

Supporting Information

Pyrazolo[1,5-a]pyrimidine with similar “amino-nitro-amino” arrangement characteristics to TATB: A novel heat-resistant explosive with fused structure

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1. Experimental Section

General methods

All reagents used in this paper were purchased from energy chemical in analytical grade and without further purification. ^1H and ^{13}C spectra were recorded using a 500 MHz (AVANCE III500MHz) nuclear magnetic spectrometer operating at 500 MHz and 126 MHz, respectively, and the chemical shifts in ^1H and ^{13}C NMR spectra are reported relative to d_6 -DMSO. The phase transition temperature and decomposition (onset) point were obtained by a differential scanning calorimeter (Mettler Toledo DSC823e) at a heating rate of $5\text{ }^\circ\text{C min}^{-1}$ in a closed Al crucibles with a nitrogen flow of 50 ml min^{-1} . IR spectra were recorded using KBr pellets for solids on a Thermo Nicolet iS10 spectrometer. Density was measured at $25\text{ }^\circ\text{C}$ by using a gas pycnometer. The heats of formation were calculated by using Gaussian 09[1], and the detonation velocities (D) and pressures (P) were calculated with EXPLO5 v6.01[2]. Impact and friction sensitivity measurements were performed with a BAM Fallhammer and a BAM friction tester [3]. The two-dimensional (2D)-fingerprint of crystals, associated Hirshfeld surfaces and noncovalent interaction analysis were investigated through CrystalExplorer [4] and Multiwfn [5] software package.

2. X-ray crystallographic study

Crystals 2, 3 and 4 were performed on a Bruker Smart ApexII diffractometer at 296K. Integration and scaling of intensity data were accomplished using the SAINT program. Corrections for Lorentz and polarization effects and for absorption (ψ scan) were applied. The structure was solved by direct methods using SHELXS-2014 and refined by full-matrix least-squares calculation on F2 with SHELXL-2014. All non-hydrogen atoms were refined anisotropically. All hydrogen were placed in calculated positions and were assigned fixed isotropic thermal parameters at 1.2 times. Data were corrected for the effects of absorption using SADABS Relevant crystal data and refinement results are summarized in Table S1. For the structure determination of compounds 4 and 5, As it was not possible to see clear electron-density peaks in difference maps which would correspond with acceptable locations for the O8 water H atoms, the refinement was completed with no allowance for these H atoms in the model.

Table S1. Crystallographic data for 2, 3, 4 and 5.

Chemical formula	$\text{C}_6\text{H}_5\text{ClN}_4$	$(\text{C}_6\text{H}_3\text{ClN}_6\text{O}_4)\cdot$	$(\text{C}_6\text{H}_5\text{N}_7\text{O}_4)\cdot$	$(\text{C}_6\text{H}_4\text{N}_6\text{O}_5)\cdot(\text{C}_2\text{H}_4\text{O}_2)\cdot$
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		(C ₂ H ₃ N)	2.5(H ₂ O)	0.125(H ₂ O)
Formula mass	168.59	299.65	568.42	302.46
Crystal system	monoclinic	Monoclinic	Triclinic	Monoclinic
a/Å	3.9124(3)	11.0127(13)	3.538(2)	4.5803(3)
b/Å	15.4255(12)	4.6953(7)	12.804(6)	27.1194(17)
c/Å	11.8549(9)	23.988(3)	13.613(7)	10.7559(7)
α/°	90	90	64.235(12)	90
β/°	93.293(3)	93.872	83.900(16)	99.380(2)
γ/°	90	90	82.879(16)	90
Volume/Å ³	714.27(10)	1237.6(3)	550.2(5)	1318.18(15)
Temperature/K	296(2)	296(2)	296(2)	296(2)
Space group	P2 ₁ /c	P2 ₁ /c	P-1	P2 ₁ /c
Z	4	4	1	4
Radiation type	Mo-Kα	Mo-Kα	Mo-Kα	Mo-Kα
μ/mm ⁻¹	0.464	0.336	0.154	0.135
Densitycalcd/g cm ⁻³	1.568	1.608	1.716	1.524
F(000)	344	608	294	621
2θ range for data collection/°	2.169 to 27.564	2.430 to 27.566	1.773 to 24.996	2.437 to 24.991
Index ranges	-5/5; 0/20; 0/15	-12/14; -25/31	-5/6; -4/4; -16/16	-15/15; -5/5;-28/2;-12/12
Reflections collected	2565	11982	5639	11523
Independent reflections	2565	2846	1858	2297
R _{int}	0.0461	0.0691	0.0658	0.0347
Data/restraints/parameters	2565/0/101	2846 / 35 / 192	1858 / 12 / 182	2297 / 0 / 199
R1 / wR2 [all data]	0.0714/ 0.1241	0.1559/0.1769	0.1986/0.3309	0.0783/0.1700
R1 / wR2 [I > 2σ(I)]	0.0461/ 0.1137	0.0657/0.1433	0.1553/0.3126	0.0565/0.1552
Goodness-of-fit on F ²	1.052	1.012	1.136	1.080
CCDC number	2005560	2016542	2007915	2053258

Table S2. Hydrogen bonds for compound **2** [Å and °].

D-H···A	D-H(Å)	H···A(Å)	D···A(Å)	D-H···A(°)
N(4)-H(4B)...N(1)#1	0.86	2.31	3.101(3)	152
N(4)-H(4A)...N(3)#2	0.86	2.22	3.008(3)	153

Symmetry transformations used to generate equivalent atoms:

#1 $x, -y+1/2, z+1/2$ #2 $-x, -y+1, -z+1$ **Table S3.** Bond lengths [Å] and angles [°] for compound **2**.

Bond length		Bond angle	
C(1)-N(1)	1.305(3)	N(1)-C(1)-C(2)	127.6(2)
C(1)-C(2)	1.381(4)	N(1)-C(1)-Cl(1)	115.4(2)
C(1)-Cl(1)	1.745(3)	C(2)-C(1)-Cl(1)	116.9(2)
C(2)-C(3)	1.381(3)	C(3)-C(2)-C(1)	118.3(2)
C(2)-H(2)	0.9300	C(3)-C(2)-H(2)	120.9
C(3)-N(4)	1.320(3)	C(1)-C(2)-H(2)	120.9
C(3)-N(2)	1.368(3)	N(4)-C(3)-N(2)	118.6(2)
C(4)-N(1)	1.356(3)	N(4)-C(3)-C(2)	126.1(2)
C(4)-C(5)	1.377(4)	N(2)-C(3)-C(2)	115.3(2)
C(4)-N(2)	1.388(3)	N(1)-C(4)-C(5)	133.8(2)
C(5)-C(6)	1.374(4)	N(1)-C(4)-N(2)	121.3(2)
C(5)-H(5)	0.9300	C(5)-C(4)-N(2)	104.9(2)
C(6)-N(3)	1.332(3)	C(6)-C(5)-C(4)	105.5(2)
C(6)-H(6)	0.9300	C(6)-C(5)-H(5)	127.2
N(2)-N(3)	1.363(3)	C(4)-C(5)-H(5)	127.2
N(4)-H(4A)	0.8600	N(3)-C(6)-C(5)	114.2(3)
N(4)-H(4B)	0.8600	N(3)-C(6)-H(6)	122.9
		C(5)-C(6)-H(6)	122.9
		C(1)-N(1)-C(4)	114.5(2)

	N(3)-N(2)-C(3)	124.2(2)
	N(3)-N(2)-C(4)	112.8(2)
	C(3)-N(2)-C(4)	123.0(2)
	C(6)-N(3)-N(2)	102.5(2)
	C(3)-N(4)-H(4A)	120.0
	C(3)-N(4)-H(4B)	120.0
	H(4A)-N(4)-H(4B)	120.0

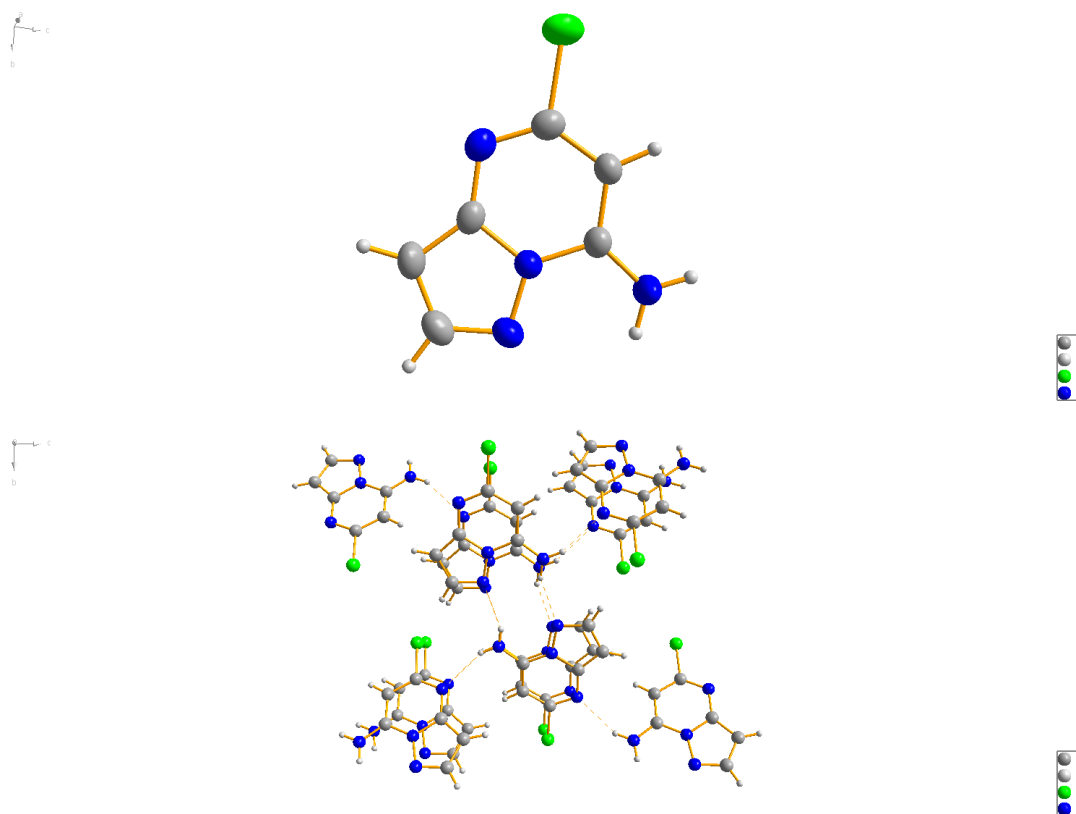


Fig. S1. Molecular structure and packing diagram of **2** (The yellow dotted line represents the hydrogen bond).

Table S4. Hydrogen bonds for compound **3** [\AA and $^\circ$].

D-H \cdots A	D-H(\AA)	H \cdots A(\AA)	D \cdots A(\AA)	D-H \cdots A($^\circ$)
C(8)-H(6) \cdots O(3A ^a)#1	0.96	2.73	3.379(11)	125
N(6)-H(6B) \cdots O(4)#2	0.86	2.33	3.095(4)	148
N(6)-H(6B) \cdots O(4)	0.86	2.07	2.637(5)	123

N(6)-H(6A)...N(7)	0.86	2.20	2.969(6)	149
C(1)-H(1)...O(1)#3	0.93	2.49	3.338(4)	151

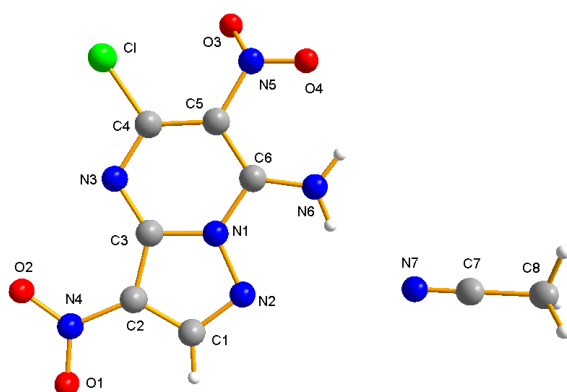
Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+3/2,-z+1/2 #2 -x+1,y+1/2,-z+1/2 #3 -x,-y+1,-z+1

Table S5. Bond lengths [Å] and angles [°] for compound **3**.

Bond length		Bond angle	
C(1)-N(2)	1.315(4)	N(2)-C(1)-C(2)	113.3(3)
C(1)-C(2)	1.383(4)	N(2)-C(1)-H(1)	123.3
C(1)-H(1)	0.9300	C(2)-C(1)-H(1)	123.3
C(2)-C(3)	1.408(4)	C(1)-C(2)-C(3)	106.4(3)
C(2)-N(4)	1.415(4)	C(1)-C(2)-N(4)	127.2(3)
C(3)-N(3)	1.337(4)	C(3)-C(2)-N(4)	126.4(3)
C(3)-N(1)	1.363(4)	N(3)-C(3)-N(1)	123.0(3)
C(4)-N(3)	1.323(4)	N(3)-C(3)-C(2)	133.8(3)
C(4)-C(5)	1.409(5)	N(1)-C(3)-C(2)	103.2(3)
C(4)-Cl(1)	1.686(4)	N(3)-C(4)-C(5)	124.0(3)
C(5)-C(6)	1.404(5)	N(3)-C(4)-Cl(1)	113.9(3)
C(5)-N(5)	1.455(5)	C(5)-C(4)-Cl(1)	122.1(3)
C(6)-N(6)	1.301(4)	C(6)-C(5)-C(4)	120.3(3)
C(6)-N(1)	1.380(4)	C(6)-C(5)-N(5)	117.3(4)
N(1)-N(2)	1.382(3)	C(4)-C(5)-N(5)	122.4(4)
N(4)-O(2)	1.222(4)	N(6)-C(6)-N(1)	116.4(3)
N(4)-O(1)	1.227(3)	N(6)-C(6)-C(5)	130.5(3)
N(5)-O(4)	1.150(5)	N(1)-C(6)-C(5)	113.2(3)
N(5)-O(3A)	1.207(10)	C(3)-N(1)-C(6)	123.7(3)
N(5)-O(3B)	1.302(8)	C(3)-N(1)-N(2)	114.3(2)
N(6)-H(6A)	0.8600	C(6)-N(1)-N(2)	122.0(3)
N(6)-H(6B)	0.8600	C(1)-N(2)-N(1)	102.8(2)
N(7)-C(7)	1.117(5)	C(4)-N(3)-C(3)	115.8(3)
C(7)-C(8)	1.436(7)	O(2)-N(4)-O(1)	123.2(3)

C(8)-H(6)	0.9600	O(2)-N(4)-C(2)	119.3(3)
C(8)-H(5)	0.9600	O(1)-N(4)-C(2)	117.5(3)
C(8)-H(4)	0.9600	O(4)-N(5)-O(3A)	109.9(6)
		O(4)-N(5)-O(3B)	118.1(4)
		O(4)-N(5)-C(5)	120.8(4)
		O(3A)-N(5)-C(5)	118.1(6)
		O(3B)-N(5)-C(5)	116.0(5)
		C(6)-N(6)-H(6A)	120.0
		C(6)-N(6)-H(6B)	120.0
		H(6A)-N(6)-H(6B)	120.0
		N(7)-C(7)-C(8)	179.4(6)
		C(7)-C(8)-H(6)	109.5
		C(7)-C(8)-H(5)	109.5
		H(6)-C(8)-H(5)	109.5
		C(7)-C(8)-H(4)	109.5
		H(6)-C(8)-H(4)	109.5
		H(5)-C(8)-H(4)	109.5



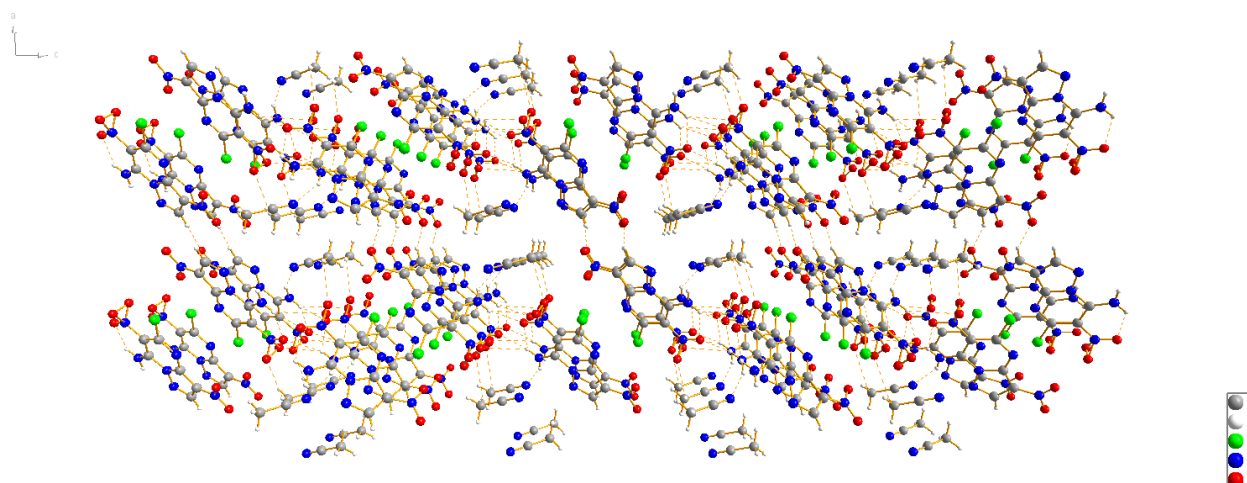


Fig. S2. Molecular structure and packing diagram of **3** (The yellow dotted line represents the hydrogen bond).

Table S6. Hydrogen bonds for **4** [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
C(6)-H(6)...O(4)#1	0.93	2.44	3.284(12)	151
N(6)-H(6A)...N(1)#2	0.86	2.20	3.048(10)	170
N(6)-H(6B)...O(2)	0.86	1.94	2.578(11)	130
N(6)-H(6B)...O(3)#2	0.86	2.32	2.757(10)	112

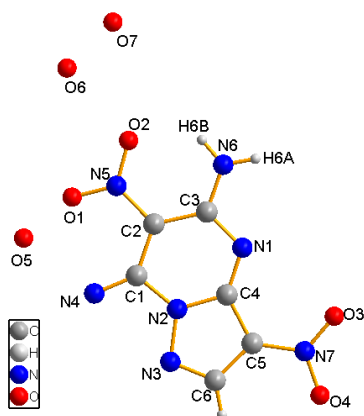
Symmetry transformations used to generate equivalent atoms:

#1 $-x+1, -y, -z$ #2 $-x+2, -y+1, -z$

Table S7. Bond lengths [\AA] and angles [$^\circ$] for compound **4**.

Bond length		Bond angle	
C(1)-N(4)	1.209(11)	N(4)-C(1)-N(2)	117.7(8)
C(1)-N(2)	1.379(11)	N(4)-C(1)-C(2)	131.3(9)
C(1)-C(2)	1.427(12)	N(2)-C(1)-C(2)	111.0(8)
C(2)-N(5)	1.411(12)	N(5)-C(2)-C(1)	116.8(8)
C(2)-C(3)	1.429(12)	N(5)-C(2)-C(3)	121.7(8)
C(3)-N(6)	1.312(11)	C(1)-C(2)-C(3)	121.4(9)
C(3)-N(1)	1.326(11)	N(6)-C(3)-N(1)	115.7(8)
C(4)-N(1)	1.304(11)	N(6)-C(3)-C(2)	122.2(8)
C(4)-N(2)	1.363(11)	N(1)-C(3)-C(2)	122.1(8)

C(4)-C(5)	1.437(13)	N(1)-C(4)-N(2)	124.2(8)
C(5)-C(6)	1.376(13)	N(1)-C(4)-C(5)	134.1(8)
C(5)-N(7)	1.394(11)	N(2)-C(4)-C(5)	101.6(7)
C(6)-N(3)	1.270(12)	C(6)-C(5)-N(7)	126.6(9)
C(6)-H(6)	0.9300	C(6)-C(5)-C(4)	107.1(8)
N(2)-N(3)	1.392(10)	N(7)-C(5)-C(4)	126.2(8)
N(5)-O(1)	1.217(10)	N(3)-C(6)-C(5)	112.8(9)
N(5)-O(2)	1.234(10)	N(3)-C(6)-H(6)	123.6
N(6)-H(6A)	0.8600	C(5)-C(6)-H(6)	123.6
N(6)-H(6B)	0.8600	C(4)-N(1)-C(3)	116.6(7)
N(7)-O(3)	1.213(10)	C(4)-N(2)-C(1)	124.4(7)
N(7)-O(4)	1.227(9)	C(4)-N(2)-N(3)	113.2(7)
		C(1)-N(2)-N(3)	122.3(7)
		C(6)-N(3)-N(2)	105.2(7)
		O(1)-N(5)-O(2)	119.2(8)
		O(1)-N(5)-C(2)	120.7(8)
		O(2)-N(5)-C(2)	120.1(8)
		C(3)-N(6)-H(6A)	120.0
		C(3)-N(6)-H(6B)	120.0
		H(6A)-N(6)-H(6B)	120.0
		O(3)-N(7)-O(4)	120.8(8)
		O(3)-N(7)-C(5)	121.3(8)
		O(4)-N(7)-C(5)	117.8(8)



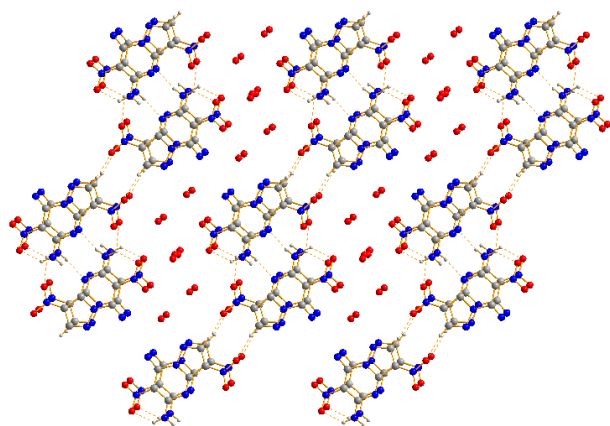


Fig. S3. Molecular structure and packing diagram of **4** (The yellow dotted line represents the hydrogen bond).



Fig. S4. The crystal morphology of compound **4**.

Table S8 Hydrogen bonds for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5)...O(7)	0.82	2.05	2.858(3)	169
O(5)-H(5)...O(2)	0.82	2.27	2.698(3)	113

N(4)-H(4B)...O(1)	0.86	1.99	2.588(3)	126
N(4)-H(4B)...N(3)#1	0.86	2.24	3.013(3)	149
N(4)-H(4A)...O(7)#1	0.86	2.57	3.114(3)	122
N(4)-H(4A)...O(6)#1	0.86	2.02	2.800(3)	150
N(1)-H(1)...O(6)#1	0.86	2.02	2.790(3)	149
N(1)-H(1)...O(4)	0.86	2.37	2.871(3)	118
C(7)-H(7A)...O(4)#2	0.96	2.44	3.273(4)	144
C(6)-H(6)...O(1)#2	0.93	2.55	3.009(4)	111

Symmetry transformations used to generate equivalent atoms:

#1 $x-1, -y+3/2, z+1/2$ #2 $x+1, -y+3/2, z-1/2$

Table S9. Bond lengths [Å] and angles [°] for compound **5**.

Bond length		Bond angle	
C(1)-N(4)	1.312(3)	N(4)-C(1)-N(1)	115.0(2)
C(1)-N(1)	1.371(3)	N(4)-C(1)-C(2)	127.3(2)
C(1)-C(2)	1.417(4)	N(1)-C(1)-C(2)	117.7(2)
C(2)-N(5)	1.425(3)	C(1)-C(2)-N(5)	119.2(2)
C(2)-C(3)	1.440(4)	C(1)-C(2)-C(3)	123.2(2)
C(3)-O(7)	1.218(3)	N(5)-C(2)-C(3)	117.6(2)
C(3)-N(2)	1.415(3)	O(7)-C(3)-N(2)	117.8(2)
C(4)-N(2)	1.349(3)	O(7)-C(3)-C(2)	130.3(2)
C(4)-N(1)	1.352(3)	N(2)-C(3)-C(2)	111.9(2)
C(4)-C(5)	1.381(4)	N(2)-C(4)-N(1)	119.8(2)
C(5)-C(6)	1.394(4)	N(2)-C(4)-C(5)	105.9(2)
C(5)-N(7)	1.413(4)	N(1)-C(4)-C(5)	134.3(2)
C(6)-N(3)	1.318(4)	C(4)-C(5)-C(6)	106.0(2)
C(6)-H(6)	0.9300	C(4)-C(5)-N(7)	125.1(2)
C(7)-C(8)	1.480(4)	C(6)-C(5)-N(7)	128.9(2)
C(7)-H(7A)	0.9600	N(3)-C(6)-C(5)	111.9(2)
C(7)-H(7B)	0.9600	N(3)-C(6)-H(6)	124.1
C(7)-H(7C)	0.9600	C(5)-C(6)-H(6)	124.1
C(8)-O(6)	1.208(3)	C(8)-C(7)-H(7A)	109.5

C(8)-O(5)	1.311(4)	C(8)-C(7)-H(7B)	109.4
N(1)-H(1)	0.8600	H(7A)-C(7)-H(7B)	109.5
N(2)-N(3)	1.388(3)	C(8)-C(7)-H(7C)	109.5
N(4)-H(4A)	0.8600	H(7A)-C(7)-H(7C)	109.5
N(4)-H(4B)	0.8600	H(7B)-C(7)-H(7C)	109.5
N(5)-O(2)	1.206(3)	O(6)-C(8)-O(5)	122.2(3)
N(5)-O(1)	1.227(3)	O(6)-C(8)-C(7)	124.6(3)
N(7)-O(3)	1.219(3)	O(5)-C(8)-C(7)	113.2(3)
N(7)-O(4)	1.228(3)	C(4)-N(1)-C(1)	121.9(2)
O(5)-H(5)	0.8200	C(4)-N(1)-H(1)	119.1
		C(1)-N(1)-H(1)	119.1
		C(4)-N(2)-N(3)	112.0(2)
		C(4)-N(2)-C(3)	125.5(2)
		N(3)-N(2)-C(3)	122.5(2)
		C(6)-N(3)-N(2)	104.2(2)
		C(1)-N(4)-H(4A)	120.0
		C(1)-N(4)-H(4B)	120.0
		H(4A)-N(4)-H(4B)	120.0
		O(2)-N(5)-O(1)	120.4(2)
		O(2)-N(5)-C(2)	120.3(2)
		O(1)-N(5)-C(2)	119.3(2)
		O(3)-N(7)-O(4)	124.1(3)
		O(3)-N(7)-C(5)	118.6(3)
		O(4)-N(7)-C(5)	117.3(2)
		C(8)-O(5)-H(5)	109.5

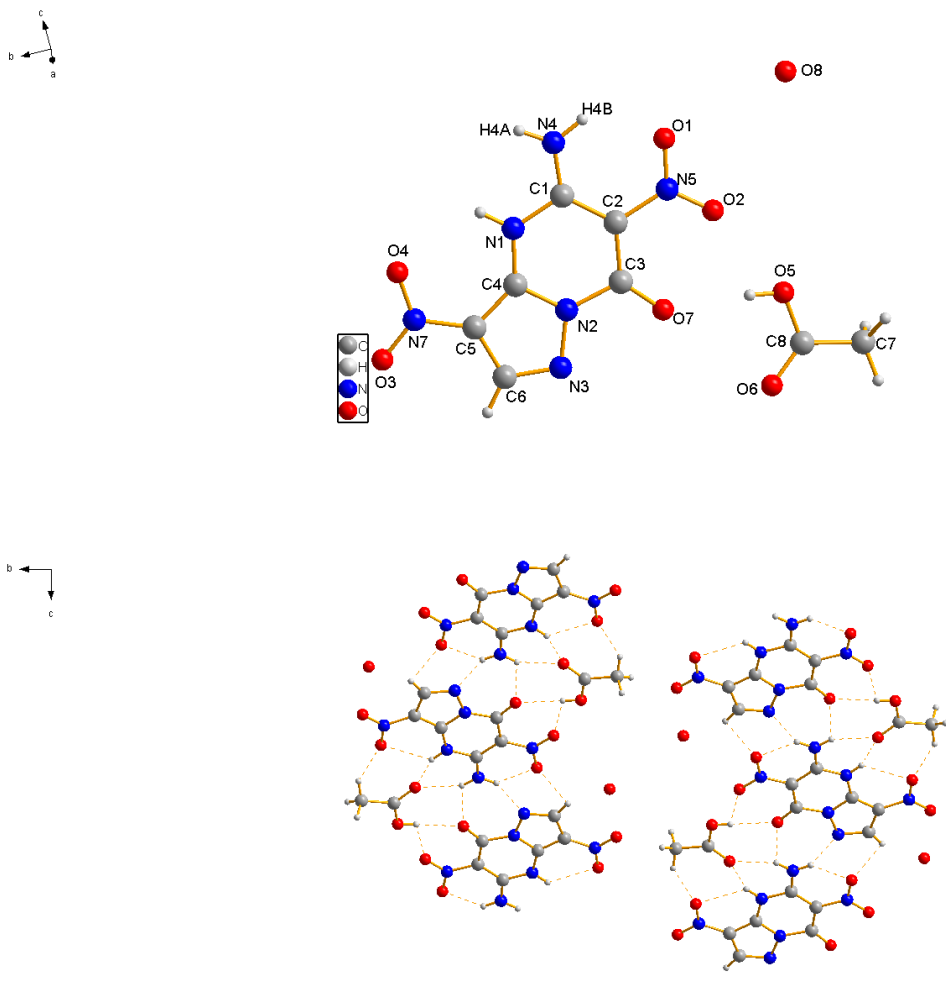


Fig. S5. Molecular structure and packing diagram of **5** (The yellow dotted line represents the hydrogen bond).

3. IR and NMR spectra

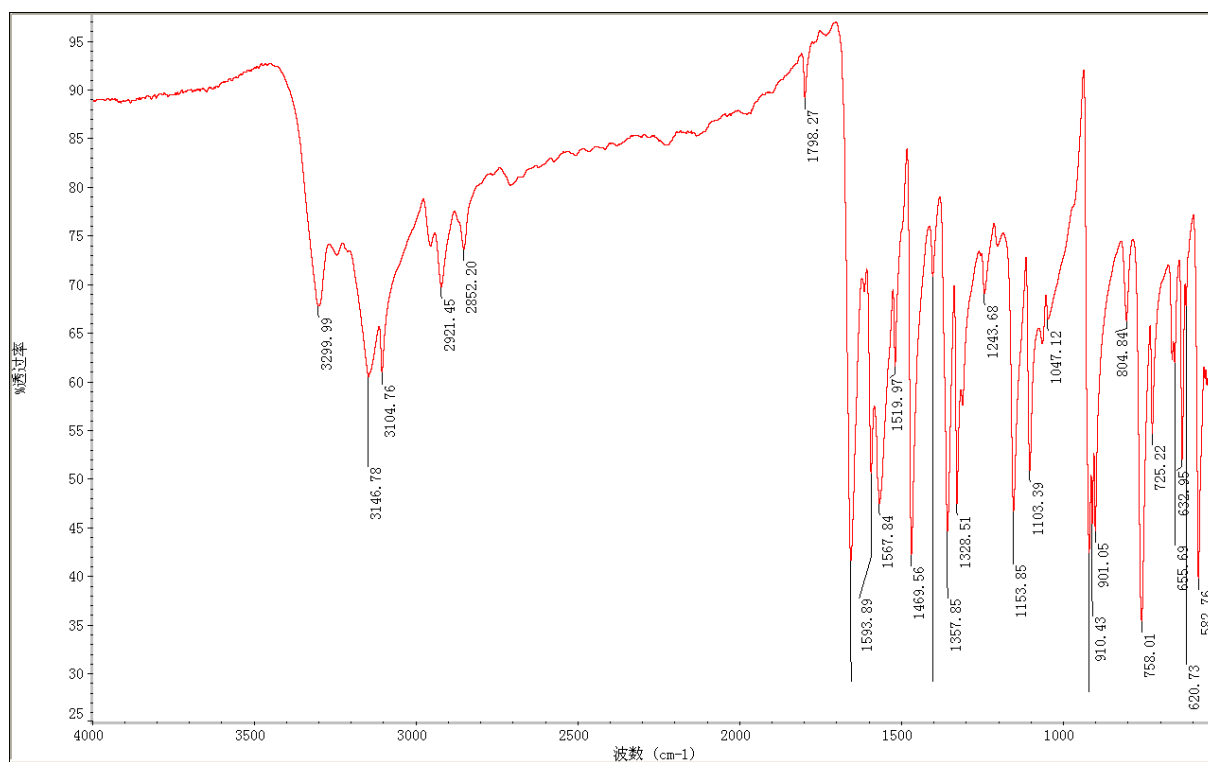


Fig. S5. IR spectra of compound 2.

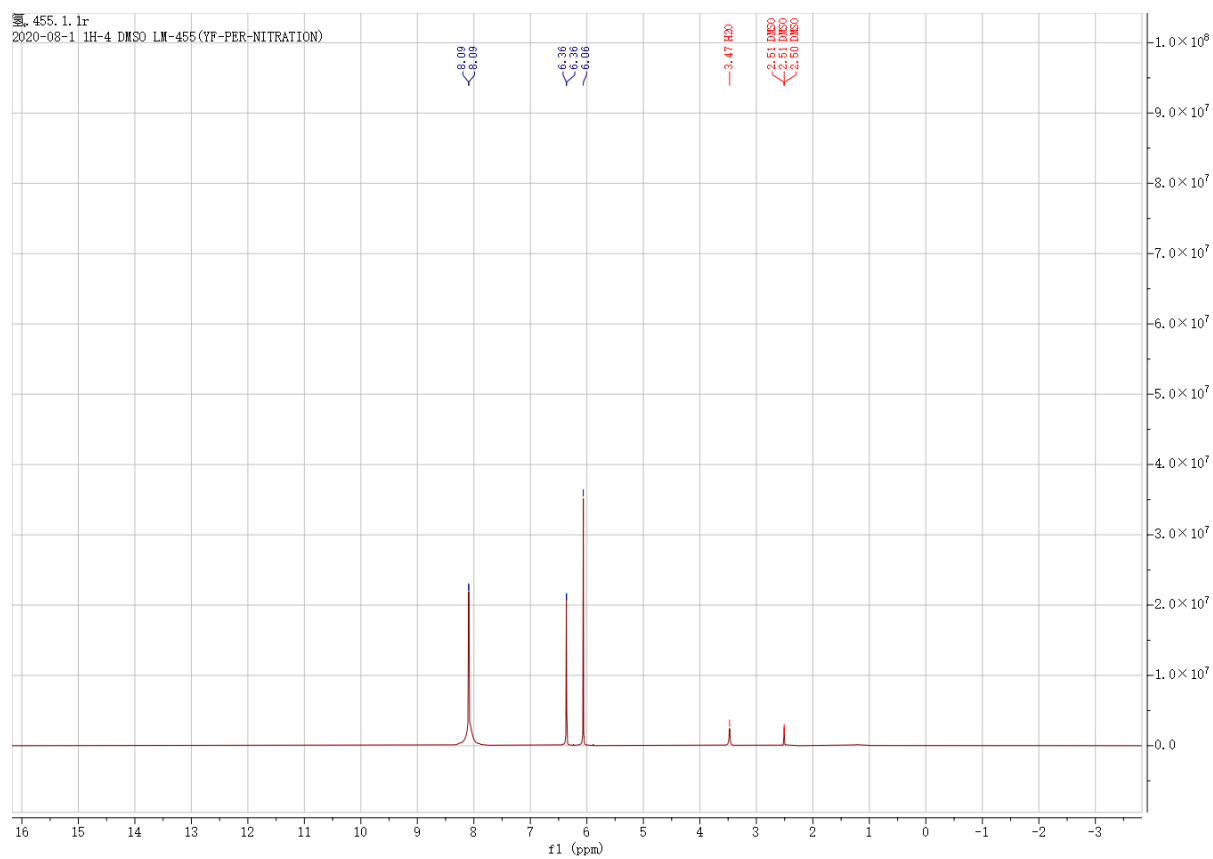


Fig. S6. ¹H NMR spectra of compound 2.

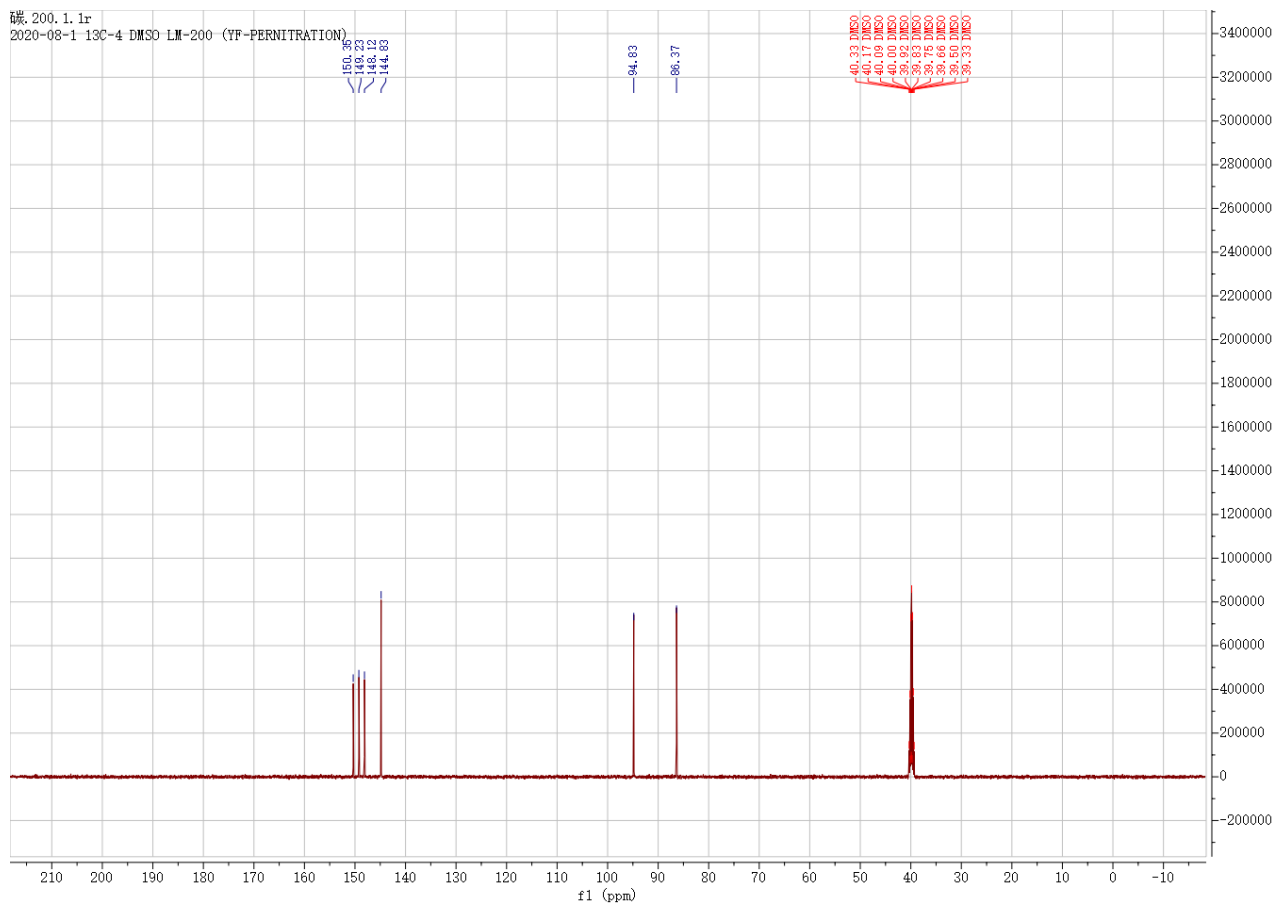


Fig. S7. ^{13}C NMR spectra of compound 2.

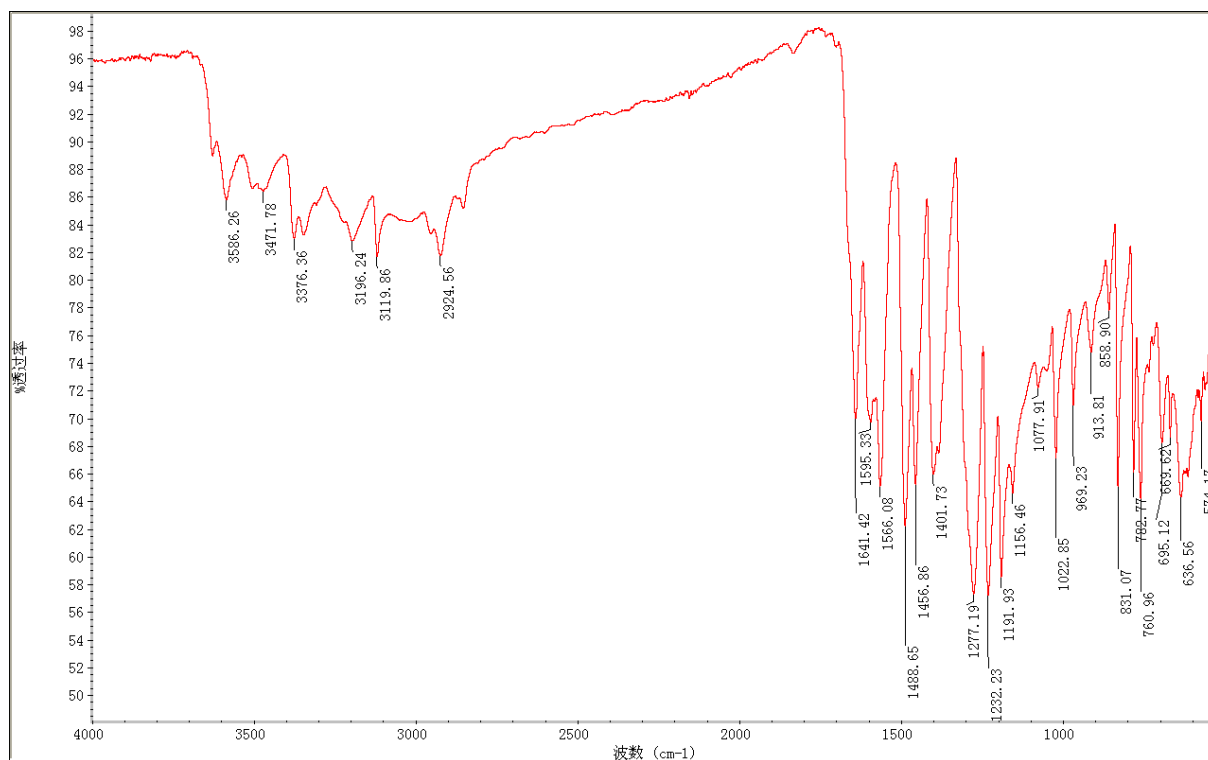


Fig. S8. IR spectra of compound 3.

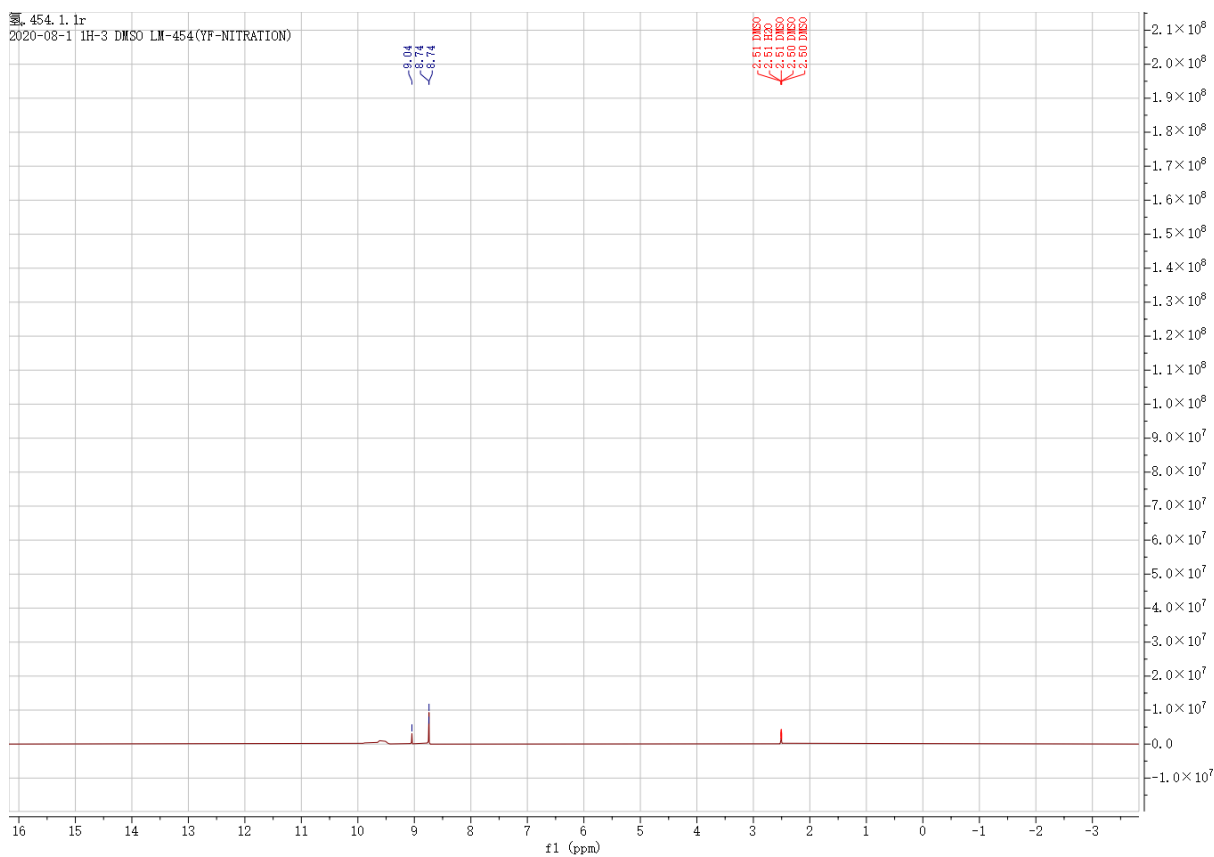


Fig. S9. ^1H NMR spectra of compound **3**.

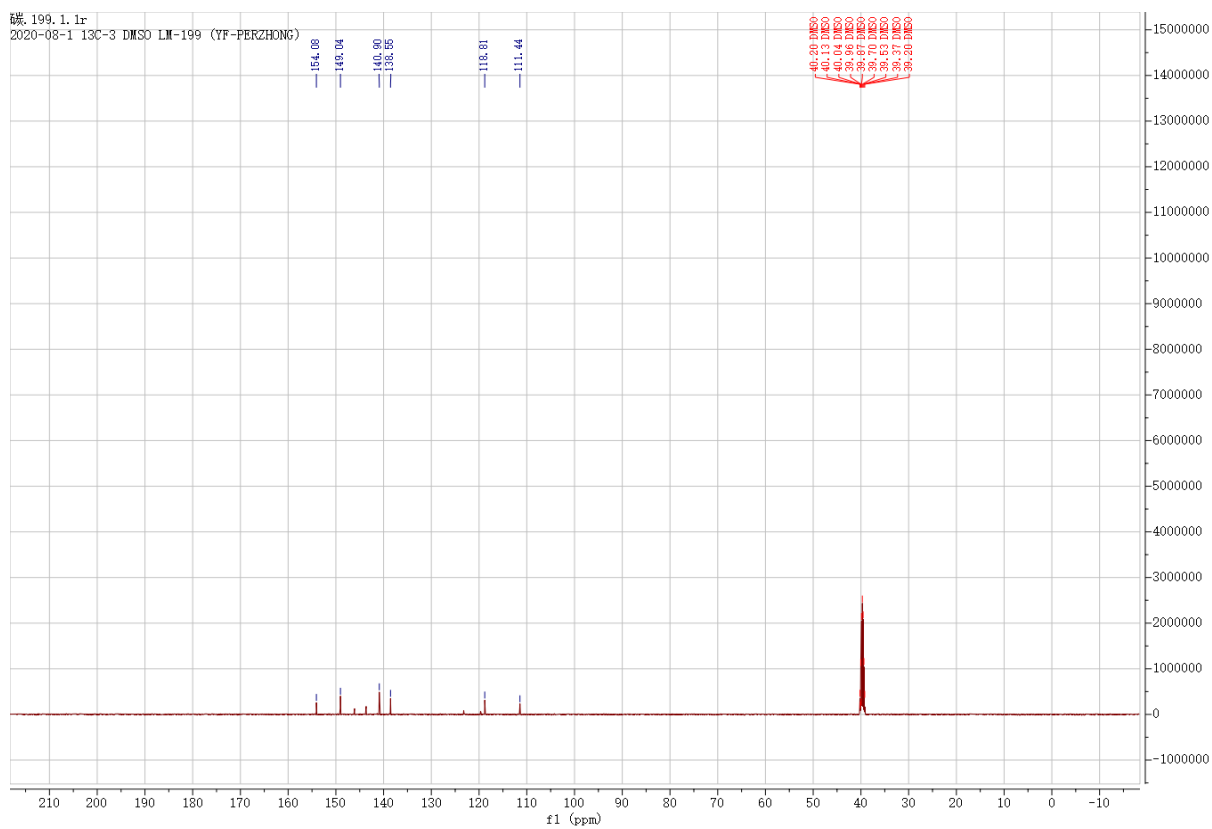


Fig. S10. ^{13}C NMR spectra of compound **3**.

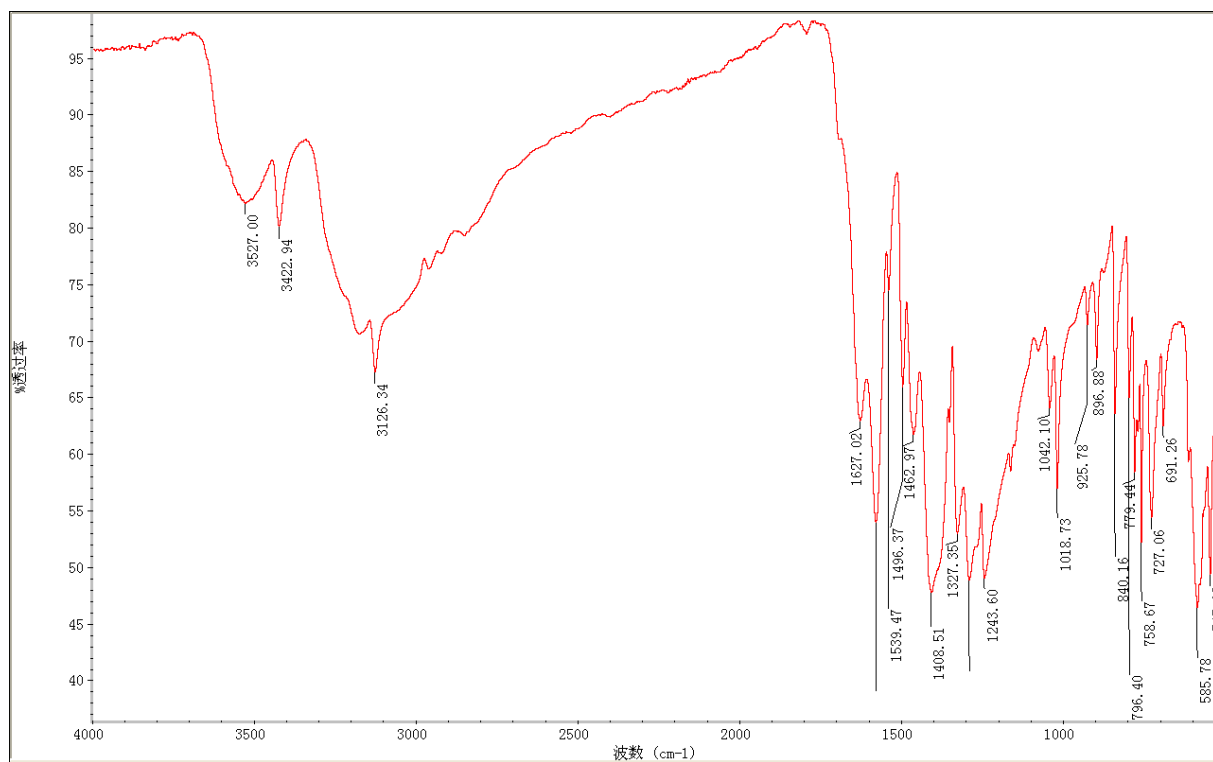


Fig. S11. IR spectra of compound 4.

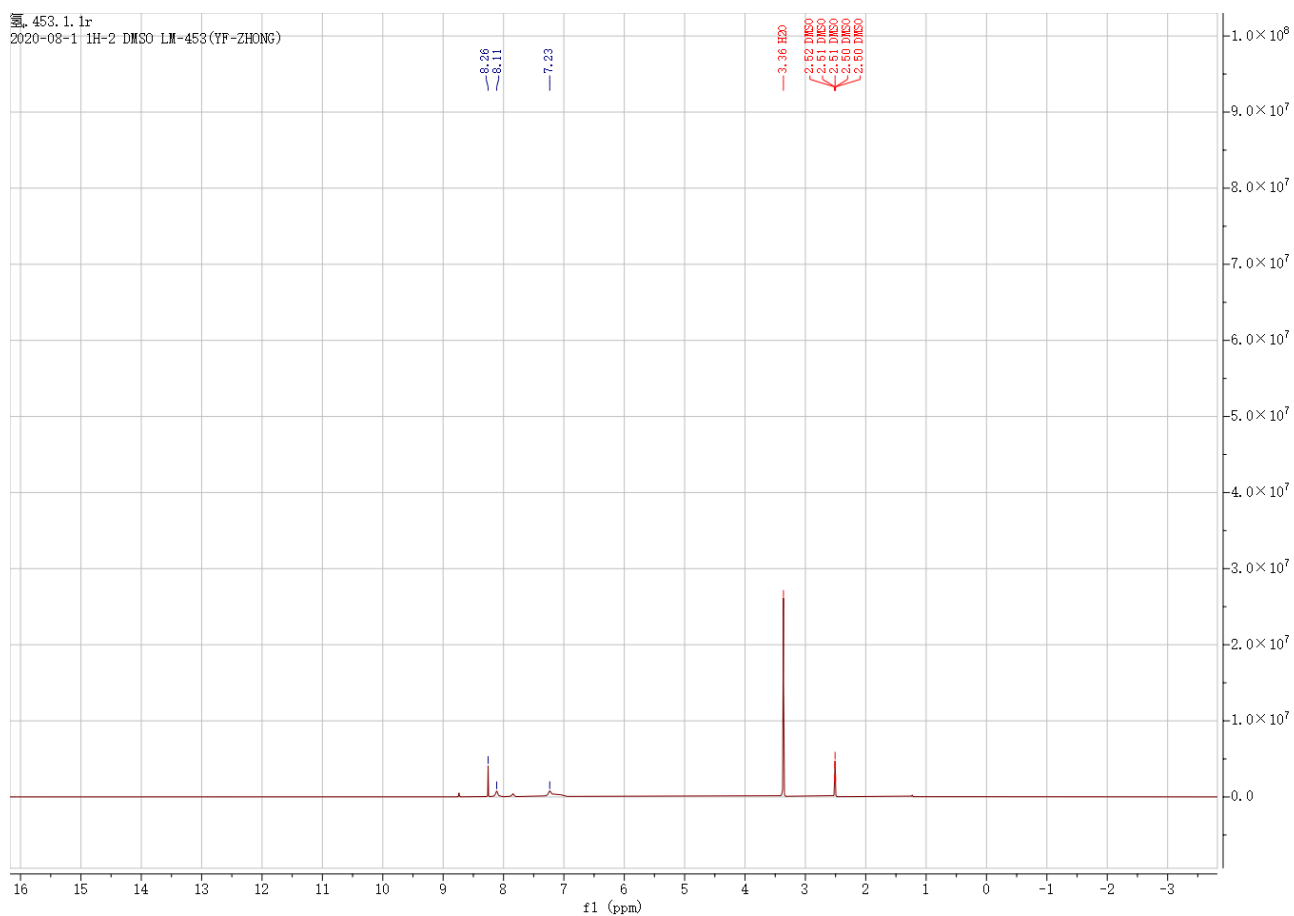


Fig. S12. ¹H NMR spectra of compound 4.

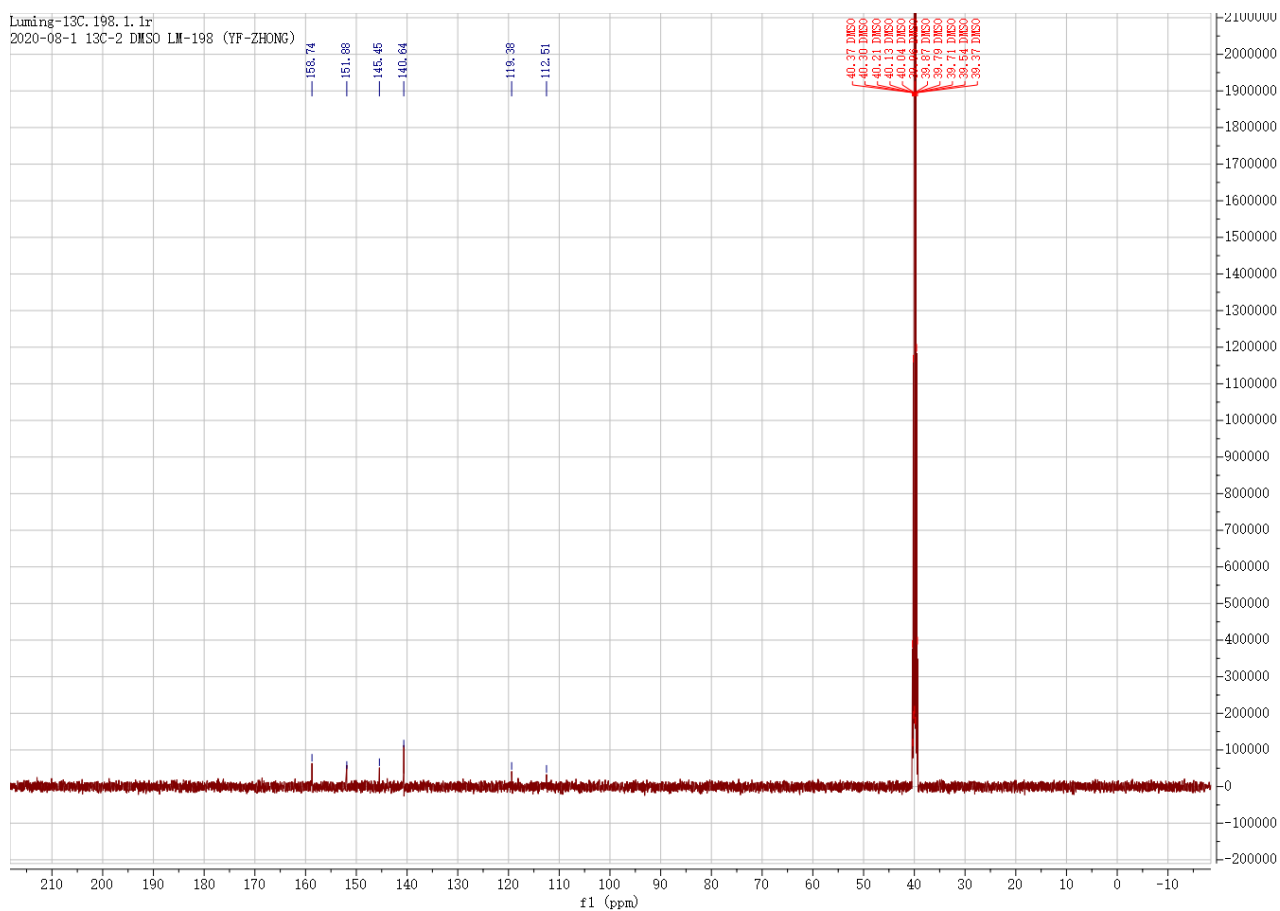


Fig. S13. ^{13}C NMR spectra of compound 4.

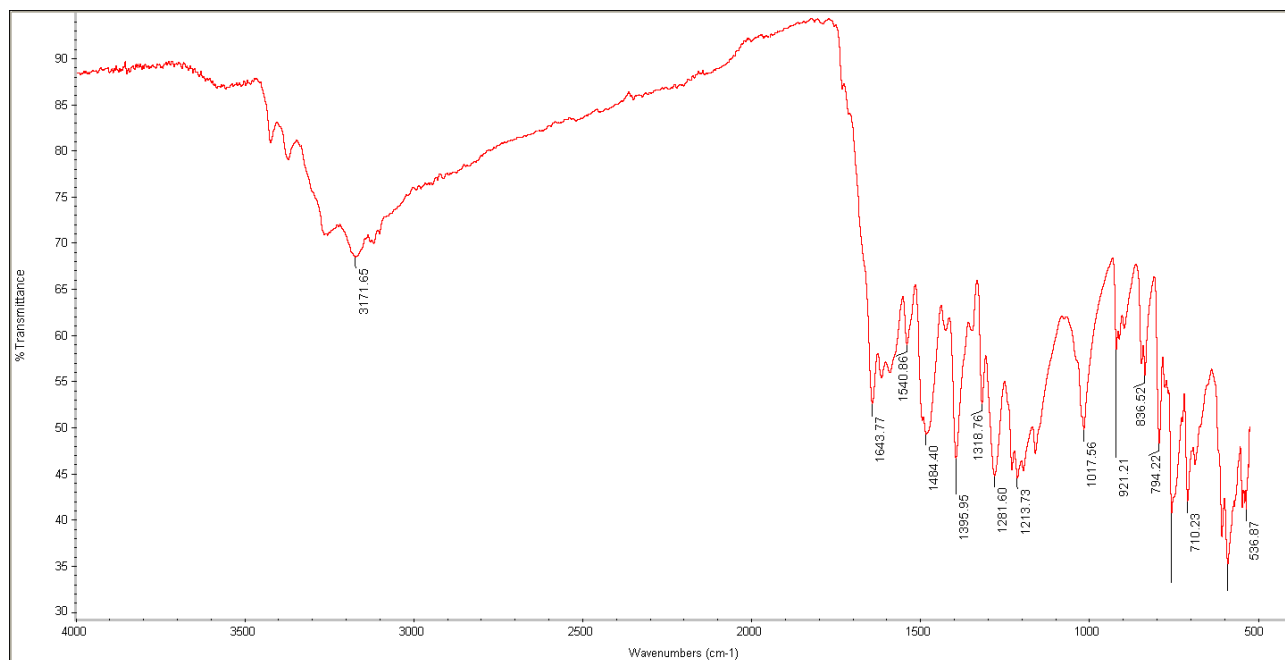


Fig. S14. IR spectra of compound 5.

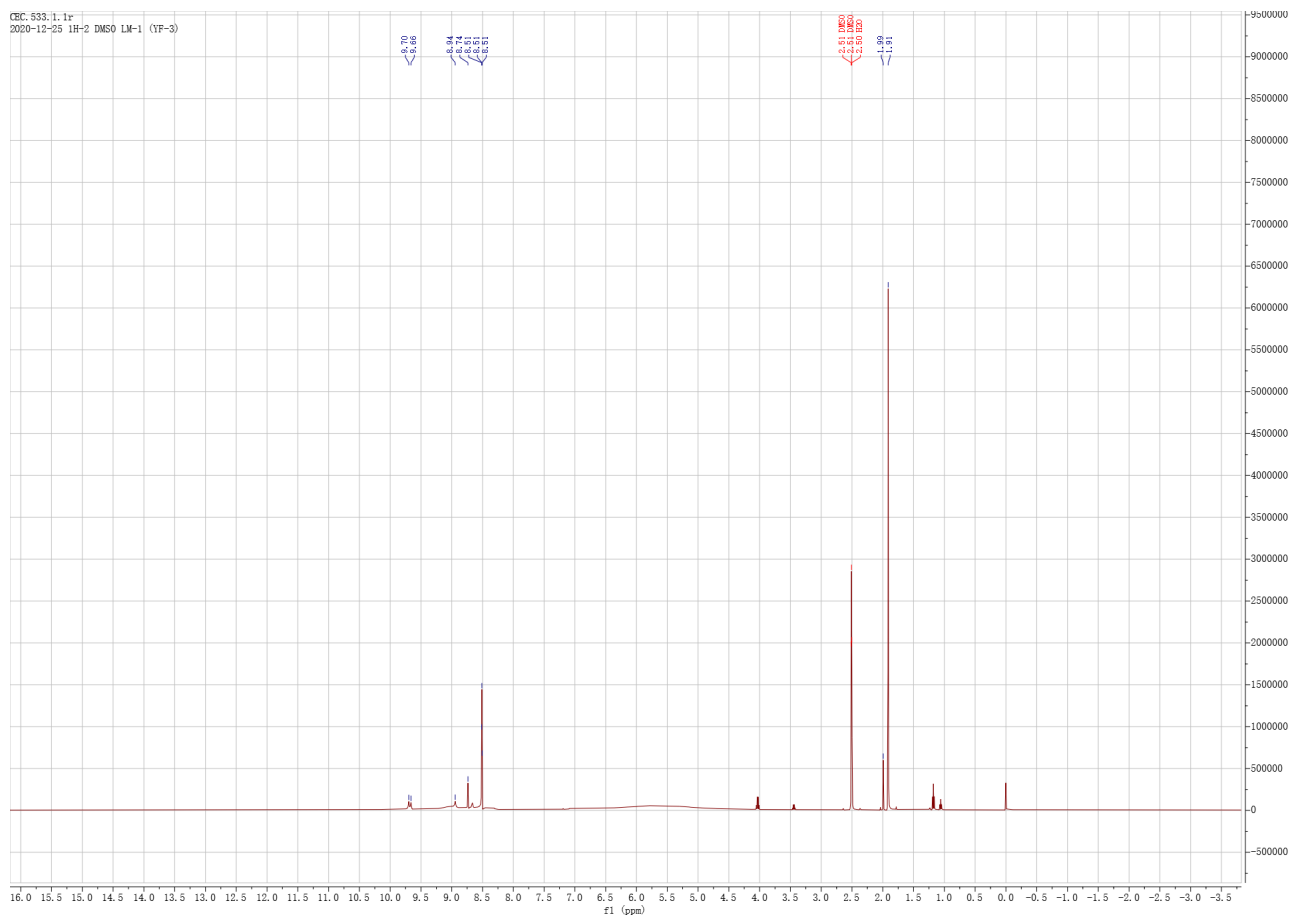
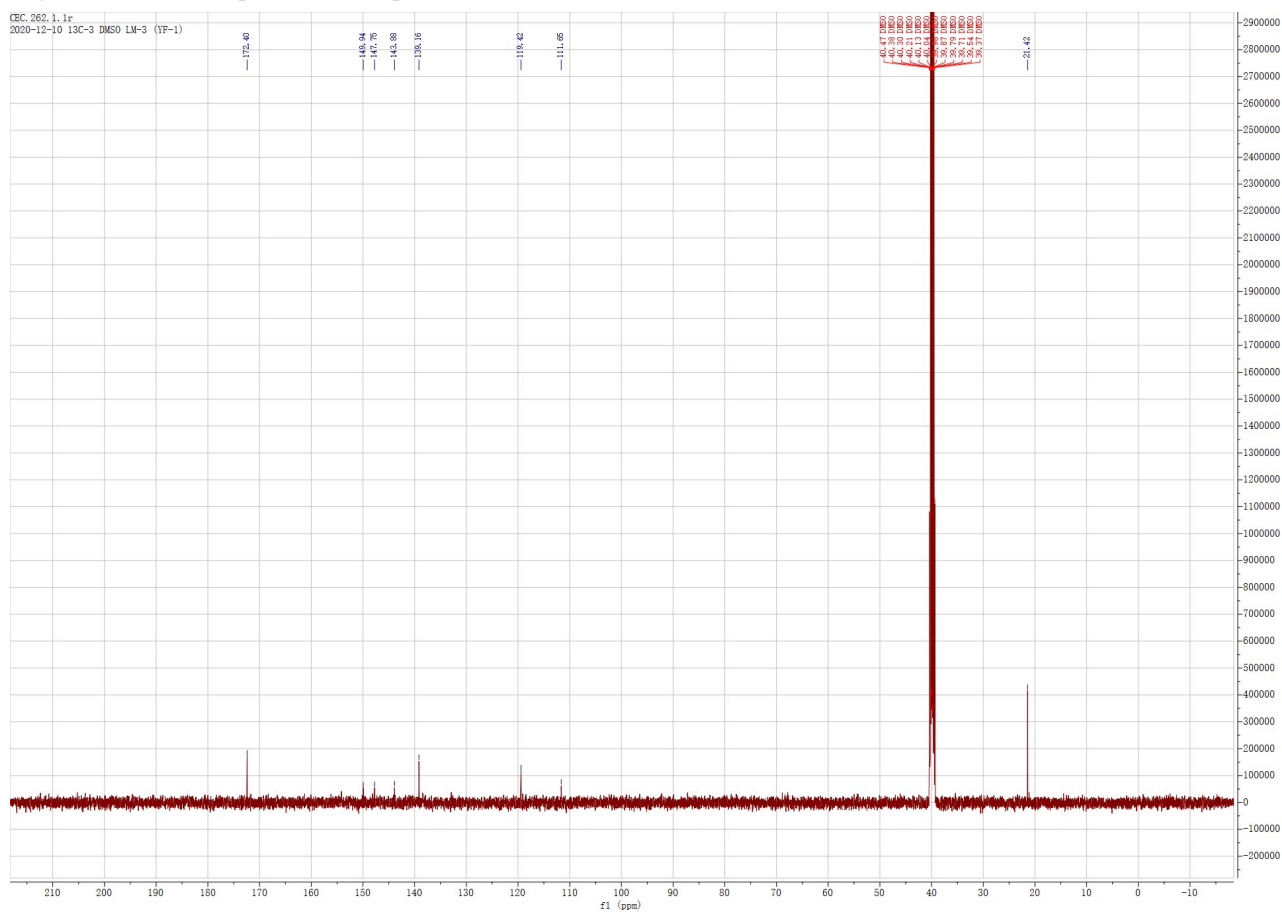


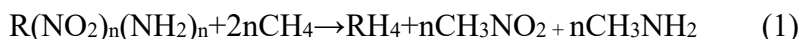
Fig. S15. ^1H NMR spectra of compound **5**.



4. Computational Details

All of the calculations involved in this work were carried out using the Gaussian 09 suite of programs and using the B3LYP functional with the 6-31G(d) basis set. All of the optimized structures were characterized to be true local energy minima on the potential energy surface without imaginary frequencies. Total energy (E_0) and zero-point energy (ZPE) were calculated with vibration frequencies analysis.

The heat of formation in gas states is calculated based on follows:⁵



According to Hess' law of constant heat summation condensed-phase heats of formation can be determined.⁶

$$\Delta H_{solid} = \Delta H_{gas} - \Delta H_{sub} \quad (2)$$

The enthalpy of sublimation can be represented as eq (4) and on the basis of the predicted electrostatic potential of a molecule.⁷

$$\Delta H_{sub} = a(SA)^2 + b\sqrt{\nu\sigma_{tot}^2} + c \quad (3)$$

Here SA is the surface area of the 0.001 electrons bohr⁻³ isosurface of the electronic density of the compounds, $\nu\sigma_{tot}^2$ is derived from the molecular electrostatic potential calculation, and a, b, c are fitting parameters reported by Politzer et al.⁷

Table S8. Calculated total energy (E_0), zero-point energy (ZPE), thermal correction to enthalpy (H_T), and heats of formation (HOF) in gas state.

Compound	E_0 / a. u.	ZPE / kJ mol ⁻¹	ΔH_T / a. u.	HOF/kJ mol ⁻¹
3	-1319.8142788	310.96	0.132809	125.597
4	-915.6081442	382.27	0.159952	362.066
5	-935.4598018	346.95	0.145785	211.942
CH ₄	-40.5240195	118.22	0.048836	-74.600
CH ₃ NO ₂	-245.0133749	131.32	0.055294	-74.300
CH ₃ NH ₂	-95.8532042	169.15	0.068745	-23.000

Reference

- (1) M. J. Frisch, Gaussian 09. Revision a. 02, Gaussian, Inc., Wallingford CT, 2009.
- (2) M. Suceska, EXPLO5 Program. Croatia, Zagreb, 2011.
- (3) J. Zhang, H. Du, F. Wang, X. Gong and Y. Huang, *J. Phys. Chem. A* 2011, **115**, 6617.
- (4) M. J. Turner, J. J. McKinnon and S. K. Wolff, CrystalExplorer 17.5, University of Western Australia: Perth, Australia, 2017.
- (5) T. Lu, F. J. Chen, Multiwfn: A multifunctional wavefunction analyzer, *J. Comput. Chem.* 2012, **33**, 580-592.
- (6) P. W. Atkins, Physical Chemistry. Oxford University Press, Oxford, U. K., 1982.
- (7) a) P. J. Politzer, S. Murray, T. Brinck and P. Lane, Immunoanalysis of agrochemicals. ACS Symposium Series 586, American Chemical Society, Washington, DC, 1994; b) J. S. Murray and P. Politzer, In quantitative treatment of solute / solvent interactions. theoretical and computational chemistry. Elsevier, Amsterdam, 1994.
- (8) Y. Tang, C. He, L. A. Mitchell, D. A. Parrish and J. M. Shreeve, C-N bonded energetic biheterocyclic compounds with good detonation performance and high thermal stability, *J. Mater. Chem. A* 2016, **4**, 3879-3885.
- (9) P. Politzer and J. S. Murray, Impact sensitivity and crystal lattice compressibility / free space, *J. Mol. Model.* 2014, **20**, 2223-2231.