

Supplementary Information

Synthesis, characterization and properties of new heat resistant energetic materials based on two C-C bridged pyrazole and benzene skeletons

Rogzheng Zhang ^a, Yuangang Xu ^{a*}, Feng Yang ^a, Pengcheng Wang ^a,
Qiuhan Lin ^a, Hui Huang ^b, Ming Lu ^{a,*}

^a School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

^b Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621900, China

* Corresponding authors: luming@njjust.edu.cn, yuangangxu@163.com

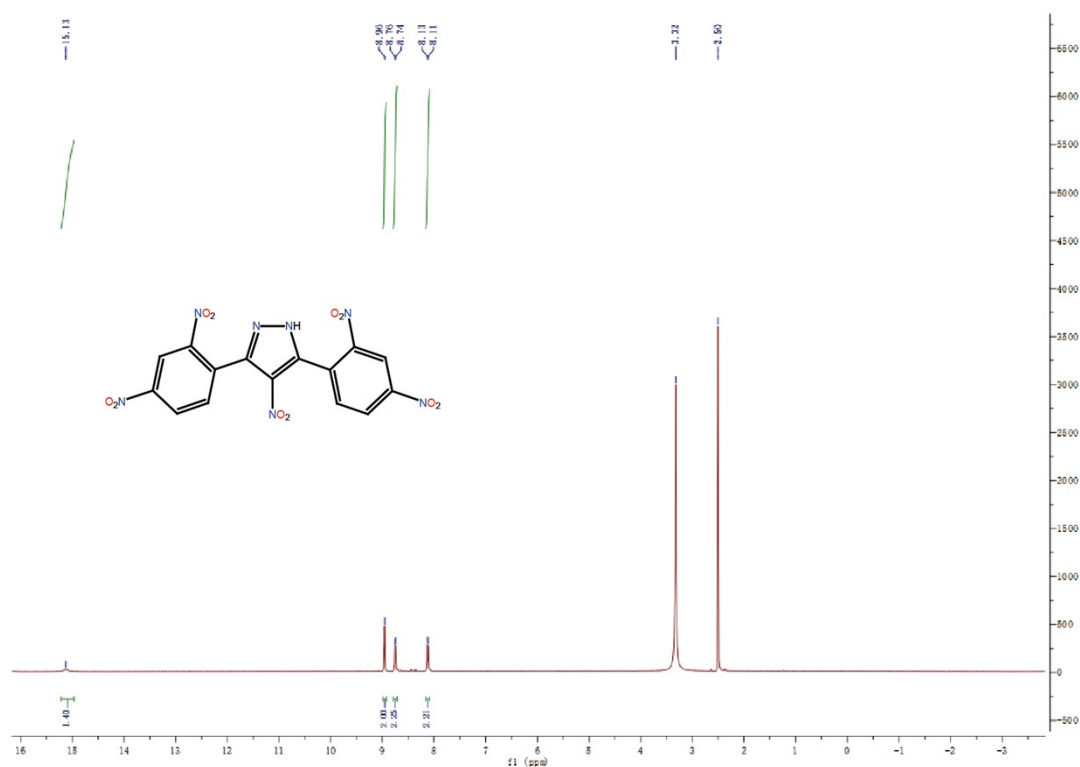


Fig. S1 ¹H NMR of **1C** (DMSO-*d*₆)

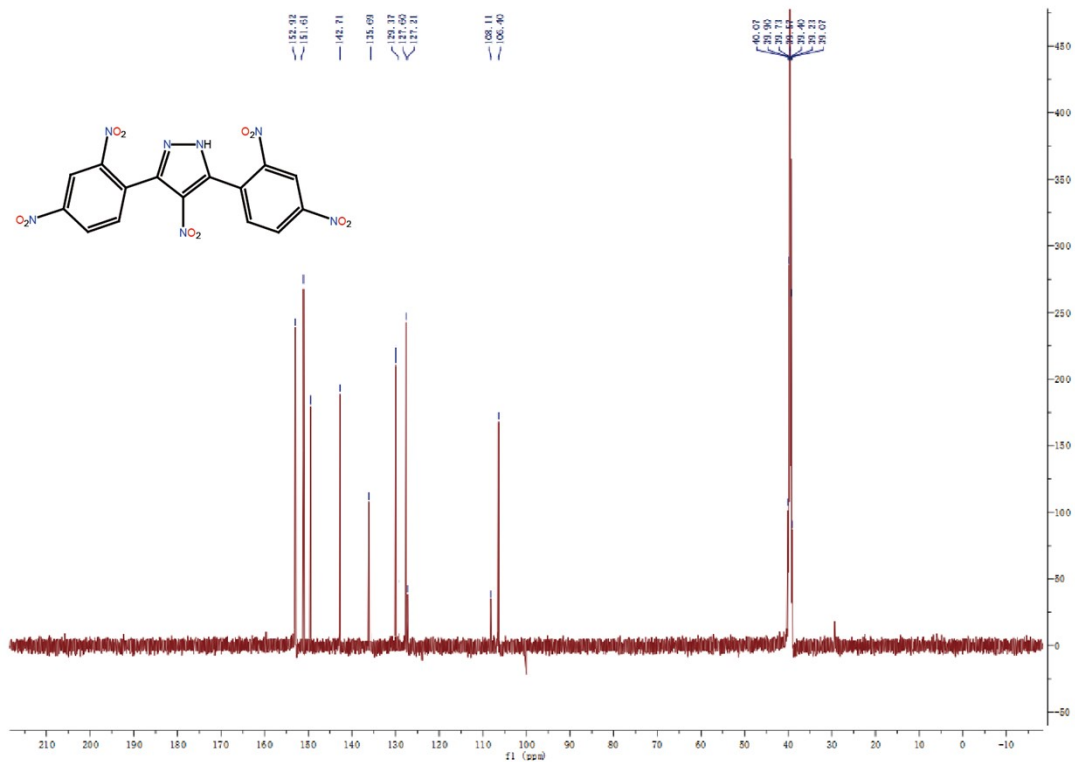


Fig. S2 ^{13}C NMR of 1C (DMSO- d_6)

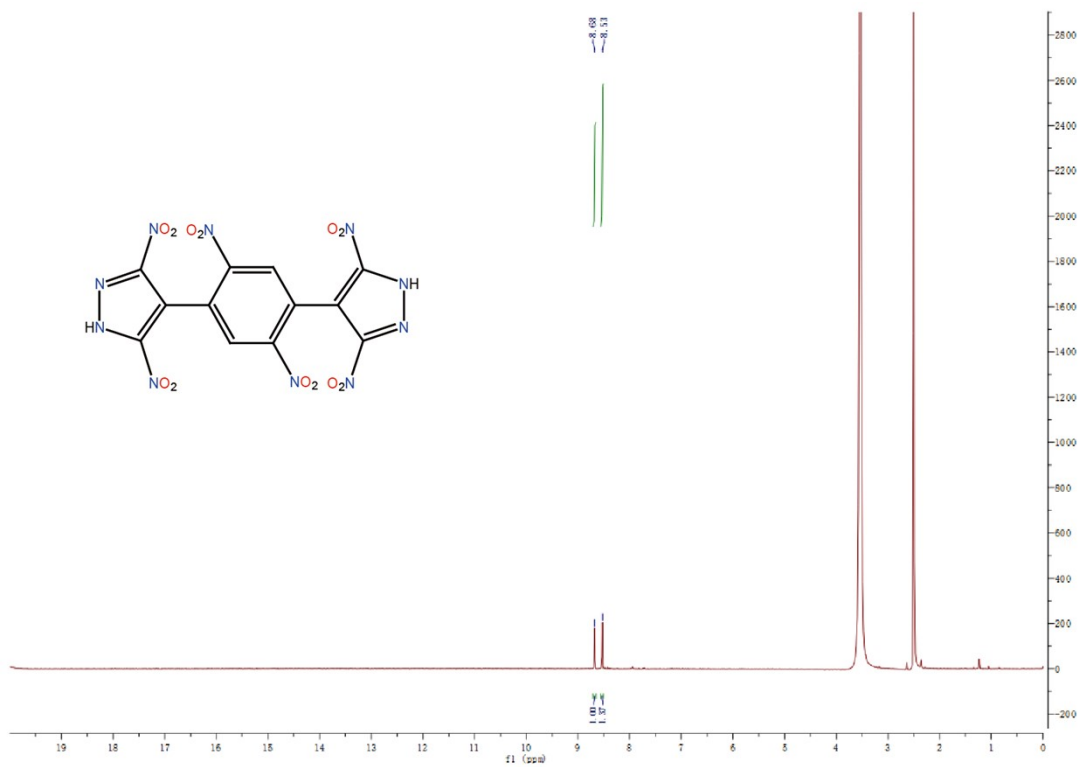


Fig. S3 ^1H NMR of 2C (DMSO- d_6)

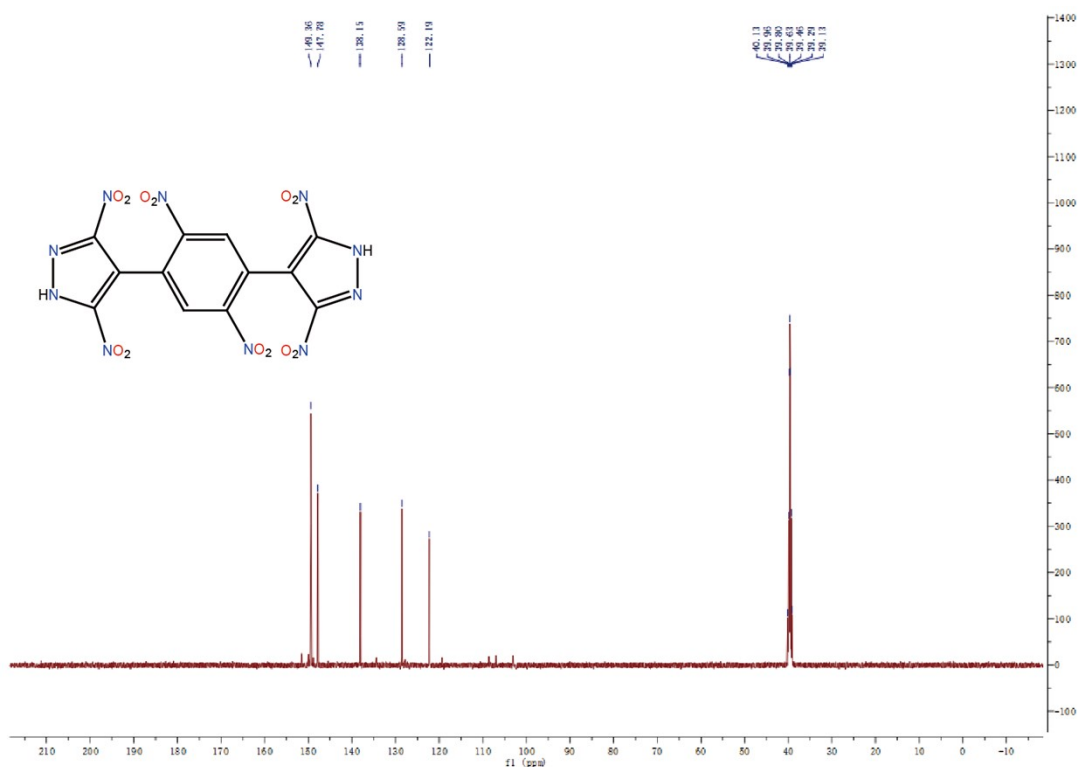


Fig. S4 ^{13}C NMR of **2C** ($\text{DMSO-}d_6$)

Table.S1 Crystal data and structure refinement for $1\text{c}\cdot\text{CH}_3\text{OH}$ and $2\text{c}\cdot\text{CH}_3\text{OH}$

Empirical formula	$\text{C}_{16}\text{H}_{11}\text{N}_7\text{O}_{11}$	$\text{C}_{14}\text{H}_{12}\text{N}_{10}\text{O}_{14}$
Formula weight	477.32	544.34
Temperature/K	296	296
Crystal system	Monoclinic	Triclinic
Space group	$\text{P } 2_1/c$	$\text{P } -1$
$a/\text{\AA}$	26.806(4)	6.2299(6)
$b/\text{\AA}$	7.7681(10)	7.4168(7)
$c/\text{\AA}$	20.357(3)	12.7696(12)
$\alpha/^\circ$	90	103.819(3)
$\beta/^\circ$	112.251	90.179(3)
$\gamma/^\circ$	90	95.701(3)
Volume/ \AA^3	3923.3(10)	569.90(9)
Z	8	1
$\rho_{\text{calc}}/\text{g/cm}^3$	1.616	1.586

μ/mm^{-1}	0.140	0.144
F(000)	1952	278
Crystal size/ mm^3	0.220×0.200×0.120	0.220×0.200×0.120
Radiation	MoK α ($\lambda=0.71073$)	MoK α ($\lambda = 0.71073$)
Theta range for data collection/ $^\circ$	0.821 to 24.997	2.843 to 27.551
Index ranges	-31 $\leq h \leq$ 31, -9 $\leq k \leq$ 9, -21 $\leq l \leq$ 20	-8 $\leq h \leq$ 7, -9 $\leq k \leq$ 9, -16 $\leq l \leq$ 16
Reflections collected	27370	8294
Independent reflections	6638 [R(int) = 0.0818]	2614 [R(int) = 0.0315]
Data/restraints/parameters	6638/0/617	2614/0/174
Goodness-of-fit on F ²	1.054	1.016
Final R indexes [I $\geq 2\sigma$ (I)]	R1 = 0.0702, wR2 = 0.1647	R1 = 0.0503, wR2 = 0.1166
Final R indexes [all data]	R1 = 0.1105, wR2 = 0.1870	R1 = 0.0898, wR2 = 0.1346
Largest diff. peak/hole / e \AA^{-3}	0.291 and -0.291	0.220 and -0.249
CCDC	2248516	2248513