Supplementary Materials

Boosting the Energetic Performance of Trinitrome-thyl-1,2,4-oxadiazole Moiety by Increasing Nitrogen-Oxygen in the Bridge

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Table of Contents

Crystal data and structure refinement

Table S1 Crystal data and structure refinement for **2**.

Identification code	**2**
CCDC number	2182869
Empirical formula	$C_{10}N_{16}O_{16}$
Formula weight	600.26
Temperature/K	170
Crystal system	triclinic
Space group	*P*-1
a/Å	9.8874(8)
b/Å	10.4237(10)
c/Å	11.3885(9)
α/°	116.162(3)
β/°	95.794(3)
γ/°	91.412(4)
Volume/Å^3	1044.96(16)
Z	2
ρ_{calc}g/cm^3	1.908
μ/mm^{-1}	0.182
F(000)	600.0
Crystal size/mm^3	$0.08 \times 0.06 \times 0.04$
Radiation	MoKα ($\lambda = 0.71073$)
2Θ range for data collection/°	4.016 to 52.956
Index ranges	$-12 \leq h \leq 11$, $-12 \leq k \leq 13$, $-14 \leq l \leq 14$
Reflections collected	12351
Independent reflections	4289 [$R_{int} = 0.0715$, $R_{sigma} = 0.0782$]
Data/restraints/parameters	4289/0/379
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	$R_1 = 0.0463$, $wR_2 = 0.1003$
Final R indexes [all data]	$R_1 = 0.0783$, $wR_2 = 0.1197$
Largest diff. peak/hole / e Å^{-3}	0.26/-0.31

¹³C NMR and ¹⁵N NMR spectra
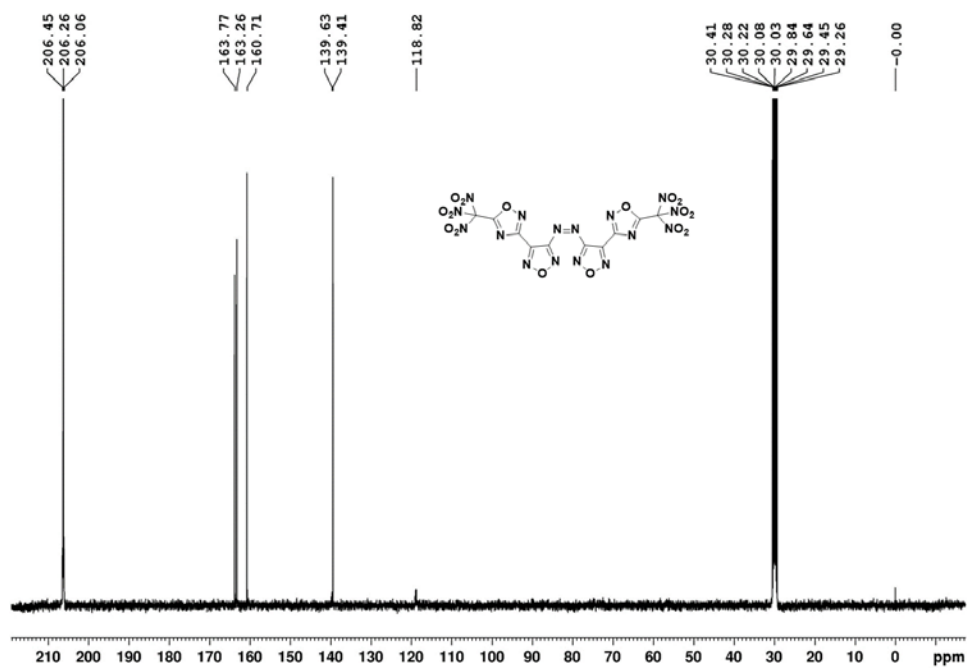

Figure S1. ¹³C NMR of **2**.
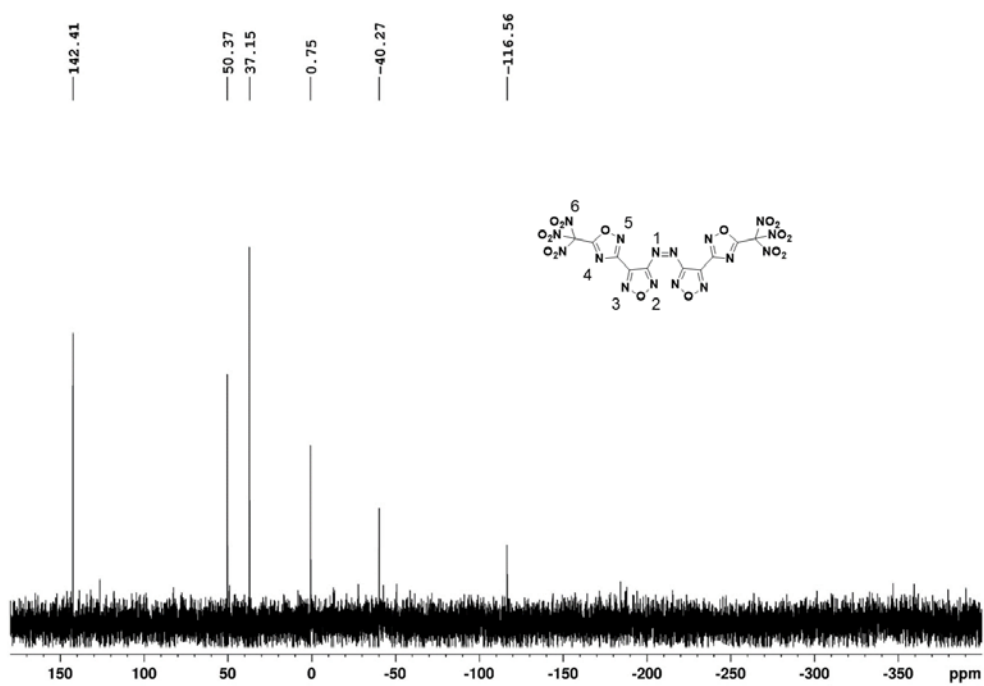

Figure S2. ¹⁵N NMR of **2**.

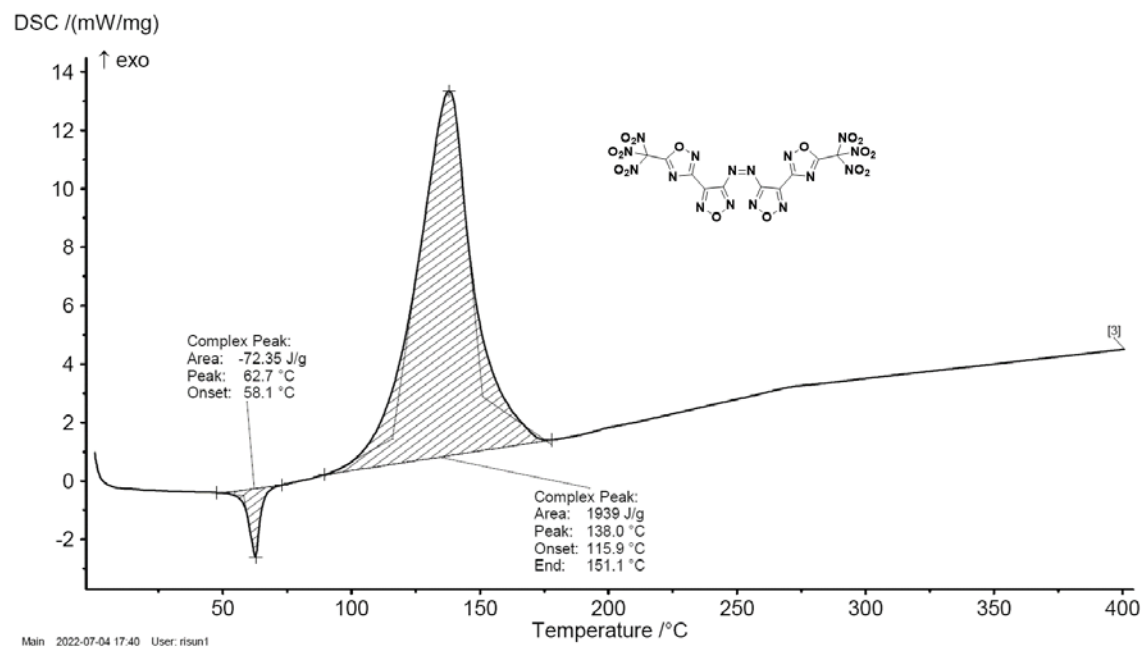## Differential scanning calorimetry (DSC) scans

Figure S3. DSC curves of 2 under nitrogen with a heating rate of 5 °C min^{-1}

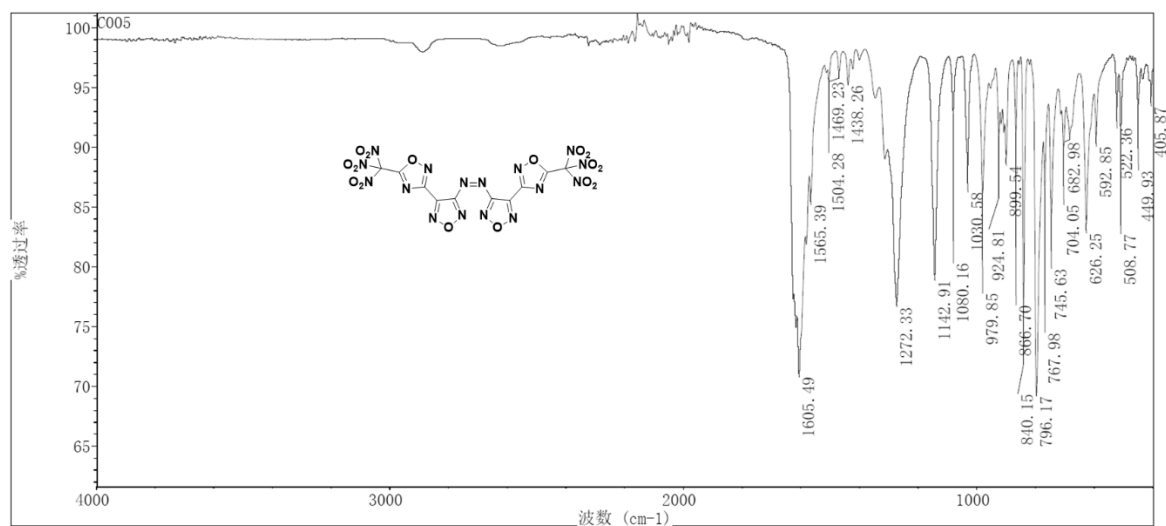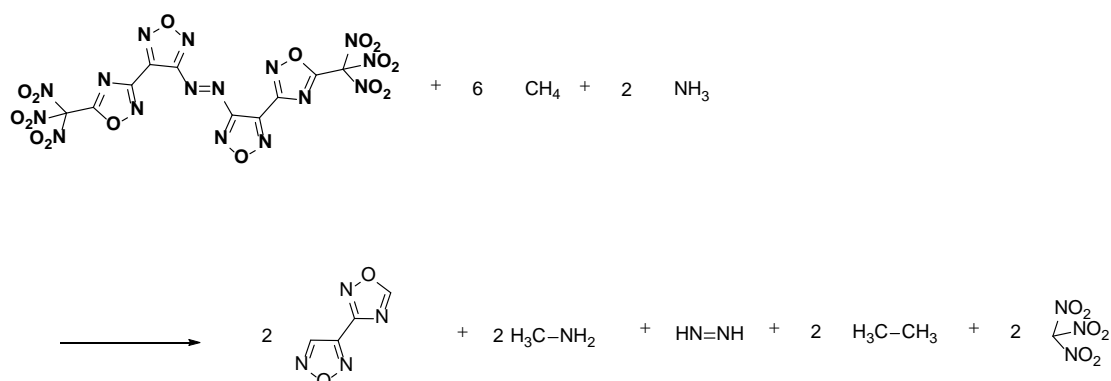## Fourier Transform Infrared (FT-IR)

Figure S4. FT-IR curves of 2

3

Gaussian Calculation

Scheme S1. Isodesmic reactions for calculating heats of formation for the anions of **2**.

Table S2. Calculated (B3LYP-D3BJ/6-31+G(d,p) // M062x/def2QZVPP) total energy(E_0), zero-point energy (*ZPE*), values of the correction (H_r), and heats of formation (HOF) for anions.

	ZPE	Hr	E_0	Corrected E_0	HOF (KJ mol^{-1})
	0.072807	0.080642	-522.9863084	-522.90858	306.17[b]
CH$_3$CH$_3$	0.074962	0.079382	-79.8143982	-79.73801	-84[a]
N$_2$H$_2$	0.028522	0.032322	110.6471796	-110.61600	200.41[b]
CH$_3$NH$_2$	0.064305	0.068654	-95.8543147	-95.78823	-23[a]
CH$_4$	0.045014	0.048823	-40.5062133	-40.45919	-74.6[a]
NH$_3$	0.034517	0.038327	-56.5578458	-56.52090	-45.9[a]
Nitrofrom	0.054646	0.064483	-654.0296587	-653.96736	-27.74[b]
2	0.201407	0.237123	-2459.86609	-2459.63702	1047.07[b]

[a] Data from NIST, [b] Calculated from G2.

Table S3. Calculation of Heat of formation by Atomization G2

	E_{298} (G2)	MW	D_0 (Hartree)	ΔH_f^{298} (Kcal/mol)	ΔH_f^{298} (KJ/mol)
	-522.2	138.0844	2.022031	73.17633821	306.1697991
N$_2$H$_2$	-110.48	30.02936	0.440344	47.89995673	200.413419
Nitrofrom	-653.18	151.0353	1.448821	-6.6289413	-27.7354904

Solid-state heats of formation of the resulting compound **2** were calculated with Equation (S1) in which T_{dec} is the decomposition temperature.

$$\Delta Hf = \Delta Hf(g) - \Delta Hsub = \Delta Hf(g) - 188[J\ mol^{-1}\ K^{-1}] \times Tm \cdots\cdots\cdots\cdots (S1)$$