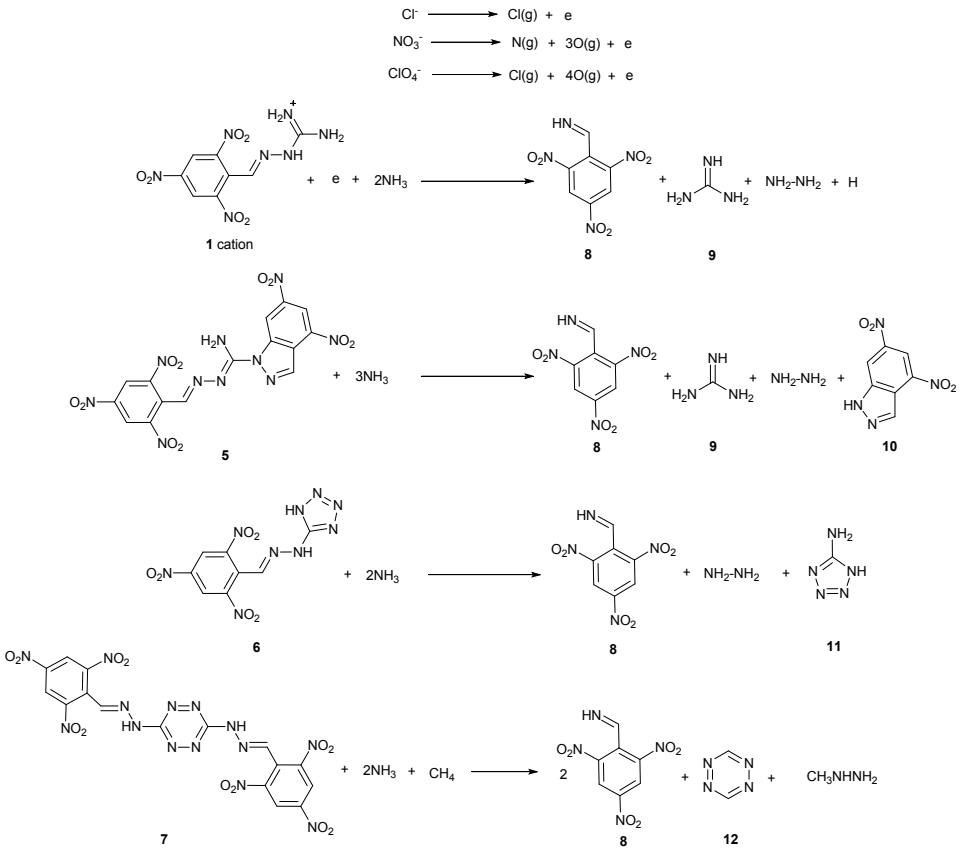
Computations were carried out by using the Gaussian09 suite of programs. The elementary geometric optimization and the frequency analysis were performed at the level of Becke three Lee-Yan-Parr (B3LYP) Functionals[1] with 6-311+G** basis set.[2] All of the optimized structures were characterized to be local energy minima on the potential surface without any imaginary frequencies. The predictions of heats of formation (HOF) adopt the hybrid DFT-B3LYP methods with 6-311+G** basis set via designed isodesmic reactions. The isodesmic reaction processes, i.e., the number of each kind of formal bond is conserved, are used with application of the bond separation reaction (BSR) rules. The molecule is broken down into a set of two heavy-atom molecules containing the same component bonds. The isodesmic reactions used to derive the HOF of these compounds are in Scheme S1. The change of enthalpy for the reactions at 298 K can be expressed as:

$$\Delta H_{298} = \sum \Delta_f H_P - \sum \Delta_f H_R \qquad (1)$$

Where $\Delta_f H_R$ and $\Delta_f H_P$ are the HOF of reactants and products at 298 K, respectively, and ΔH_{298} can be calculated using the following expression:

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

Where 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 thermal correction from 0 to 298 K. The $\Delta(PV)$ value in eq (2) is the PV work term. It equals ΔnRT for the reactions of ideal gas. For the isodesmic reactions, $\Delta n = 0$, so $\Delta(PV) = 0$. On the left side of Eq. (1), apart from target compound, all the others are called reference compounds. The HOF of reference compounds are available either from the experiments[3-5] or from the high level computing like CBS-4M.



Scheme S1 The isodesmic reactions for the calculation of HOF

For compounds **5-7**, the theoretical density was obtained from the molecular weight divided by the average molecular volume of 100 single point calculations. The volume was defined as the space inside an electronic isodensity contour of 0.001 electron/bohr3 evaluated using a Monte Carlo integrator. This method has been successfully applied to various energetic molecules.[6-7]

For an ionic crystal with formula unit M_pX_q, its volume is simply the sum of the volumes of the ions contained in the formula unit:[6-8]

$$V = pV_{M+} + qV_{X-} \quad (3)$$

where M denotes the cation and X denotes the anion. Because the volumes of individual ions able to be evaluated using the DFT procedure, eq 3 was used to calculate formula unit volumes for ionic crystal. For those compounds that contain hydrogen atoms, a "correct" molecular volume using a molecular structure optimized at the DFT level can be calculated using:

V(corrected)Opt = V(uncorrected)Opt - [0.6763 + 0.9418×（no. of hydrogen atoms in the ion） （4）

Based on a Born-Haber enegy cycle,the heat of formation of energetic salt **1-3** can be simplified by the formula (5):

$$\Delta H_f^o(\text{salt},298\ \text{K}) = \Delta H_f^o(\text{cation},298\ \text{K}) + \Delta H_f^o(\text{anion},298\ \text{K}) - \Delta H_L \quad (5)$$

where ΔH_L is the lattice energy of the salt.

The ΔH_L value could be predicted by the formula suggested by Jenkins et al.[9] (equation 6), in which U_{POT} is the lattice potential energy and n_M and n_X depend on the nature of the ions M_p^+ and X_q^-, respectively, and is equal to three for monatomic ions, five for linear polyatomic ions, and six for nonlinear polyatomic ions.

$$\Delta H_L = U_{POT} + [\, p(n_M/2 - 2) + q(n_X/2 - 2)]RT \quad (6)$$

The equation for the lattice potential energy, U_{POT}, takes the form of equation (7), where ρ_m is the density (g cm^{-3}), M_m is the chemical formula mass of the ionic material (g), and the coefficients γ (kJ mol^{-1} cm) and δ (kJ mol^{-1}) are assigned literature values.[9]

$$U_{POT}\ (\text{kJ·mol}^{-1}) = \gamma\,(\rho_m/M_m)^{1/3} + \delta \quad (7)$$

Table S11 Calculated total energy (E_0), zero-point energy (ZPE), thermal correction (H_T), and enthalpy of formation (HOF) of reference compounds

	E_0 /a.u.	ZPE/ kJ·mol^{-1}	H_T/ kJ·mol^{-1}	HOF/ kJ·mol^{-1}
H	-0.5021559	0.00	6.20	218.00[b]
NH_3	-56.5826356	86.27	10.05	-45.90[b]
H_2N-NH_2	-111.9105763	134.28	11.16	95.40[b]
CH_3NHNH_2	-151.2295206	204.89	13.79	94.70[b]
1cation	-1144.0386864	492.56	56.04	895.03[c]
8	-939.4577013	322.67	41.27	147.84[c]

9	-205.4417653	184.19	14.19	30.52[c]
10	-789.0629081	307.27	33.36	173.78[c]
11	-313.7044074	157.30	14.81	330.58[c]
12	-296.3983124	128.90	13.87	469.38[c]
5	-1876.1274612	677.07	81.40	525.42
6	-1251.891433	430.92	54.92	652.06
7	-2283.572454	756.21	99.81	989.52

、[a] E_0 in a.u. ZPE (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.

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